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, metric learning, 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: $x \in X$
 - 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.

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

Supervised Learning: Classification

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

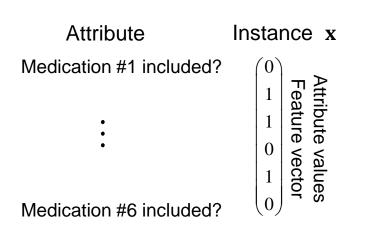
$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$$

- 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

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

Classification: Example

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



Medication combination



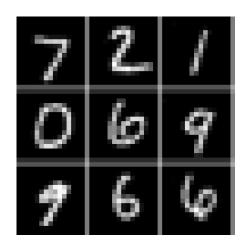
• Output: $y \in Y = \{\text{toxic, ok}\}$



Classification: Example

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

Attribute	Instance x
Gray value of pixel 1	0.1 0.3 0.45 : 0.65 0.87
	0.3
•	0.45
•	: 3 va
	0.65
Gray value of pixel 256	(0.87) $^{\circ}$

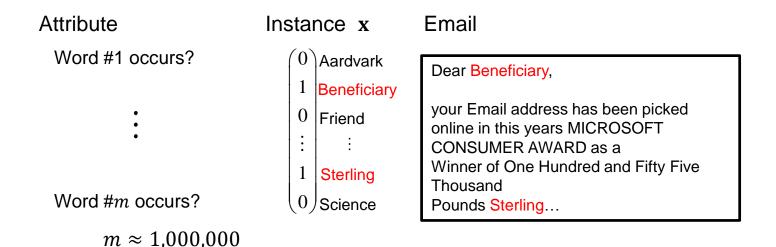


• Output: $y \in Y = \{0,1,2,3,4,5,6,7,8,9\}$: recognized digit

$$\rightarrow$$
 classifier \rightarrow "6"

Classification: Example

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



• Output: $y \in Y = \{\text{spam, 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 Steffing...

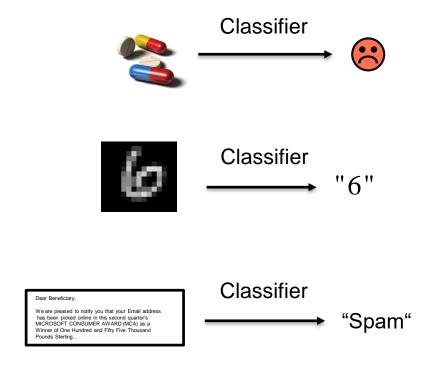
Classifier Toward Pounds Steffing...

**Classifier Toward Pounds Steffing...

Classifier Toward Pounds Steffing...

Classification

Classifier should be learned from training data.



Classifier Learning

Input to the Learner: Training data T_n .

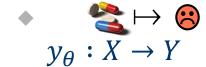
$$\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix}$$
 for example:

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \mathbf{y}$$

Training Data:

$$T_n = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$$

Output: a Model



$$y_{\mathbf{\theta}}(\mathbf{x}) = \begin{cases} \mathbf{\Theta} & \text{if } \mathbf{x}^{\mathrm{T}} \mathbf{\theta} \ge 0 \\ & \text{otherwise} \end{cases}$$

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

Classifier Learning

• Input to the Learner: Training data T_n .

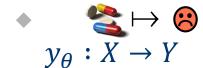
$$\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix}$$

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Training Data:

$$T_n = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$$

Output: a model



- Model classes
 - (Generalized) linear model
 - Decision tree
 - Ensemble classifier
 - **...**

Supervised Learning: Regression

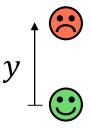
- Input: Instance $x \in X$.
 - e.g., feature vector

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



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 .

$$\mathbf{x} = \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix}$$

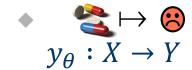
$$\mathbf{y}_{\theta} : X \to Y$$
For example
$$\mathbf{y}_{\theta}(\mathbf{x}) = \mathbf{x}^{T} \mathbf{\theta}$$

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Training Data:

$$T_n = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$$

Output: a model

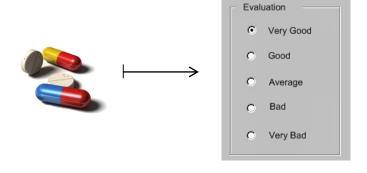


$$y_{\mathbf{\theta}}(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{\theta}$$

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

Supervised Learning: Ordinal Regression

- Input: Instance $x \in X$.
- 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.



Satisfied with the outcome?

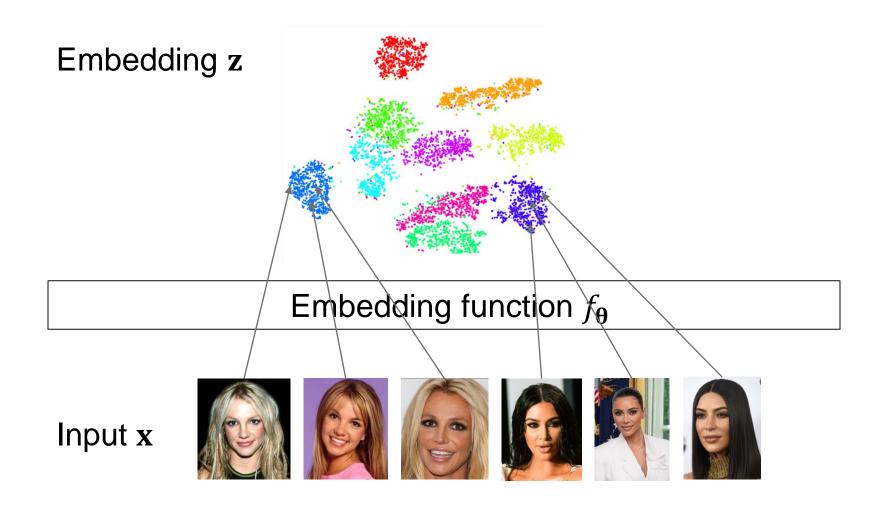
Metric Learning

- For classification problem, the classes are defined and fixed at training time.
- In some applications, one may want the model to identify previously unseen classes.
- For example, biometric identification:
 - All facial images (or fingerprint scans, or iris scans)
 of one individuals can be seen as one class.
 - New individuals should be recognized as such.
- Example object classification:
 - Images of new, previously unseen types of objects should be recognized as belonging to the same class.

Metric Learning

- Given: similarity metric $s(\mathbf{z}, \mathbf{z}')$.
- Input: Instance $x \in X$.
- Output: embedding vector z.
- Input to the learner:
 - Training instances x with classes y.
 - $T_n = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}.$
- Output of the learner: a model $f: \mathbf{x} \mapsto \mathbf{z}$ such that
 - All instances \mathbf{x}, \mathbf{x}' with the same class y are similar: $s(f_{\theta}(\mathbf{x}), f_{\theta}(\mathbf{x}')) > \varepsilon$.
 - Instances $\tilde{\mathbf{x}}$, $\tilde{\mathbf{x}}'$ with different classes y, y' are dissimilar: $s(f_{\theta}(\tilde{\mathbf{x}}), f_{\theta}(\tilde{\mathbf{x}}')) < \varepsilon$.

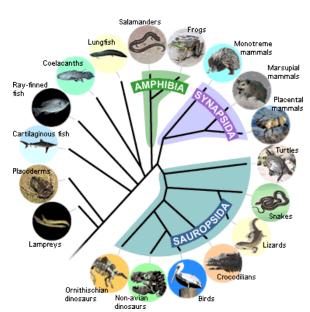
Metric Learning



Supervised Learning: Taxonomy Classification

- Input: Instance $x \in X$.
- 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 farer apart the predicted and actual nodes are.

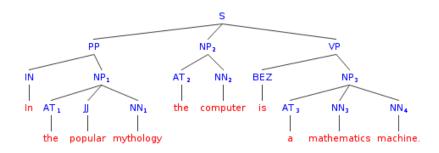


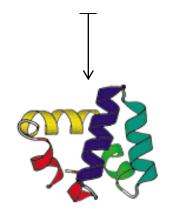


Supervised Learning: Sequence and Structure Prediction

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

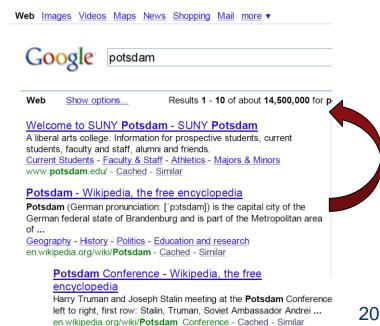
...AAGCTTGCACTGCCGT...





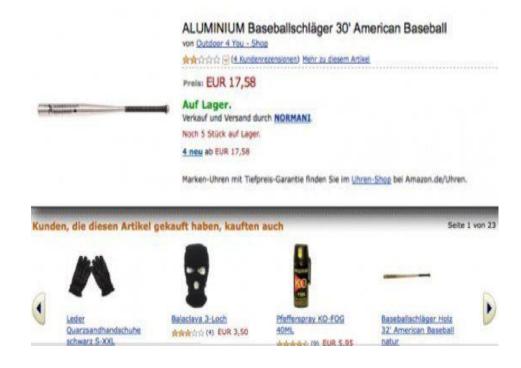
Supervised Learning: Rankings

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



Supervised Learning: Recommendations

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

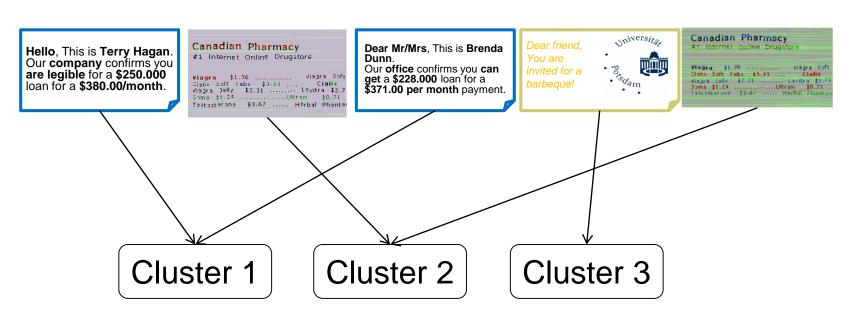


Unsupervised Learning

- Training data for unsupervised learning: Set of instances $x \in X$.
- 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

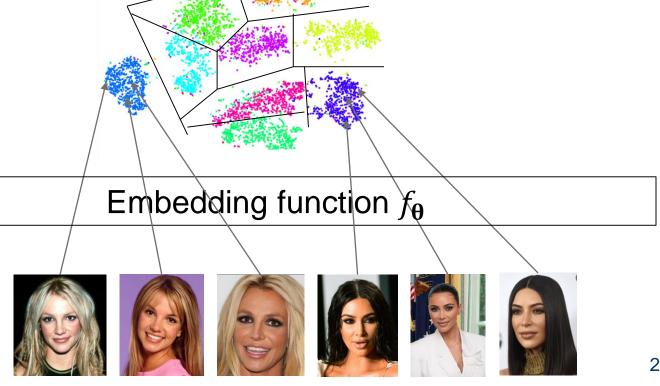
- Input: a stream of emails.
- Output: a partitioning into subsets that belong to the same email campaign.



Example: Clustering Embedding Space

Input: embeddings $f(\mathbf{x})$ of images.

Output: a partitioning into clusters that correspond to individuals.



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 timelagging 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 ones, sales are lost.



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:
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 - 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 .

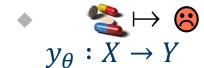
$$\mathbf{X} = \begin{pmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nm} \end{pmatrix} \qquad \mathbf{How can a learning}$$

$$\mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Training Data:

$$T_n = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$$

Output: a classifier



- 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 θ ∈ Θ.
 - ◆ 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

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

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

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

We average the loss over the entire training data T_n :

• Empirical risk
$$\widehat{R}(\mathbf{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_{\mathbf{\theta}}(\mathbf{x}_i), y_i)$$

Example: Binary classification problem with positive class (+1) and negative class (-1). False positives and false negatives are equally bad.

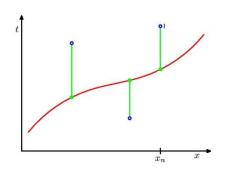
• Zero-One Loss:
$$\ell_{0/1}(y_{\theta}(\mathbf{x}_i), y_i) = \begin{cases} 0 & \text{if } y_{\theta}(\mathbf{x}_i) = y_i \\ 1 & \text{otherwise} \end{cases}$$

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

$$\ell_{c_{FP},c_{FN}}(y_{\boldsymbol{\theta}}(\mathbf{x}_i), y_i) = \begin{cases} y_{\boldsymbol{\theta}}(\mathbf{x}_i) = +1 & y_i = -1 \\ y_{\boldsymbol{\theta}}(\mathbf{x}_i) = +1 & 0 & c_{FP} \\ y_{\boldsymbol{\theta}}(\mathbf{x}_i) = -1 & c_{FN} & 0 \end{cases}$$

- 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:

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



- 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.







Search for a Model

- Search for a Classifier of "toxic combinations".

Model space:
$$y_{\theta}(\mathbf{x}) = \begin{cases} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{cases}$$
 if $\sum_{j=1}^m x_j \theta_j \geq \theta_0$ where \mathbf{x}_1 is \mathbf{x}_2 and \mathbf{x}_3 is \mathbf{x}_4 otherwise. Approach: empirical risk should be minitial to \mathbf{x}_1 and \mathbf{x}_2 is \mathbf{x}_3 and \mathbf{x}_4 and \mathbf{x}_4 is \mathbf{x}_4 .

Training data

Medications in the combination

	X 1	<i>X</i> 2	<i>X</i> 3	X 4	X 5	X 6	y
X 1	1	1	0	0	1	1	
X 2	0	1	1	0	1	1	
X 3	1	0	1	0	1	0	\odot
X 4	0	1	1	0	0	0	\odot

Approach: empirical risk should be minimal

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

Is there such a model? Are there many?

- Search for a Classifier of "toxic combinations".

Model space:
$$y_{\theta}(\mathbf{x}) = \begin{cases} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{cases}$$
 if $\sum_{j=1}^m x_j \theta_j \geq \theta_0$ otherwise
$$\sum_{j=1}^m x_j \theta_j \geq \theta_0$$
 Models with 0 loss:

Training data

	X 1	X 2	<i>X</i> 3	X 4	X 5	X 6	y
X 1	1	1	0	0	1	1	
X 2	0	1	1	0	1	1	
X 3	1	0	1	0	1	0	\odot
X 4	0	1	1	0	0	0	\odot

- Models with 0 loss:
 - $y_{\theta}(\mathbf{x}) = \mathbf{\Theta}$, if $x_6 \ge 1$

 - $y_{\theta}(\mathbf{x}) = 3$, if $x_2 + x_5 \ge 2$ $y_{\theta}(\mathbf{x}) = 3$, if $2x_4 + x_6 \ge 1$

- Search for a Classifier of "toxic combinations".

Model space:
$$y_{\theta}(\mathbf{x}) = \begin{cases} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{cases}$$
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Training data

	X 1	X 2	Х3	X 4	X 5	X 6	y
X 1	1	1	0	0	1	1	
X 2	0	1	1	0	1	1	
X 3	1	0	1	0	1	0	\odot
X 4	0	1	1	0	0	0	\odot

- 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 Classifier of "toxic combinations".

Model space:
$$y_{\theta}(\mathbf{x}) = \begin{cases} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{cases}$$
 if $\sum_{j=1}^m x_j \theta_j \geq \theta_0$ where \mathbf{x}_1 is \mathbf{x}_2 and \mathbf{x}_3 and \mathbf{x}_4 where \mathbf{x}_2 is \mathbf{x}_3 and \mathbf{x}_4 where \mathbf{x}_3 is \mathbf{x}_4 . The Models with 0 loss:

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•
$$y_{\theta}(\mathbf{x}) = \mathbf{0}$$
, if $x_2 + x_5 \ge 2$

•
$$y_{\theta}(\mathbf{x}) = \mathbf{0}$$
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Training data

	X 1	<i>X</i> 2	<i>X</i> 3	X 4	X 5	X 6	y
X 1	1	1	0	0	1	1	
X 2	0	1	1	0	1	1	
X 3	1	0	1	0	1	0	\odot
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 if $\sum_{j=1}^m x_j \theta_j \geq \theta_0$ otherwise
$$\sum_{j=1}^m x_j \theta_j \geq \theta_0$$
 Models with 0 loss:
$$\mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \\ \mathbf{x}_4 \\ \mathbf{x}_5 \\ \mathbf{x}_6 \\ \mathbf{x}_7 \\ \mathbf{x}_8 \\ \mathbf{x}_9 \\ \mathbf{x}_{1} \\ \mathbf{x}_{2} \\ \mathbf{x}_{3} \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \mathbf{x}_{6} \\ \mathbf{x}_{1} \\ \mathbf{x}_{2} \\ \mathbf{x}_{3} \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \mathbf{x}_{6} \\ \mathbf{x}_{1} \\ \mathbf{x}_{2} \\ \mathbf{x}_{3} \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \mathbf{x}_{6} \\ \mathbf{x}_{6} \\ \mathbf{x}_{1} \\ \mathbf{x}_{2} \\ \mathbf{x}_{3} \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \mathbf{x}_{6} \\ \mathbf{x}_{1} \\ \mathbf{x}_{2} \\ \mathbf{x}_{3} \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \mathbf{x}_{6} \\ \mathbf{x}_{6} \\ \mathbf{x}_{1} \\ \mathbf{x}_{2} \\ \mathbf{x}_{3} \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \mathbf{x}_{6} \\ \mathbf{x}_{6} \\ \mathbf{x}_{1} \\ \mathbf{x}_{2} \\ \mathbf{x}_{3} \\ \mathbf{x}_{4} \\ \mathbf{x}_{5} \\ \mathbf{x}_{6} \\ \mathbf{x}_{6} \\ \mathbf{x}_{6} \\ \mathbf{x}_{6} \\ \mathbf{x}_{6} \\ \mathbf{x}_{7} \\ \mathbf{x}_{8} \\ \mathbf{x}_{8} \\ \mathbf{x}_{8} \\ \mathbf{x}_{9} \\ \mathbf{x}_{9}$$

Models with 0 loss:

•
$$y_{\theta}(\mathbf{x}) = \mathbf{\Theta}$$
, if $x_6 \ge 1$
• $y_{\theta}(\mathbf{x}) = \mathbf{\Theta}$, if $x_2 + x_5 \ge 2$
• $y_{\theta}(\mathbf{x}) = \mathbf{\Theta}$, if $2x_4 + x_6 \ge 1$

•
$$y_{\theta}(\mathbf{x}) = \mathbf{0}$$
, if $x_2 + x_5 \ge 2$

•
$$y_{\theta}(\mathbf{x}) = 0$$
, if $2x_4 + x_6 \ge 1$

Training data

	X 1	<i>X</i> 2	<i>X</i> 3	X 4	X 5	X 6	y
X 1	1	1	0	0	1	1	
X 2	0	1	1	0	1	1	
X 3	1	0	1	0	1	0	\odot
X 4	0	1	1	0	0	0	\odot

- 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 Ω(θ):
 - Expresses assumptions about whether the model θ is a priori probable.
 - $\bullet \Omega$ 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 weights, L_0 -Regularization
 - Sum of the attribute weights, L₁-Regularization
 - Sum of the squared attribute weights, L_2 -Regularization.

Regularizer

Candidates:

$$(\theta_0, \theta_1, \theta_2, \theta_3, \theta_4, \theta_5, \theta_6)$$

$$y_{\theta}(\mathbf{x}) = \mathbf{e}$$
, if $x_6 \ge 1$

$$\mathbf{\theta}_1 = (1,0,0,0,0,0,1)^{\mathrm{T}}$$

•
$$y_{\theta}(\mathbf{x}) = \mathbf{\Theta}$$
, if $x_2 + x_5 \ge 2$ $\theta_2 = (2,0,1,0,0,1,0)^T$

$$\mathbf{\theta}_2 = (2,0,1,0,0,1,0)^{\mathrm{T}}$$

•
$$y_{\theta}(\mathbf{x}) = \mathbf{\Theta}$$
, if $2x_4 + x_6 \ge 1$ $\theta_3 = (1,0,0,0,2,0,1)^T$

$$\theta_3 = (1,0,0,0,2,0,1)^{\mathrm{T}}$$

Regularizer:

 L_0 -Regularisierung L_1 -Regularisierung L_2 -Regularisierung

$$\Omega_0(\boldsymbol{\theta}_1) = 2$$

$$\Omega_1(\boldsymbol{\theta}_1) = 2$$

$$\Omega_2(\mathbf{\theta}_1) = 2$$

$$\Omega_0(\boldsymbol{\theta}_2) = 3$$

$$\Omega_1(\mathbf{\theta}_2) = 4$$

$$\Omega_2(\mathbf{\theta}_2) = 6$$

$$\Omega_0(\mathbf{\theta}_3) = 3$$

$$\Omega_1(\mathbf{\theta}_3) = 4$$

$$\Omega_2(\boldsymbol{\theta}_3) = 6$$

Optimization Criterion

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

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

■ 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 $|\theta|$ (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:
$$y_{\theta}(\mathbf{x}) = \begin{cases} \mathbf{if} \ \sum_{j=1}^{m} x_{j} \theta_{j} \geq \theta_{0} \\ otherwise \end{cases}$$
Regularized empirical risk:
$$1 \sum_{j=1}^{n} \mathbf{if} \ \mathbf{x}_{j} \mathbf$$

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

Model with minimal regularized empirical risk

$$y_{\theta}(\mathbf{x}) = \begin{cases} \mathbf{S} & \text{if } x_6 \ge 1 \\ \mathbf{O} & \text{otherwise} \end{cases}$$

Training data

	X 1	<i>X</i> 2	<i>X</i> 3	X 4	X 5	X 6	y
X 1	1	1	0	0	1	1	
X 2	0	1	1	0	1	1	
X 3	1	0	1	0	1	0	\odot
X 4	0	1	1	0	0	0	\odot

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 $p(\mathbf{x}, y)$.

$$R(\mathbf{\theta}) = \sum_{v} \int \ell((y_{\mathbf{\theta}}(\mathbf{x}), y)) p(\mathbf{x}, y) d\mathbf{x}$$

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

Evaluation of Models

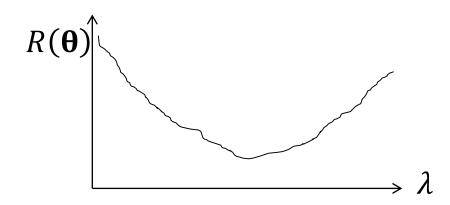
- How good will a model function in the future?
- Future instances will be drawn according to an (unknown) probability distribution $p(\mathbf{x}, y)$.
- Risk: expected loss under distribution $p(\mathbf{x}, y)$.
- Is the empirical risk on the training data a useful estimator for the risk?
 - Problem: 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 instances 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.