Chapter ML:II

II. Machine Learning Basics

- On Data
- Regression
- Concept Learning: Search in Hypothesis Space
- Concept Learning: Search in Version Space
- Measuring Performance

On Data [Tan et al. 2005]

- An object $o \in O$ is described by a set of attributes.
  An object is also known as record, point, case, sample, entity, or instance.
- An attribute A is a property of an object.
  An attribute is also known as variable, field, characteristic, or feature.
- A measurement scale is a system (often a convention) of assigning a numerical or symbolic value to an attribute of an object.

Attributes

Objects

ID	Check	Status	Income	Risk
1	+	single	125 000	No
2	-	married	100 000	No
3	-	single	70 000	No
4	+	married	120 000	No
5	-	divorced	95 000	Yes
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7	+	divorced	220 000	No
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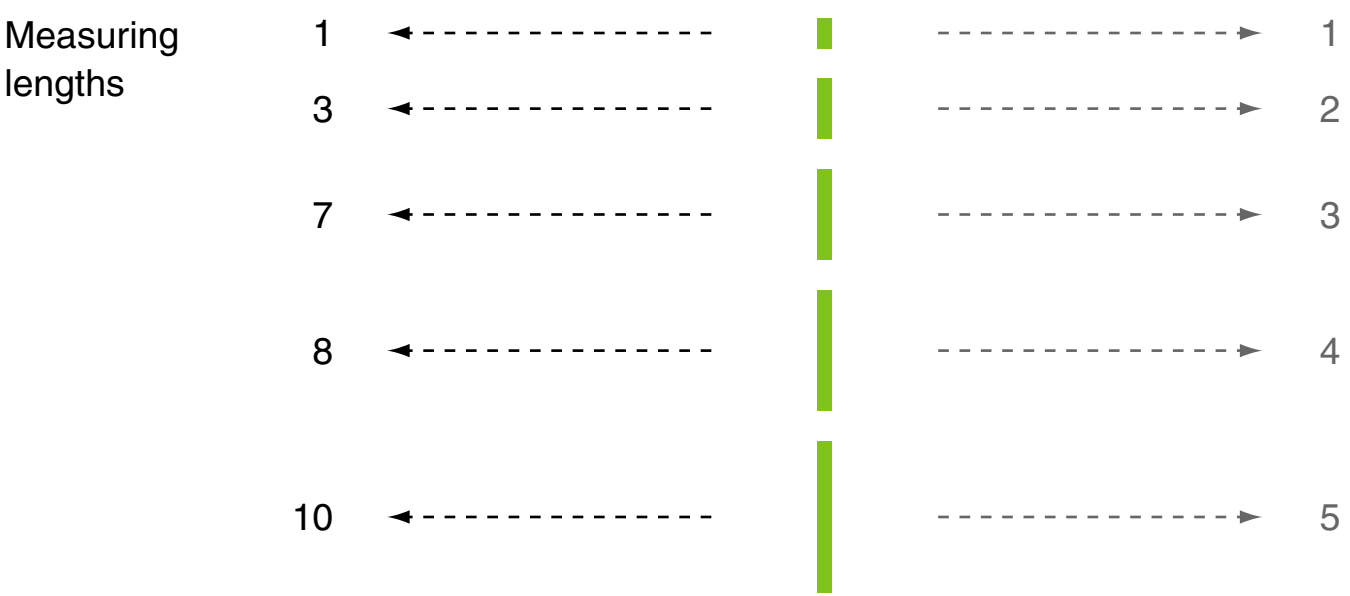
On Data [Tan et al. 2005]

- Attribute values may vary from one object to another or one time to another.
- The same attribute can be mapped to different attribute values.
  Example: height can be measured in feet or meters.
- Different attributes can be mapped to the same set of values.
  Example: attribute values for person ID and age are integers.

The way an attribute is measured may not match the attribute's properties:



On Data [Tan et al. 2005]

Types of Attributes

Type		Comparison	Statistics	Examples
categorical (qualitative)	nominal	values are names, only information to distinguish objects $=$ $\neq$	mode, entropy, contingency, correlation, χ^2 test	zip codes, employee IDs, eye color, gender: {male, female}

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numeric (quantitative)	interval	differences are meaningful, a unit of measurement exists $+$ $-$	mean, standard deviation, Pearson's correlation, t-test, F-test	calendar dates, temperature in Celsius, temperature in Fahrenheit

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numeric (quantitative)	interval	differences are meaningful, a unit of measurement exists $+$ $-$	mean, standard deviation, Pearson's correlation, t-test, F-test	calendar dates, temperature in Celsius, temperature in Fahrenheit
	ratio	differences and ratios are meaningful $*$ $/$	geometric mean, harmonic mean, percent variation	temperature in Kelvin, monetary quantities, counts, age, length, electrical current

On Data [Tan et al. 2005]

Types of Attributes

Type		Permissible transformation	Comment
categorical (qualitative)	nominal	any one-to-one mapping, permutation of values	A reassignment of employee ID numbers will not make any difference.

On Data [Tan et al. 2005]

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On Data [Tan et al. 2005]

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numeric (quantitative)	interval	$x \to a \cdot x + b$, where a and b are constants	Thus, the Fahrenheit and Celsius temperature scales differ in terms of where their zero value is and the size of a unit (degree).
	ratio	$x \to a \cdot x$, where a is a constant	Length can be measured in meters or feet.

Remarks:

- Identifying, considering, and measuring an attribute A of an object O is the heart of model formation and always goes along with a sort of abstraction. Formally, this abstraction is operationalized by a model formation function $\alpha : O \to X$. [ML Introduction]
- The terms “attribute” and “feature” can be used synonymously. However, a slight distinction is the following: attributes are often associated with objects, O, while features usually designate the dimensions of the feature space, X.
- The type of an attribute is also referred to as the type of a *measurement scale* or *level of measurement*.
- We call a transformation of an attribute *permissible* if its meaning is unchanged after the transformation.
- Distinguish between *discrete* attributes and *continuous* attributes. The former can only take a finite or countably infinite set of values, the latter can be measured in infinitely small units. Be careful when deriving from this distinction an attribute’s type.
- We will encode attributes of interval type or ratio type by real numbers. Note that attributes of nominal type and ordinal type can also be encoded by real numbers.
- Particular learning methods require particular attribute types.

On Data [Tan et al. 2005]

Types of Data Sets

Data sets may not be a homogeneous collection of objects but come along with differently intricate characteristics:

1. Inhomogeneity of attributes:

2. Inhomogeneity of objects:

3. Inhomogeneity of distributions:

4. Curse of dimensionality:

5. Resolution:

On Data [Tan et al. 2005]

Types of Data Sets

Data sets may not be a homogeneous collection of objects but come along with differently intricate characteristics:

1. Inhomogeneity of attributes:
   Consider the combination of different attribute types within a single object.

2. Inhomogeneity of objects:
   Consider the combination of different objects in a single data set.

3. Inhomogeneity of distributions:
   The correlation between attributes varies in the sample space.

4. Curse of dimensionality:
   Attribute number and object density stand in exponential relation.

5. Resolution:
   The number of objects or attributes may be given at different resolutions.

On Data [Tan et al. 2005]

Types of Data Sets: Record Data

Collection of records, each of which consists of a fixed set of attributes:

ID	Check	Status	Income	Risk
1	+	single	125 000	No
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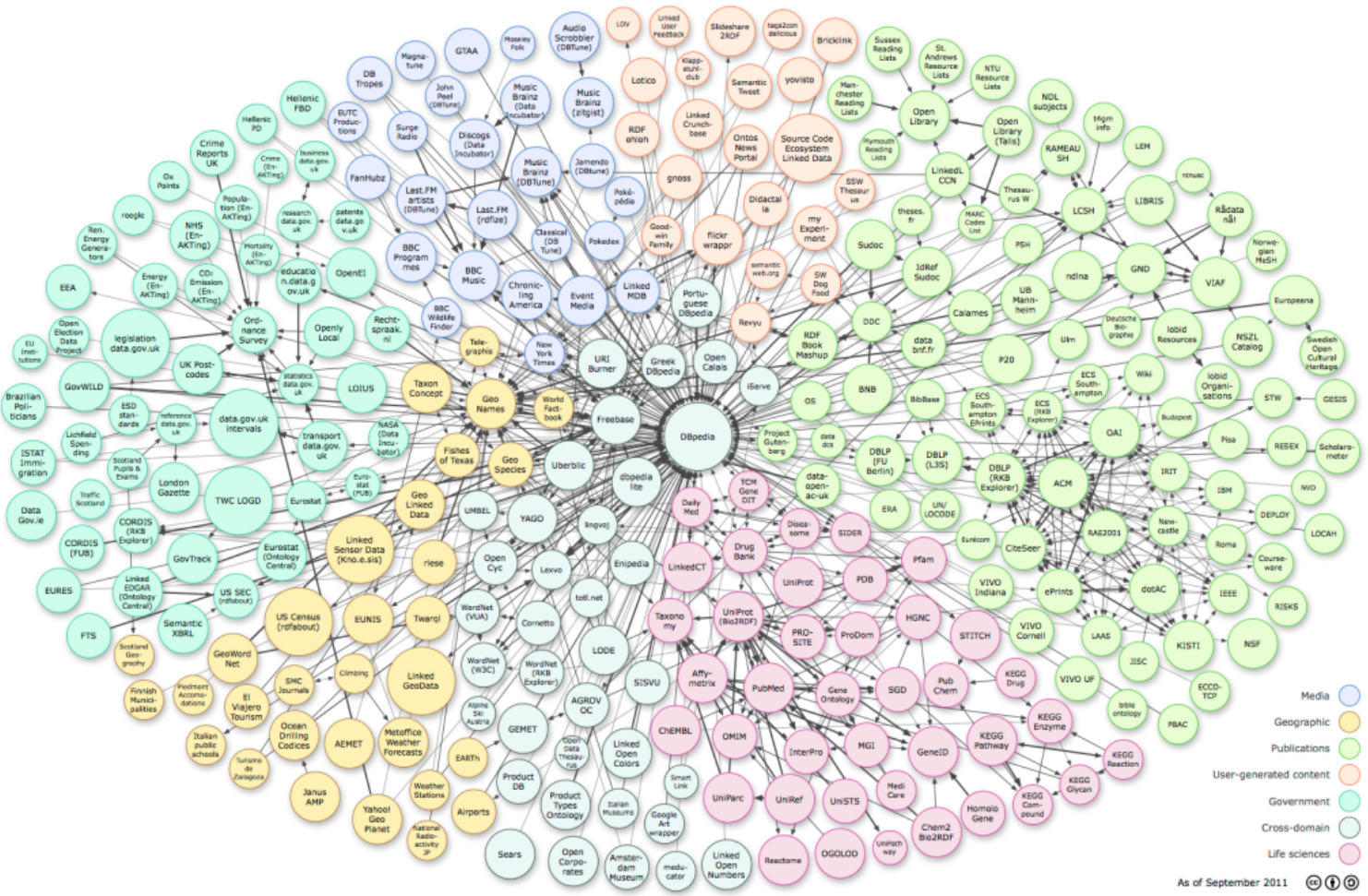
- If all elements in a data set have the same fixed set of numeric attributes, they can be thought of as points in a multi-dimensional space.
- Such data can be represented by a matrix, where each row stores an object and each column stores an attribute.
  Example: term-document matrices in information retrieval.

On Data [Tan et al. 2005]

Types of Data Sets: Graph Data

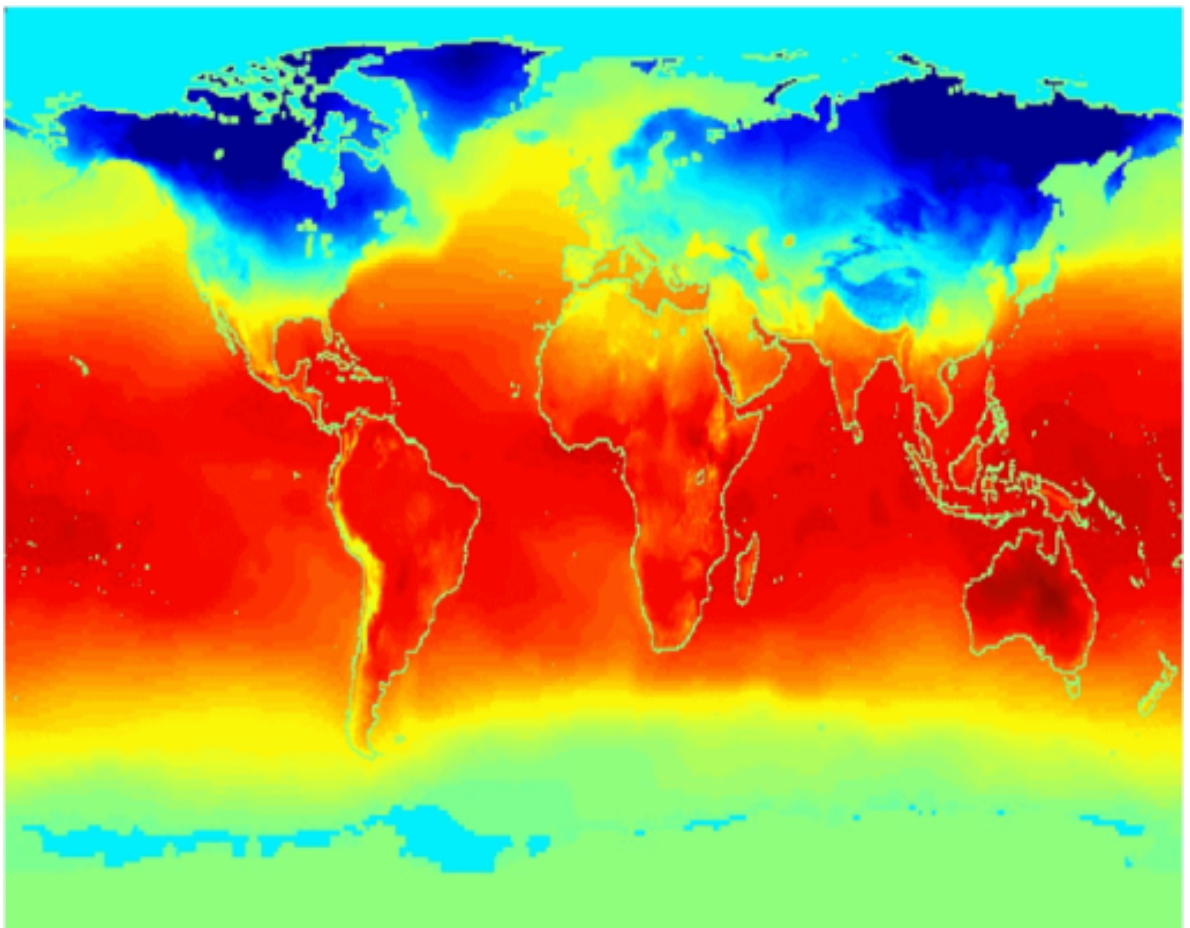
Graph of the Linked Open Data cloud [richard.cyganiak.de]:



On Data [Tan et al. 2005]

Types of Data Sets: Ordered Data

Average monthly temperature of land and ocean (= spatio-temporal data) :



On Data [Tan et al. 2005]

Data Quality

When repeating measurements of a quantity, measurement errors and data collection errors may occur during the measurement process. Questions:

1. What kinds of data quality problems exist?
2. How to detect data quality problems?
3. How to address data quality problems?

On Data [Tan et al. 2005]

Data Quality

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Definition 1 (Precision, Bias, Accuracy)

Given a set of repeated measurements of the same quantity. Then, the closeness of the measurements to one another is called *precision*, a possible systematic variation is called *bias*, and the closeness to the true value is called *accuracy*.

On Data [Tan et al. 2005]

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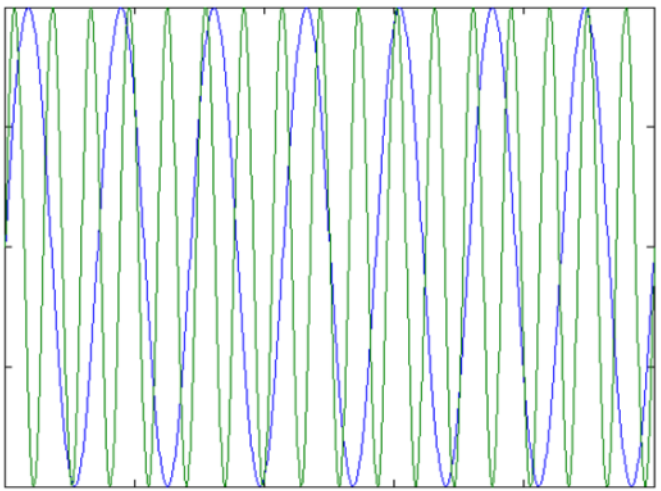
Examples for data quality problems:

- noise, artifacts, outliers
- missing values
- duplicate data

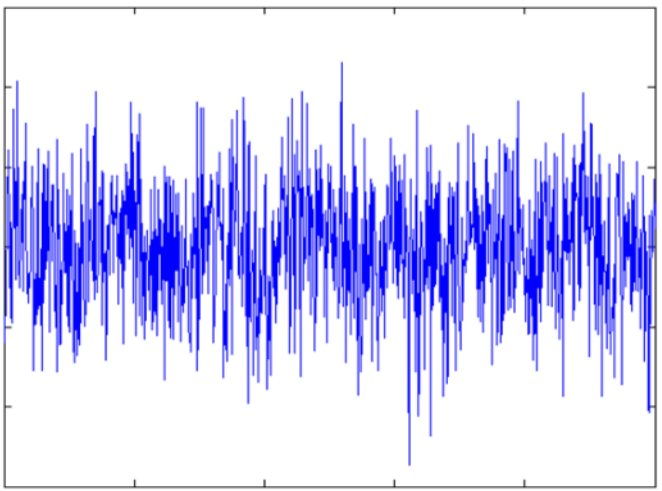
On Data [Tan et al. 2005]

Data Quality: Noise

Noise refers to random modifications of attributes that often have a spatial or temporal characteristics:



sin waves



sin waves with noise

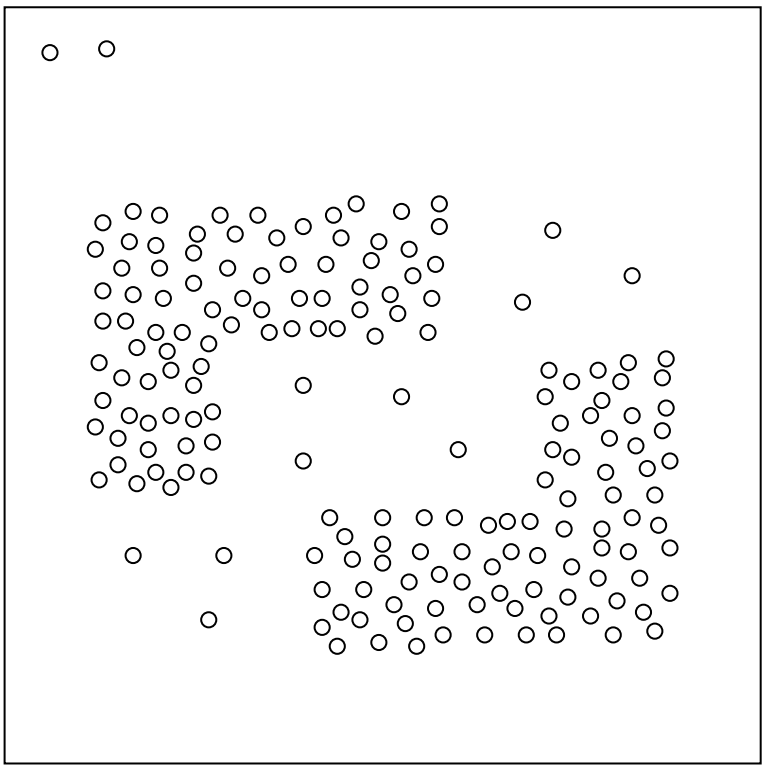
Noise represents the intrinsic variability of data. [Bishop 2006, p.47]

Artifacts refer to more deterministic distortions of a measurement process.

On Data [Tan et al. 2005]

Data Quality: Outliers

Outliers are members in the data set with characteristics that are considerably different than most of the other elements:



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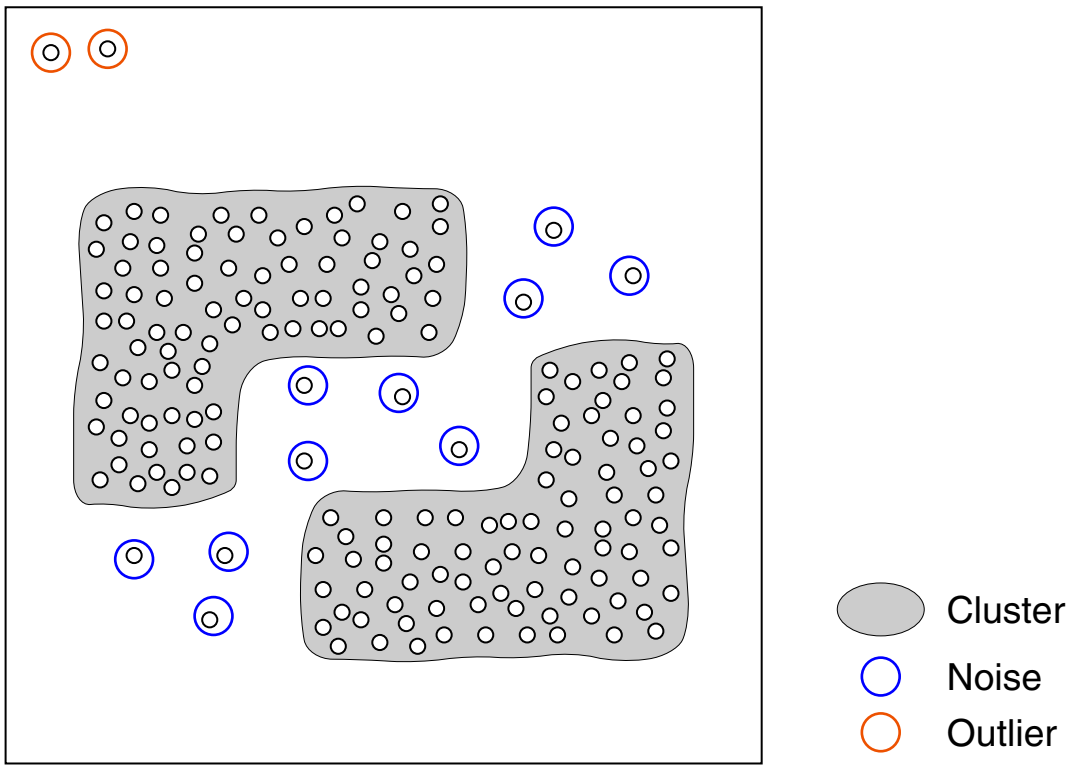

On Data [Tan et al. 2005]

Data Quality: Missing Values

Main reasons for missing values:

1. Information is not collected.
   Example: people decline to give their age or weight.
2. Attributes may not be applicable to all elements in O.
   Example: annual income is not applicable to children.
3. Information is not trustworthy.
   Example: profile data on Facebook is intentionally misleading.

Strategies for handling missing values:

- eliminate members of the data
- estimate missing values
- ignore the missing value during analysis
- replace with all possible values weighted by their probabilities

On Data [Tan et al. 2005]

Data Preprocessing

- sampling of object set O
- modeling of objects, $\alpha : O \to X$
- sampling of feature space X [ML Introduction]
- selection of attributes (features) [attributes versus features]
- transformation of attributes (features)
- discretization and binarization of attributes (features)
- dimensionality reduction of feature space X

Chapter ML:II

II. Machine Learning Basics

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- Measuring Performance

Regression

Classification versus Regression

X is a p-dimensional feature space or input space. Example:

Customer 1	
house owner	yes
income (p.a.)	51 000 EUR
repayment (p.m.)	1 000 EUR
credit period	7 years
SCHUFA entry	no
age	37
married	yes
...	

...

Customer n	
house owner	no
income (p.a.)	55 000 EUR
repayment (p.m.)	1 200 EUR
credit period	8 years
SCHUFA entry	no
age	?
married	yes
...	

Classification:

- $C = \{-1, 1\}$ is a set of classes. Similarly: $C = \{0, 1\}$, $C = \{\text{no}, \text{yes}\}$
- $c : X \to C$ is the ideal classifier for X.
- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.

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Regression:

- $Y \subseteq \mathbf{R}$ is the output space.
- y_i is an observed credit line value for an $\mathbf{x}_i \in X$.
- $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \subseteq X \times Y$ is a set of examples.

Regression

The Linear Regression Model

- Given $\mathbf{x}$, predict a real-valued output under a linear model function:

$$y(\mathbf{x}) = w_0 + \sum_{j=1}^{p} w_j \cdot x_j$$

- Vector notation with $x_0 = 1$ and $\mathbf{w} = (w_0, w_1, \ldots, w_p)^T$:

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$$

- Given $\mathbf{x}_1, \ldots, \mathbf{x}_n$, assess goodness of fit as residual sum of squares:

$$\text{RSS}(\mathbf{w}) = \sum_{i=1}^{n} (y_i - y(\mathbf{x}_i))^2 = \sum_{i=1}^{n} (y_i - \mathbf{w}^T \mathbf{x}_i)^2 \quad (1)$$

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- Estimate $\mathbf{w}$ by minimizing the residual sum of squares:

$$\hat{\mathbf{w}} = \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\text{argmin}} \ \text{RSS}(\mathbf{w}) \tag{2}$$

Remarks:

- A *residual* is the difference between an observed value y_i and the estimated value $y(\mathbf{x}_i)$ of the model function.
- The residual sum of squares, RSS, is the sum of squares of the residuals. It is also known as the sum of squared residuals, SSR, or the sum of squared errors of prediction, SSE.
- The RSS term quantifies the regression error—or similarly, the goodness of fit—in the form of a single value.
- RSS provides several numerical and theoretical advantages, but it is not the only possibility to assess the goodness of fit (= error) between observed values and the model function. Alternative approaches for quantifying the error include absolute residual values or a polynomial in the residual values.
- The error computation is also called loss computation, cost computation, or generally, performance computation. Similarly, for the right-hand side of Equation (1) the following names are used: error function, loss function, cost function, or generally, performance term. Measures that quantify this kind of performance are called *effectiveness* measures. This must not be confused with *efficiency* measures, which quantify the computational effort or runtime performance of a method.

Remarks (continued):

- From a statistical viewpoint, $\mathbf{x} = x_1, \ldots, x_p$ and y represent *random variables* (vectorial and scalar respectively). Each feature vector, $\mathbf{x}_i$, and outcome, y_i, is the result of a random experiment and hence is governed by a—usually unknown—probability distribution.
- The distributions of the random variables y_i and $(y_i - y(\mathbf{x}_i))$ are identical.
- Equation (2): Estimating $\mathbf{w}$ by RSS minimization is based on the following assumptions:
  1. The random variables y_i are statistically independent. Actually, the conditional independence of the y_i under $\mathbf{x}_i$ is sufficient.
  2. The means $E(y_i)$ lie on a straight line, known as the true (population) regression line: $E(y_i) = \mathbf{w}^{*T}\mathbf{x}_i$. I.e., the relation between the observed $(\mathbf{x}, y) \in X \times Y$ can be completely explained by a linear model function.
  3. The probability distributions $P(y_i \mid \mathbf{x}_i)$ have the same variance.

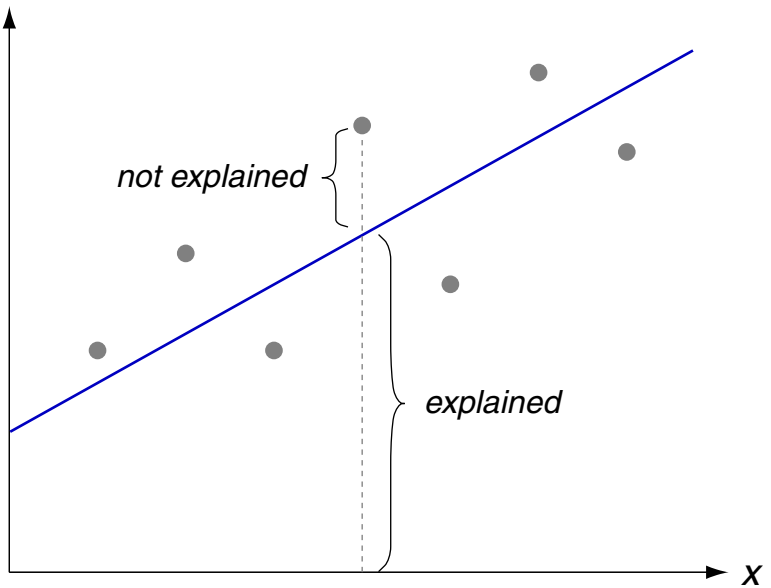
  The three assumptions are called the *weak set* (of assumptions). Along with a fourth assumption about the distribution shape of y_i they become the *strong set* of assumptions.
- In order to avoid cluttered notation, we won't use different symbols to distinguish random variables from ordinary variables. I.e., if $\mathbf{x}, x, y$ denote a (vectorial or scalar) random variable this fact will become clear from the context.

Regression

One-Dimensional Feature Space

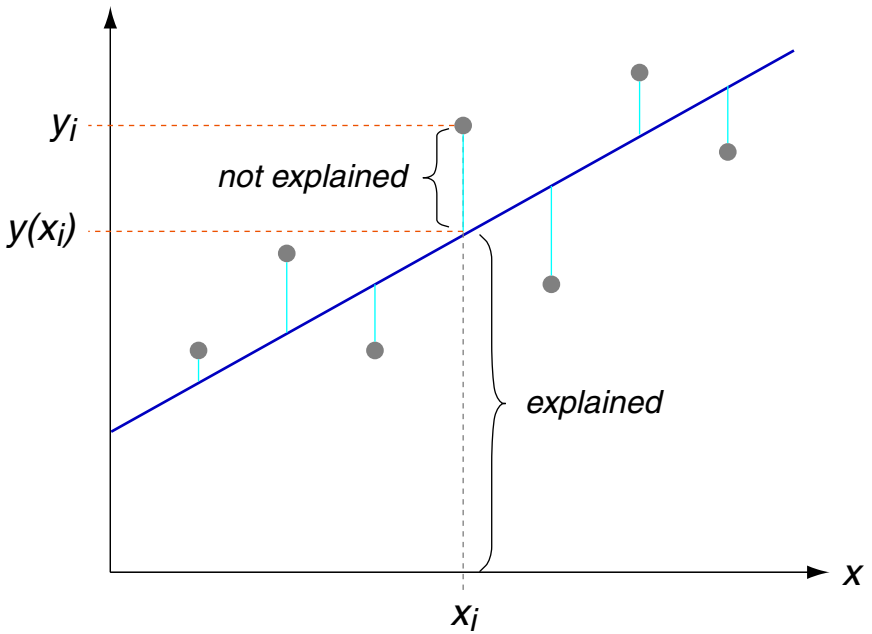
Regression

One-Dimensional Feature Space (continued)



Regression

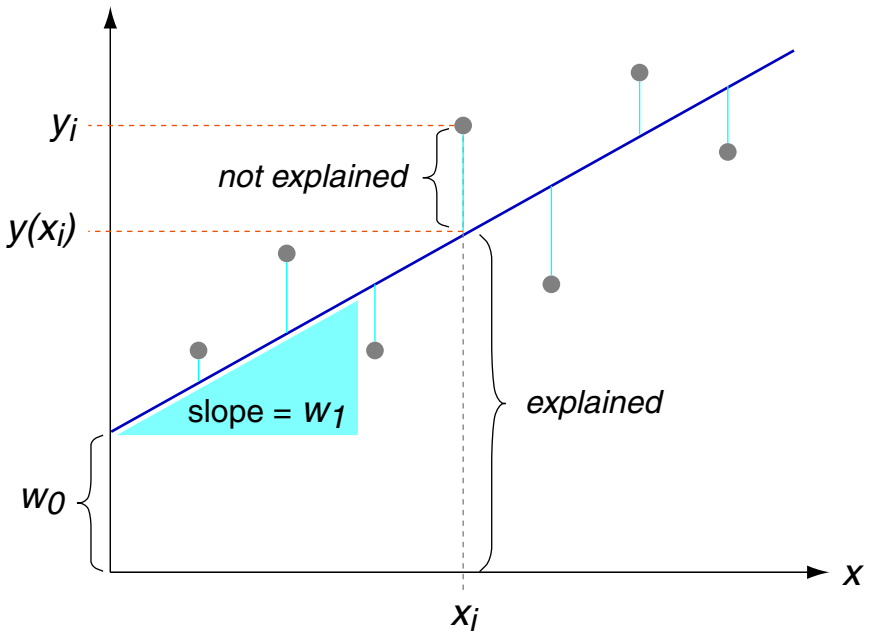
One-Dimensional Feature Space (continued)



$$\text{RSS} = \sum_{i=1}^{n} (y_i - y(x_i))^2$$

Regression

One-Dimensional Feature Space (continued)



$$y(x) = w_0 + w_1 \cdot x, \qquad \text{RSS}(w_0, w_1) = \sum_{i=1}^{n} (y_i - w_0 - w_1 \cdot x_i)^2$$

Regression

One-Dimensional Feature Space (continued) [higher-dimensional]

Minimize RSS(w_0, w_1) by a direct method:

1. $$\frac{\partial}{\partial w_0} \sum_{i=1}^{n} (y_i - w_0 - w_1 \cdot x_i)^2 \;=\; 0$$

$$\rightsquigarrow \;\ldots\; \rightsquigarrow \quad w_0 \;=\; \frac{1}{n} \sum_{i=1}^{n} y_i \;-\; \frac{w_1}{n} \sum_{i=1}^{n} x_i \;=\; \bar{y} - w_1 \cdot \bar{x}$$

Regression

One-Dimensional Feature Space (continued) [higher-dimensional]

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$$\rightsquigarrow \;\ldots\; \rightsquigarrow \qquad w_1 = \frac{\sum_{i=1}^{n} (x_i - \bar{x}) \cdot (y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2}$$

Regression

One-Dimensional Feature Space (continued) [higher-dimensional]

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Regression

Higher-Dimensional Feature Space

- Recall Equation (1):

$$\text{RSS}(\mathbf{w}) = \sum_{\mathbf{x}_i \in D} (y(\mathbf{x}_i) - \mathbf{w}^T \mathbf{x}_i)^2$$

- Let $\mathbf{X}$ denote the $n \times (p+1)$ matrix,
  where row i is the extended input vector $(1 \;\; \mathbf{x}_i^T)$, $\mathbf{x}_i \in D$.

  Let $\mathbf{y}$ denote the n-vector of outputs in the training set D.

Regression

Higher-Dimensional Feature Space

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  Let $\mathbf{y}$ denote the n-vector of outputs in the training set D.

$\rightsquigarrow$ $\text{RSS}(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^T (\mathbf{y} - \mathbf{X}\mathbf{w})$

$\text{RSS}(\mathbf{w})$ is a quadratic function in $p+1$ parameters.

Regression

Higher-Dimensional Feature Space (continued) [one-dimensional]

Minimize $\mathrm{RSS}(\mathbf{w})$ by a direct method:

$$\frac{\partial \mathrm{RSS}}{\partial \mathbf{w}} = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w}) = 0, \qquad \frac{\partial^2 \mathrm{RSS}}{\partial \mathbf{w} \partial \mathbf{w}^T} = -2\mathbf{X}^T\mathbf{X}$$ [Wikipedia 1, 2, 3]

$$\begin{aligned} \mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w}) &= 0 \\ \Leftrightarrow \quad \mathbf{X}^T\mathbf{X}\mathbf{w} &= \mathbf{X}^T\mathbf{y} \\ \rightsquigarrow \quad \mathbf{w} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\,\mathbf{y} \end{aligned}$$

Regression

Higher-Dimensional Feature Space (continued) [one-dimensional]

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Normal equations.

If $\mathbf{X}$ has full column rank $p+1$.

Pseudoinverse of $\mathbf{X}$ [Wikipedia]

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$$\Leftrightarrow \quad \mathbf{X}^T\mathbf{X}\mathbf{w} = \mathbf{X}^T\mathbf{y}$$ Normal equations.

$$\rightsquigarrow \quad \hat{\mathbf{w}} \equiv \mathbf{w} = \underbrace{(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T}\,\mathbf{y}$$ If $\mathbf{X}$ has full column rank $p+1$.

Pseudoinverse of $\mathbf{X}$ [Wikipedia]

$$\hat{y}(\mathbf{x}_i) = \mathbf{x}_i^T\,\hat{\mathbf{w}}$$ Regression function with least squares estimator $\hat{\mathbf{w}}$.

$$\hat{\mathbf{y}} = \mathbf{X}\,\hat{\mathbf{w}}$$ The n-vector of fitted values at the training input.

$$= \mathbf{X}\,(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

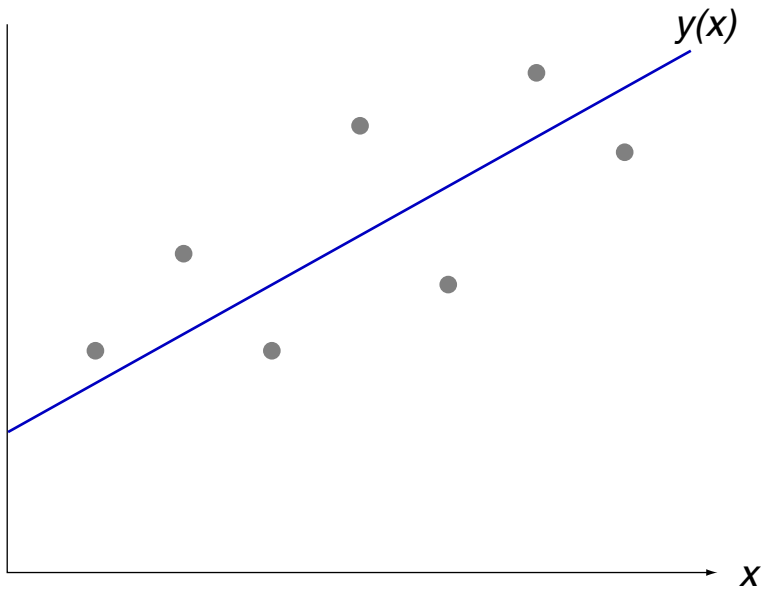
Remarks:

- A curve fitting (or regression) method that is based on the minimization of squared residuals is called a *method of least squares*.
- Various approaches for operationalizing the method of least squares have been devised, in particular for the case of linear model functions. From a numerical viewpoint one can distinguish iterative methods, such as the LMS algorithm, and direct methods, such as solving the normal equations via computing the pseudoinverse.
- More on direct methods. While solving the normal equations is usually fast, it suffers from several deficits: it is numerically sensitive and requires singularity handling. Numerically more stable and more accurate methods base on the QR decomposition and the singular value decomposition, SVD.
- QR decomposition may handle problems with up to 10^4 variables, provided a dense problem structure. For significantly larger problems (additional 1-2 orders of magnitudes) as well as for sparse matrices iterative solvers are the choice. Even larger, dense problems may be tackled with Artificial Neural Networks.

Regression

Linear Regression for Classification (illustrated for $p = 1$)

Regression learns a real-valued function given as $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$.



$$y(x) = (w_0 \;\; w_1)\begin{pmatrix}1\\ x\end{pmatrix}$$

Regression

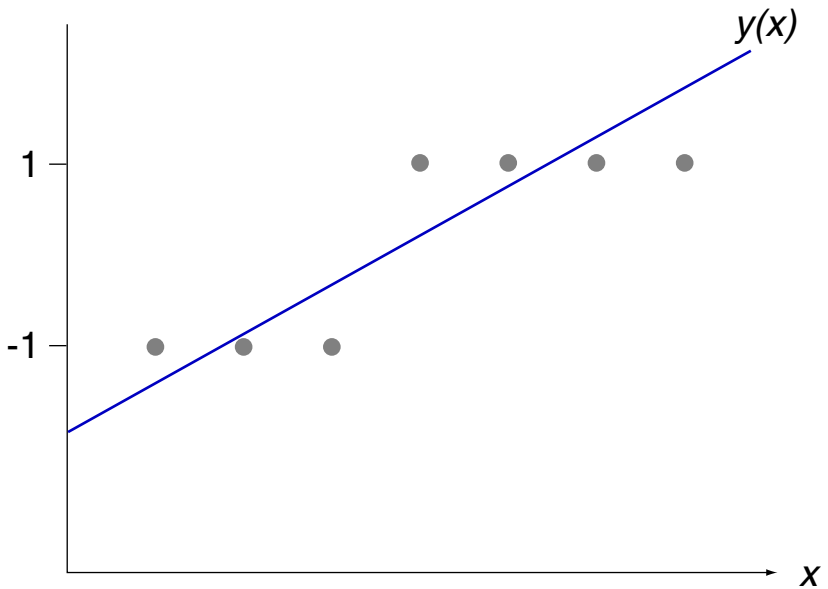
Linear Regression for Classification (illustrated for $p = 1$)

Binary-valued (± 1) functions are also real-valued.

Regression

Linear Regression for Classification (illustrated for $p = 1$)

Use linear regression to learn $\mathbf{w}$ from D, where $y_i = \pm 1 \approx y(\mathbf{x}_i) = \mathbf{w}^T \mathbf{x}_i$.



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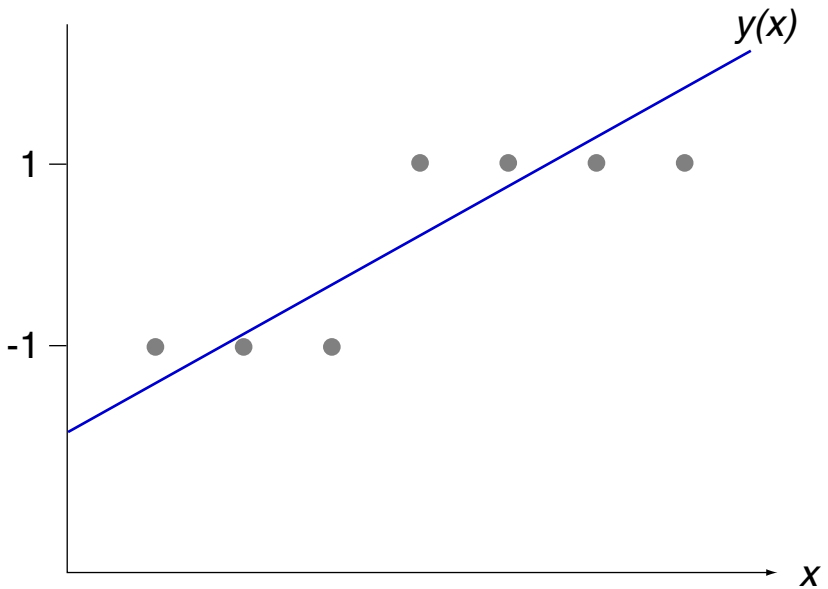

The function "sign$(\mathbf{w}^T \mathbf{x}_i)$" is likely to agree with $y_i = \pm 1$.

- Regression: $y(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$
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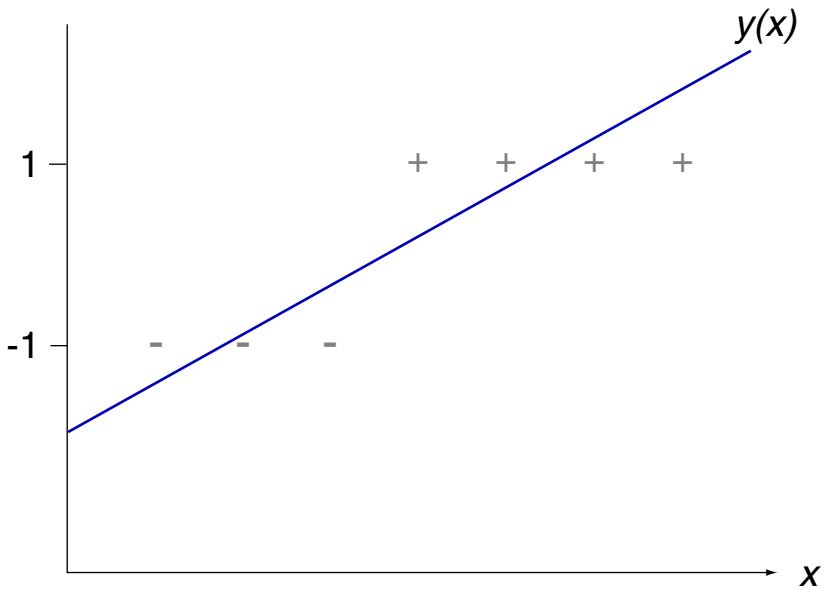

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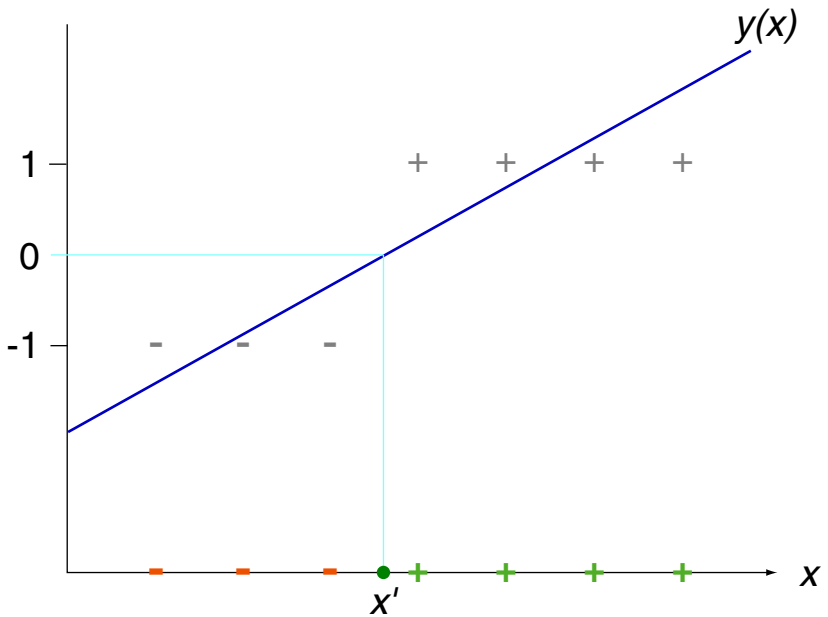

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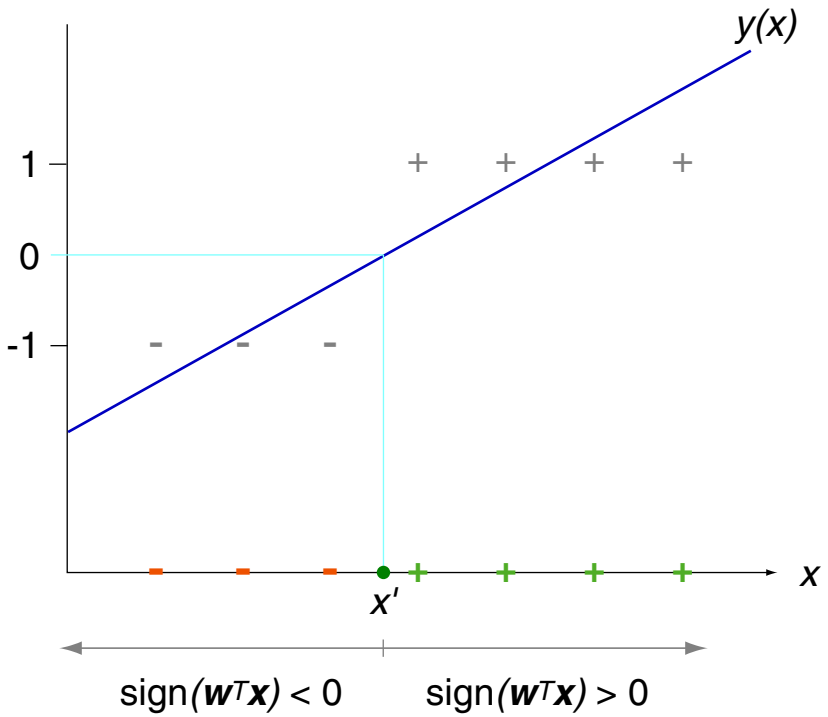
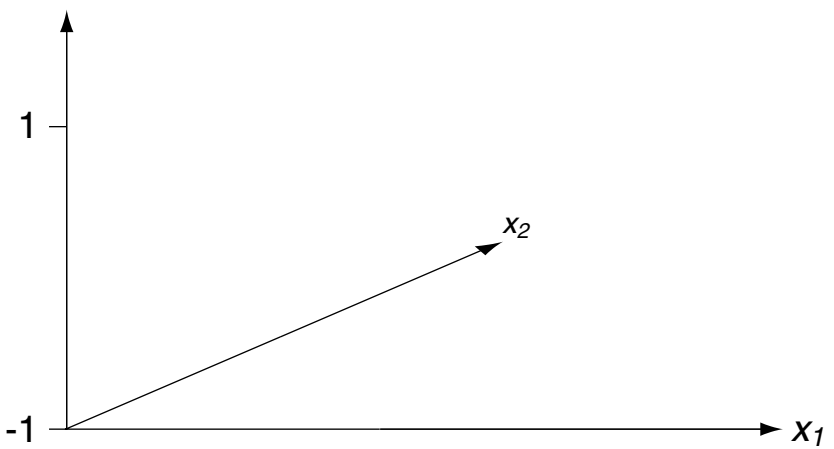


- The discrimination point, •, is defined by $w_0 + w_1 \cdot x' = 0$.
- For $p = 2$ we are given a discrimination *line*.

Regression

Linear Regression for Classification (illustrated for $p = 2$)



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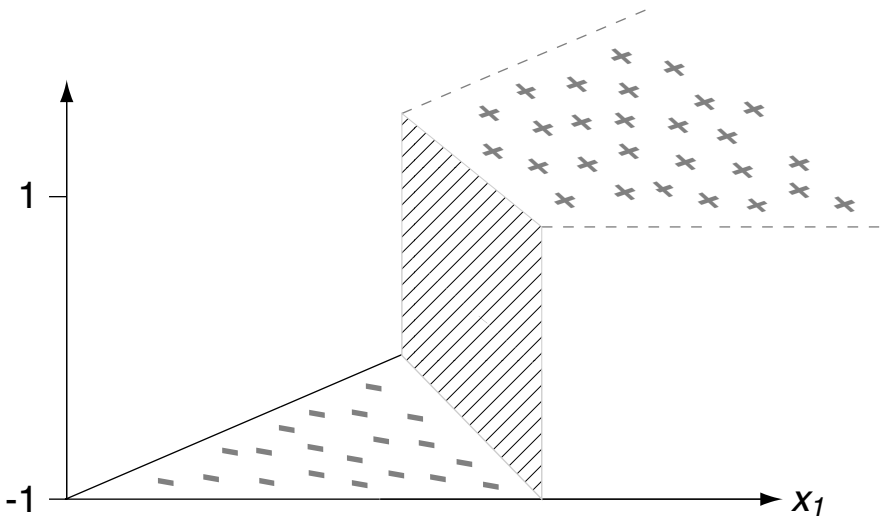

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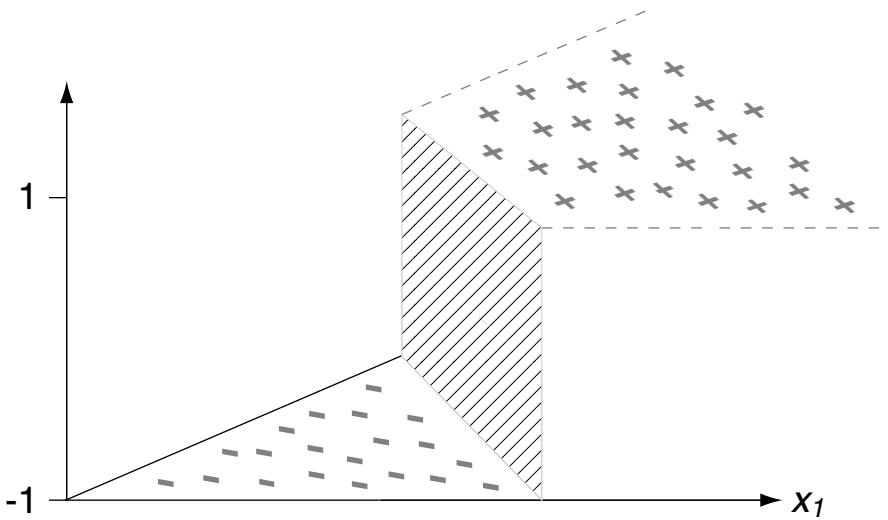

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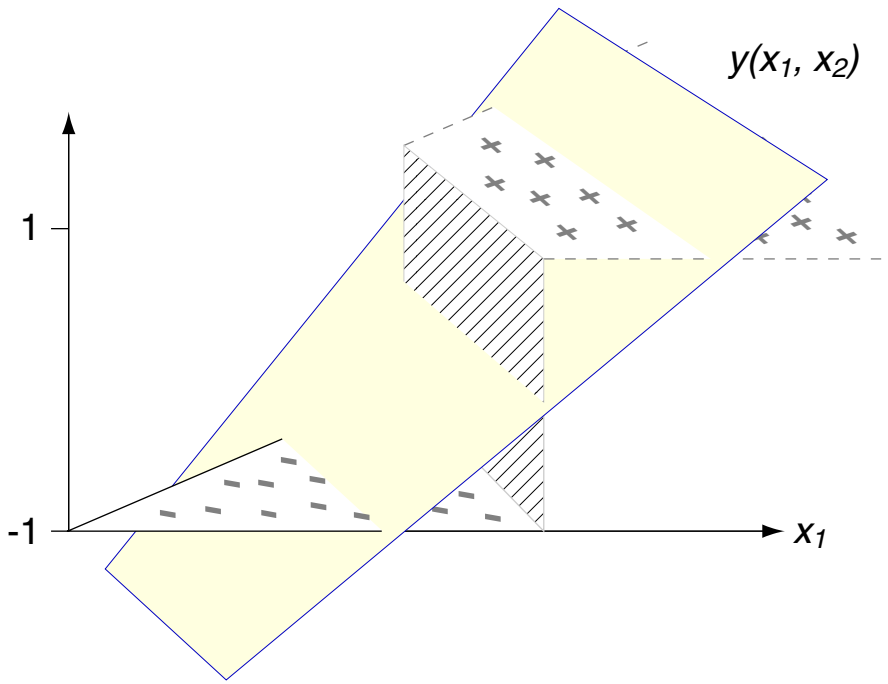

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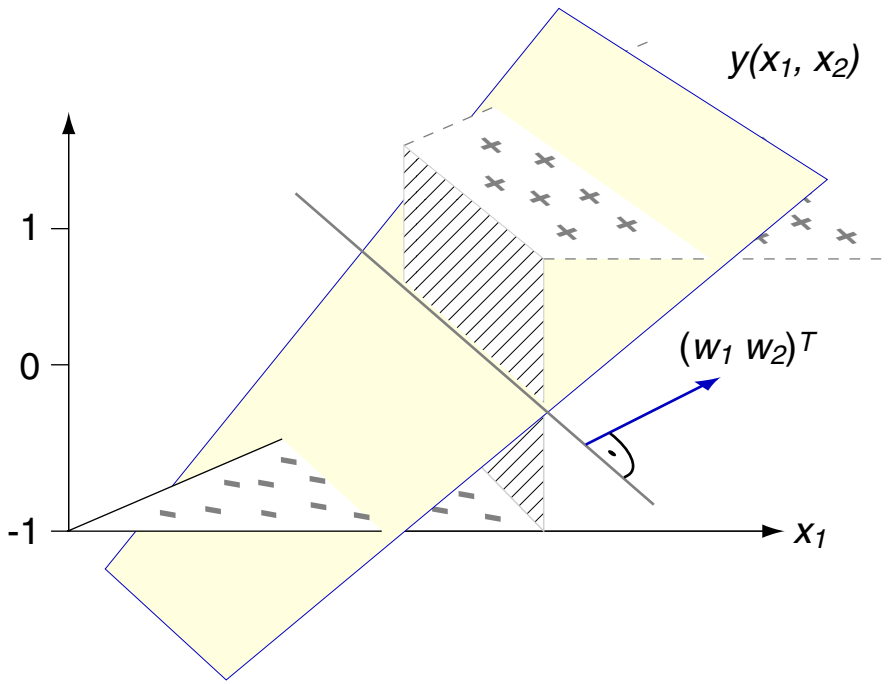

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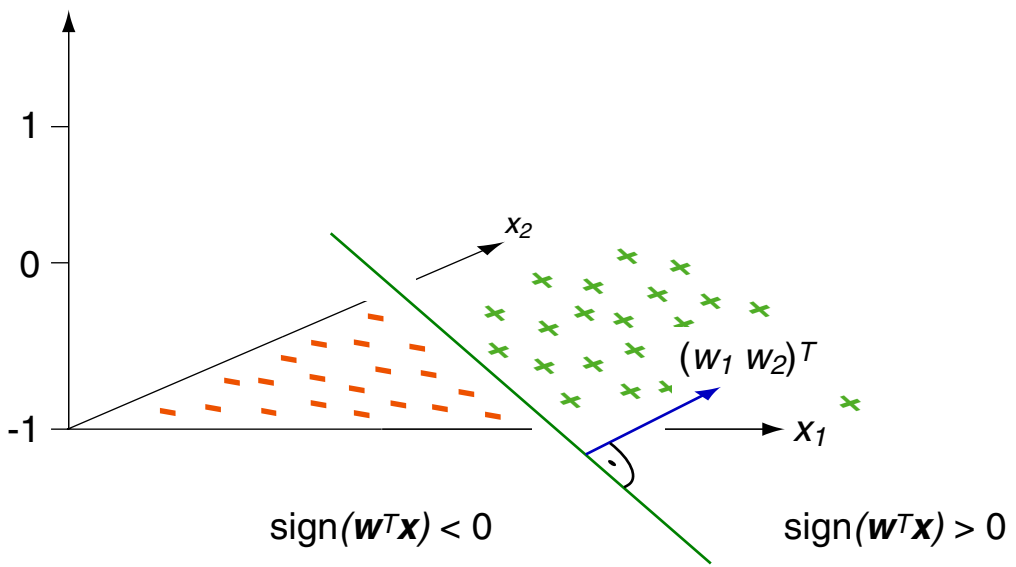

- The discrimination line, —, is defined by $w_0 + w_1 \cdot x_1 + w_2 \cdot x_2 = 0$.
- For $p = 3$ ($p > 3$) we are given a discriminating *(hyper)plane*.

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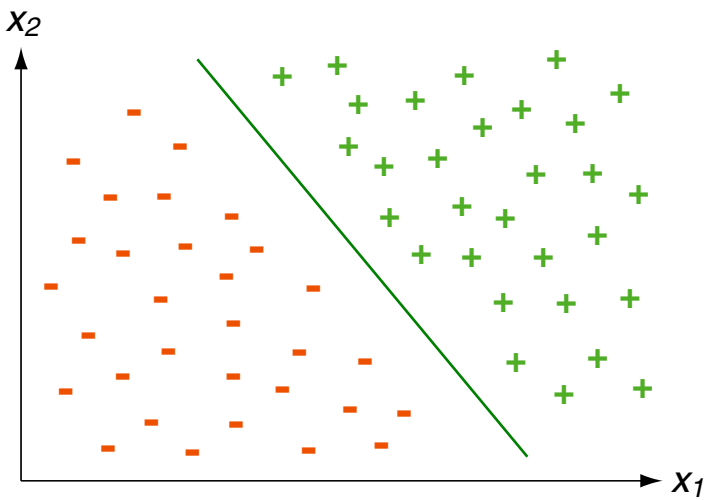

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Regression

The Linear Model Function: Variants

The components (variables, random variables) of the input vector $\mathbf{x} = (x_1, \ldots, x_p)$ can come from different sources [Hastie et al. 2001]:

1. quantitative inputs
2. transformations of quantitative inputs, such as $\log x_j$, $\sqrt{x_j}$
3. basis expansions, such as $x_j = (x_1)^j$
4. encoding of a qualitative variable g, $g \in \{1, \ldots, p\}$, as $x_j = I(g = j)$
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- basis functions: input variables (space) become feature variables (space)

Regression

The Linear Model Function: Properties of the Solution

Theorem 1 (Gauss-Markov)

Let $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$ be a set of examples to be fitted with a linear model function as $y(\mathbf{x}) = \mathbf{x}^T\mathbf{w}$. Within the class of linear unbiased estimators for $\mathbf{w}$, the least squares estimator $\hat{\mathbf{w}}$ has minimum variance, i.e., is most efficient.

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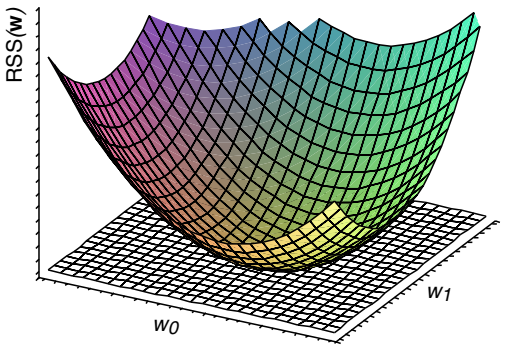
Related followup issues:

- mean and variance of $\hat{\mathbf{w}}$
- proof of the Gauss-Markov theorem
- weak set and strong set of assumptions
- efficiency and consistency of unbiased estimators
- rank deficiencies, where the feature number p exceeds $|D| = n$
- relation of mean least squares and the maximum likelihood principle

Regression

Methods of Least Squares: Iterative versus Direct Methods

$$\underset{\mathbf{w}}{\text{argmin}}\ \text{RSS}(\mathbf{w}), \quad \text{with } \text{RSS}(\mathbf{w}) = \sum_{i=1}^{n}(y_i - \mathbf{w}^T\mathbf{x}_i)^2$$



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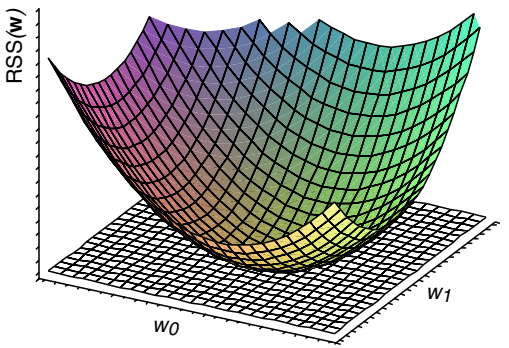
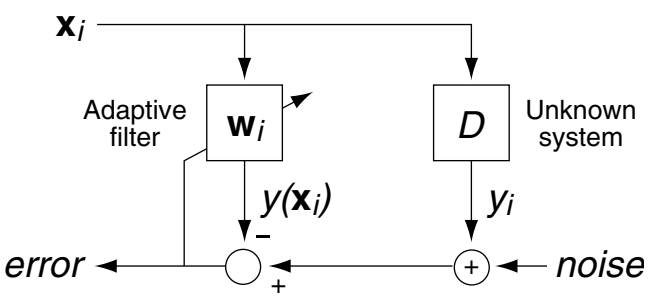


LMS algorithm:

- applicable as online algorithm
- robust algorithm structure
- unsatisfactory convergence
- allows stochastic sampling



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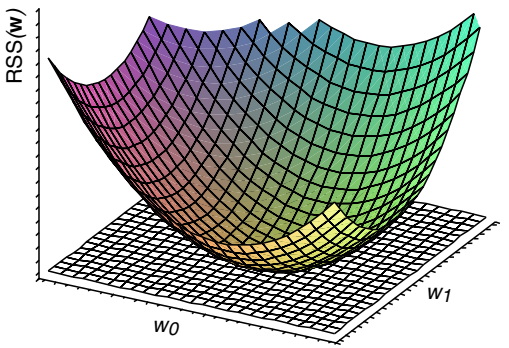

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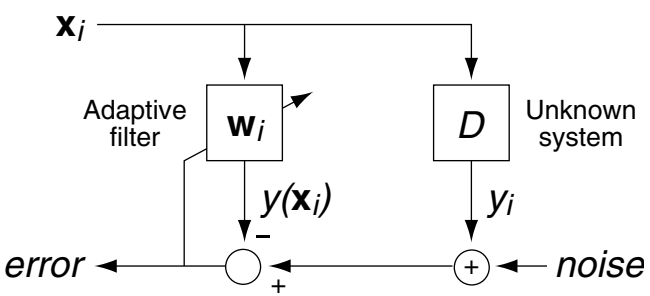


Normal equations:

- needs complete data
- numerically sensible
- requires singularity handling
- hardly applicable to big data

$$\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}\mathbf{y}$$

Remarks:

- Recall the definitions for residual and method of least squares.
- The principle of RSS minimization is orthogonal to (= independent of) the type of the model function y, i.e., independent of its dimensionality as well as its linearity or nonlinearity.
- To fit the parameters $\mathbf{w}$ of a (one-dimensional, multi-dimensional, linear, nonlinear) model function y, both the LMS algorithm and direct methods exploit information about the derivative of the RSS term with respect to $\mathbf{w}$. I.e., even if *classification* and not regression is the goal, the distance to the decision boundary (and not the zero-one-loss) is computed, since the latter is not differentiable.
- For a linear model function y, RSS$(\mathbf{w})$ is a convex function and hence a single, global optimum exists.
- Forthcoming: A main goal of machine learning approaches is to avoid overfitting. Overfitting in turn is caused by an inadequate (too high) model function complexity—or, similarly, by insufficient data. A means to reduce the model function complexity is regularization.
- Regularization will introduce additional constraints for the model function y or the parameter vector $\mathbf{w}$, respectively. With regularization the minimization expression (2) will consist of two summands: a performance term such as the RSS term, and a penalizing term such as a norm. As before, the first term captures the model function's goodness depending on $\mathbf{w}$, whereas the second term restricts the absolute values of the model function's parameters $\mathbf{w}$.

Chapter ML:II (continued)

II. Machine Learning Basics

- On Data
- Regression
- Concept Learning: Search in Hypothesis Space
- Concept Learning: Search in Version Space
- Measuring Performance

Concept Learning: Search in Hypothesis Space

A Learning Task

Given is a set D of examples: days that are characterized by the six features "Sky", "Temperature", "Humidity", "Wind", "Water", and "Forecast", along with a statement (in fact: a feature) whether or not our friend will enjoy her favorite sport.

Example	Sky	Temperature	Humidity	Wind	Water	Forecast	EnjoySport
1	sunny	warm	normal	strong	warm	same	yes
2	sunny	warm	high	strong	warm	same	yes
3	rainy	cold	high	strong	warm	change	no
4	sunny	warm	high	strong	cool	change	yes

- What is the concept behind "EnjoySport"?
- What are possible hypotheses to formalize the concept "EnjoySport"?
  Similarly: What are the elements of the set or class "EnjoySport"?

Remarks:

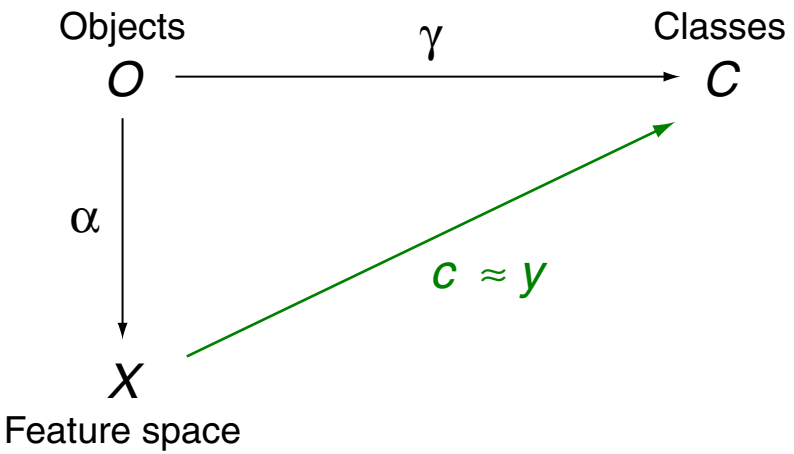
- Domains of the features in the learning task:

Sky	Temperature	Humidity	Wind	Water	Forecast
sunny	warm	normal	strong	warm	same
rainy	cold	high	weak	cool	change
cloudy					

- A hypothesis is a finding or an insight gained by inductive reasoning. A hypothesis cannot be inferred or proved by deductive reasoning.
- Within concept learning tasks, hypotheses are used to capture the target concept. A hypothesis is justified inductively, by its capability to represent (= to explain) a given set of observations, which are called examples here.

Concept Learning: Search in Hypothesis Space

Recall [ML:I Specification of Learning Problems] :



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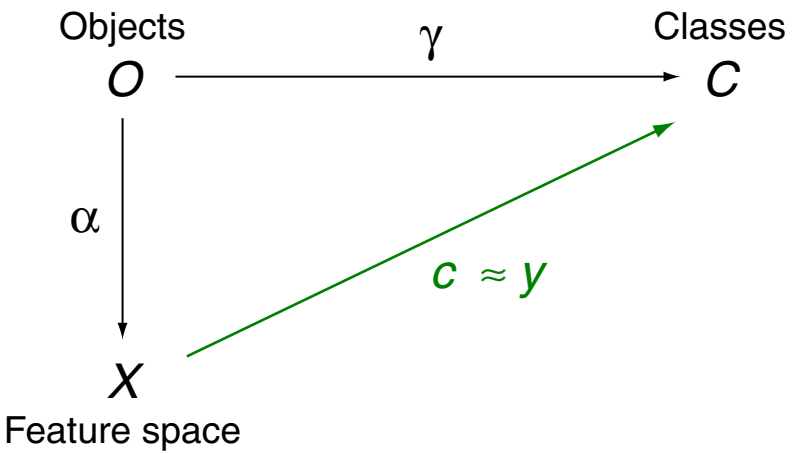

Definition 1 (Concept, Hypothesis, Hypothesis Space)

A concept is a subset of an object set O and hence determines a subset of the feature space $X = \alpha(O)$. Concept learning is the approximation of the ideal classifier $c : X \to \{0, 1\}$ by a function y, where c is defined as follows:

$$c(\mathbf{x}) = \begin{cases} 1 & \text{if } \alpha^{-1}(\mathbf{x}) \text{ belongs to the concept} \\ 0 & \text{otherwise} \end{cases}$$

A function $h : X \to \{0, 1\}$ is called hypothesis. A set H of hypotheses among which the approximation function y is searched is called hypothesis space.

Concept Learning: Search in Hypothesis Space

Usually, an example set D, $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\}$, contains positive ($c(\mathbf{x}) = 1$) and negative ($c(\mathbf{x}) = 0$) examples. [Learning Task]

Definition 2 (Hypothesis-Fulfilling, Consistency)

An example $(\mathbf{x}, c(\mathbf{x}))$ fulfills a hypothesis h iff $h(\mathbf{x}) = 1$. A hypothesis h is consistent with an example $(\mathbf{x}, c(\mathbf{x}))$ iff $h(\mathbf{x}) = c(\mathbf{x})$.

A hypothesis h is consistent with a set D of examples, denoted as *consistent*(h, D), iff:

$$\forall (\mathbf{x}, c(\mathbf{x})) \in D : \; h(\mathbf{x}) = c(\mathbf{x})$$

Remarks:

- The string “Iff” or “iff” is an abbreviation for “If and only if”, which means “necessary and sufficient”. It is a textual representation for the logical biconditional, also known as material biconditional or iff-connective. The respective symbol is “$\leftrightarrow$”. [Wolfram] [Wikipedia]
- The following terms are used synonymously: target concept, target function, ideal classifier.
- The fact that a hypothesis is consistent with an example can also be described the other way round: an example is consistent with a hypothesis.
- Given an example $(\mathbf{x}, c(\mathbf{x}))$, notice the difference between (1) hypothesis-fulfilling and (2) being consistent with a hypothesis. The former asks for $h(\mathbf{x}) = 1$, disregarding the actual target concept value $c(\mathbf{x})$. The latter asks for the equivalence between the target concept $c(\mathbf{x})$ and the hypothesis $h(\mathbf{x})$.
- The consistency of h can be analyzed for a single example as well as for a set D of examples. Given the latter, consistency requires for all elements in D that $h(\mathbf{x}) = 1$ iff $c(\mathbf{x}) = 1$. This is equivalent with the condition that $h(\mathbf{x}) = 0$ iff $c(\mathbf{x}) = 0$ for all $\mathbf{x} \in D$.
- Learning means to determine a hypothesis $h \in H$ that is consistent with D.

Concept Learning: Search in Hypothesis Space

A Learning Task (continued)

Structure of a hypothesis h:

1. conjunction of feature-value pairs
2. three kinds of values: literal, ? (wildcard), $\perp$ (contradiction)

A hypothesis in the example [Learning Task]: $\langle$ *sunny, ?, ?, strong, ?, same* $\rangle$

Concept Learning: Search in Hypothesis Space

A Learning Task (continued)

Structure of a hypothesis h:

1. conjunction of feature-value pairs
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A hypothesis in the example [Learning Task]: $\langle$ *sunny, ?, ?, strong, ?, same* $\rangle$

Definition 3 (Maximally Specific / General Hypothesis)

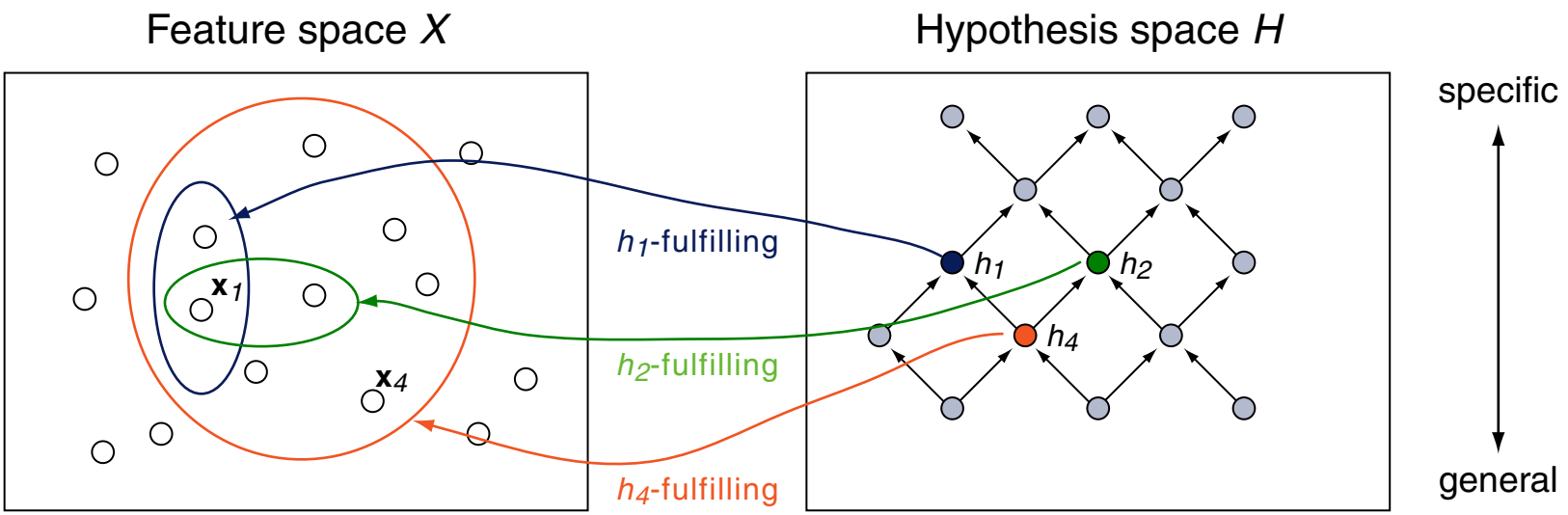
The hypotheses $s_0(\mathbf{x}) \equiv 0$ and $g_0(\mathbf{x}) \equiv 1$ are called maximally specific and maximally general hypothesis respectively. No $\mathbf{x} \in X$ fulfills s_0, and all $\mathbf{x} \in X$ fulfill g_0.

Maximally specific / general hypothesis in the example [Learning Task]:

- $s_0 = \langle \perp, \perp, \perp, \perp, \perp, \perp \rangle$
- $g_0 = \langle$ *?, ?, ?, ?, ?, ?* $\rangle$

Concept Learning: Search in Hypothesis Space

Order of Hypotheses



$\mathbf{x}_1 = (\textit{sunny, warm, normal, strong, warm, same})$ $h_1 = \langle\ \textit{sunny, ?, normal, ?, ?, ?}\ \rangle$

$h_2 = \langle\ \textit{sunny, ?, ?, ?, warm, ?}\ \rangle$

$\mathbf{x}_4 = (\textit{sunny, warm, high, strong, cool, change})$ $h_4 = \langle\ \textit{sunny, ?, ?, ?, ?, ?}\ \rangle$

Concept Learning: Search in Hypothesis Space

Order of Hypotheses

Definition 4 (More General Relation)

Let X be a feature space and let h_1 and h_2 be two boolean-valued functions with domain X. Then function h_1 is called more general than function h_2, denoted as $h_1 \geq_g h_2$, iff:

$$\forall \mathbf{x} \in X : \ (\ h_2(\mathbf{x}) = 1 \ \text{ implies } \ h_1(\mathbf{x}) = 1 \ )$$

h_1 is called stricly more general than h_2, denoted as $h_1 >_g h_2$, iff:

$$(h_1 \geq_g h_2) \ \text{ and } \ (h_2 \not\geq_g h_1)$$

Concept Learning: Search in Hypothesis Space

Order of Hypotheses

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$$(h_1 \geq_g h_2) \ \text{ and } \ (h_2 \not\geq_g h_1)$$

About the maximally specific / general hypothesis:

- s_0 is minimum and g_0 is maximum with regard to $\geq_g$: no hypothesis is more specific wrt. s_0, and no hypothesis is more general wrt. g_0.
- We will consider only hypothesis spaces that contain s_0 and g_0.

Remarks:

- If h_1 is more general than h_2, then h_2 can also be called being more specific than h_1.
- $\geq_g$ and $>_g$ are independent of a target concept c. They depend only on the fact that examples fulfill a hypothesis, i.e., whether $h(\mathbf{x}) = 1$. They require not that $c(\mathbf{x}) = 1$.
- The $\geq_g$-relation defines a partial order on the hypothesis space H : $\geq_g$ is reflexive, anti-symmetric, and transitive. The order is *partial* since (unlike in a total order) not all hypothesis pairs stand in the relation. [Wikipedia partial, total]
  I.e., we are given hypotheses h_i, h_j, for which neither $h_i \geq_g h_j$ nor $h_j \geq_g h_i$ holds, such as the hypotheses h_1 and h_2 in the hypothesis space.

Remarks: (continued)

- The semantics of the implication, in words "a implies b", denoted as $a \to b$, is as follows. $a \to b$ is true if either (1) a is true and b is true, or (2) if a is false and b is true, or (3) if a is false and b is false—in short: "if a is true then b is true as well", or, "the truth of a implies the truth of b".
- "$\to$" can be understood as "causality connective": Let a and b be two events where a is a cause for b. If we interpret the occurrence of an event as true and its non-occurrence as false, we will observe only occurrence combinations such that the formula $a \to b$ is true. The connective is also known as material conditional, material implication, material consequence, or simply, implication or conditional.
- Note in particular that the connective "$\to$" does not stand for "entails", which would be denoted as either $\Rightarrow$ or $\models$. Logical entailment (synonymously: logical inference, logical deduction, logical consequence) allows to infer or to prove a fact. From the fact $h_2(\mathbf{x}) = 1$, however, we cannot infer or prove the fact $h_1(\mathbf{x}) = 1$.
- Here, in the definition, the implication specifies a condition that is to be fulfilled by the definiendum (= the thing to be defined). The implication is used to check whether or not a thing belongs to the set of things specified by the definition: each pair of functions, h_1, h_2, is a thing that belongs to the set of things specified by the definition of the $\geq_g$-relation (i.e., stands in the $\geq_g$-relation) if and only if the implication $h_2(\mathbf{x}) = 1 \to h_1(\mathbf{x}) = 1$ is true for all $\mathbf{x} \in X$.

Remarks: (continued)

- In a nutshell: distinguish carefully between "α requires β", denoted as $\alpha \to \beta$, on the one hand, and "from α follows β", denoted as $\alpha \Rightarrow \beta$, on the other hand. $\alpha \to \beta$ is considered as a sentence from the *object language* (language of discourse) and stipulates a computing operation, whereas $\alpha \Rightarrow \beta$ is a sentence from the *meta language* and makes an assertion *about* the sentence $\alpha \to \beta$, namely: "$\alpha \to \beta$ is a tautology".
- Finally, consider the following sentences from the object language, which are synonymous: "$\alpha \to \beta$", "α implies β", "if α then β", "α causes β", "α requires β", "α is sufficient for β", "β is necessary for α".

Concept Learning: Search in Hypothesis Space

Inductive Learning Hypothesis

"Any hypothesis found to approximate the target function well over a sufficiently large set of training examples will also approximate the target function well over other unobserved examples."

[p.23, Mitchell 1997]

Concept Learning: Search in Hypothesis Space

Find-S Algorithm

1. $h = s_0$ // h is a maximally specific hypothesis in H.
2. **FOREACH** $(\mathbf{x}, c(\mathbf{x})) \in D$ **DO**
   IF $c(\mathbf{x}) = 1$ **THEN** // Use only positive examples.
   IF $h(\mathbf{x}) = 0$ **DO**
   $h = \mathit{min\_generalization}(h, \mathbf{x})$ // Relax hypothesis h wrt. $\mathbf{x}$.
   ENDIF
   ENDIF
   ENDDO
3. *return*(h)

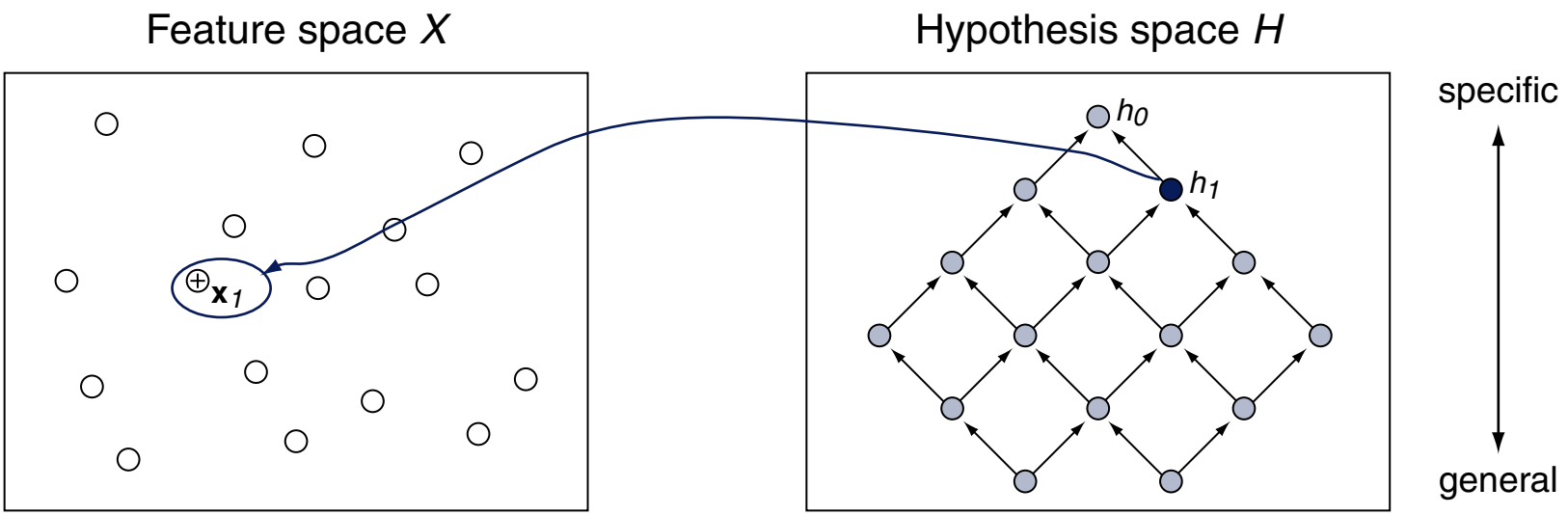
Remarks:

- Another term for “generalization” is “relaxation”.
- The function *min_generalization*$(h, \mathbf{x})$ returns a hypothesis h' that is minimally generalized wrt. h and that is consistent with $(\mathbf{x}, 1)$. Denoted formally: $h' \geq_g h$ and $h'(\mathbf{x}) = 1$ and there is no h'' with $h' >_g h'' \geq_g h$ and $h''(\mathbf{x}) = 1$.
- For more complex hypothesis structures the relaxation of h given $\mathbf{x}$, *min_generalization*$(h, \mathbf{x})$, may not be unique. In such a case one of the alternatives has to be chosen.
- If a hypothesis h needs to be relaxed towards some h' with $h' \notin H$, the maximally general hypothesis $g_0 \equiv 1$ can be added to H.
- Similar to *min_generalization*$(h, \mathbf{x})$, a function *min_specialization*$(h, \mathbf{x})$ can be defined, which returns a minimally specialized, consistent hypotheses for negative examples.

Concept Learning: Search in Hypothesis Space

Find-S Algorithm

See the example set D for the concept *EnjoySport*.



$$h_0 = s_0 = \langle \perp, \perp, \perp, \perp, \perp, \perp \rangle$$

$\mathbf{x}_1 = (\textit{sunny, warm, normal, strong, warm, same})$ $h_1 = \langle \textit{sunny, warm, normal, strong, warm, same} \rangle$

Concept Learning: Search in Hypothesis Space

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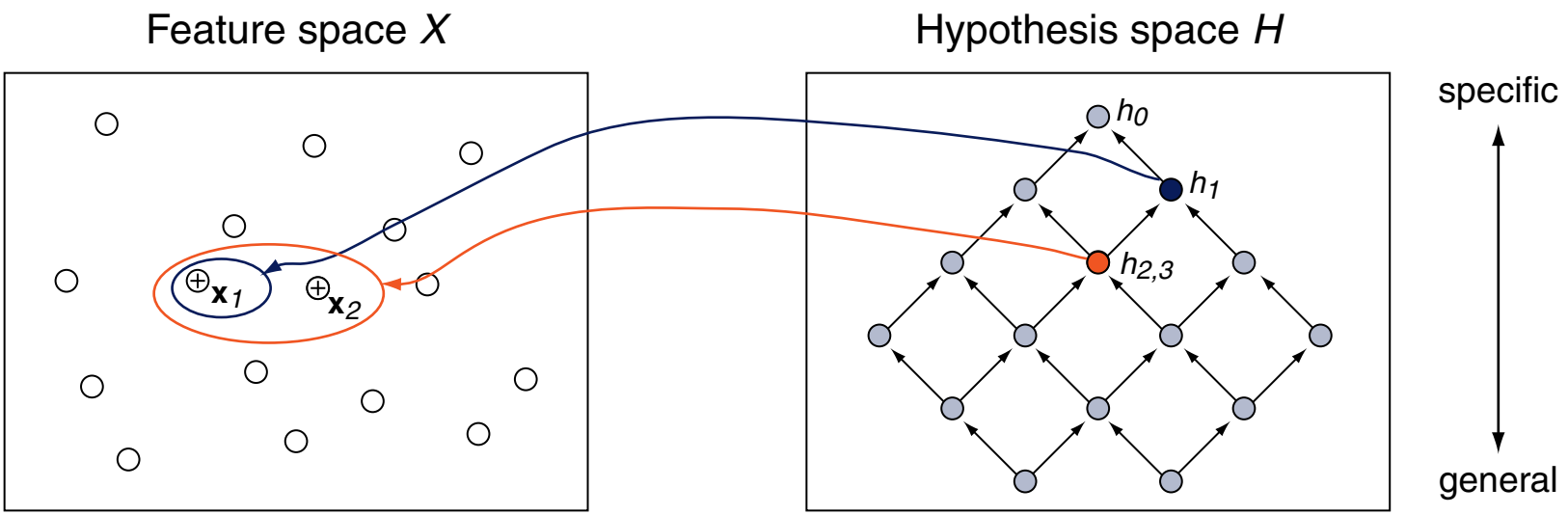

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Concept Learning: Search in Hypothesis Space

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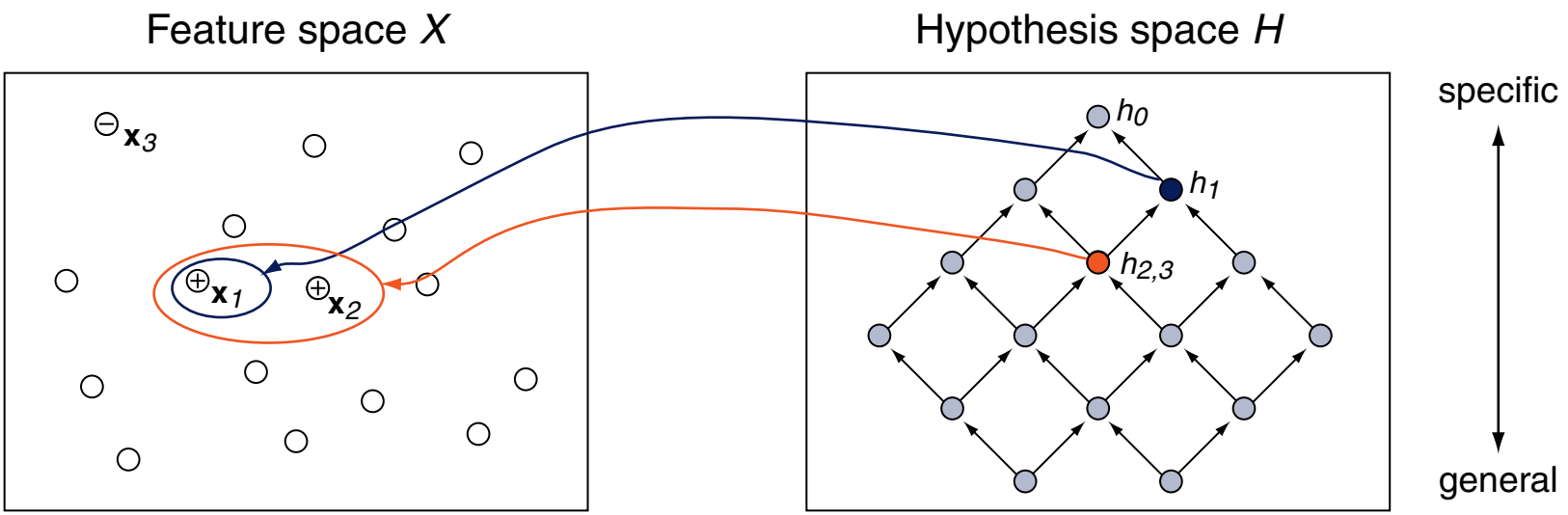

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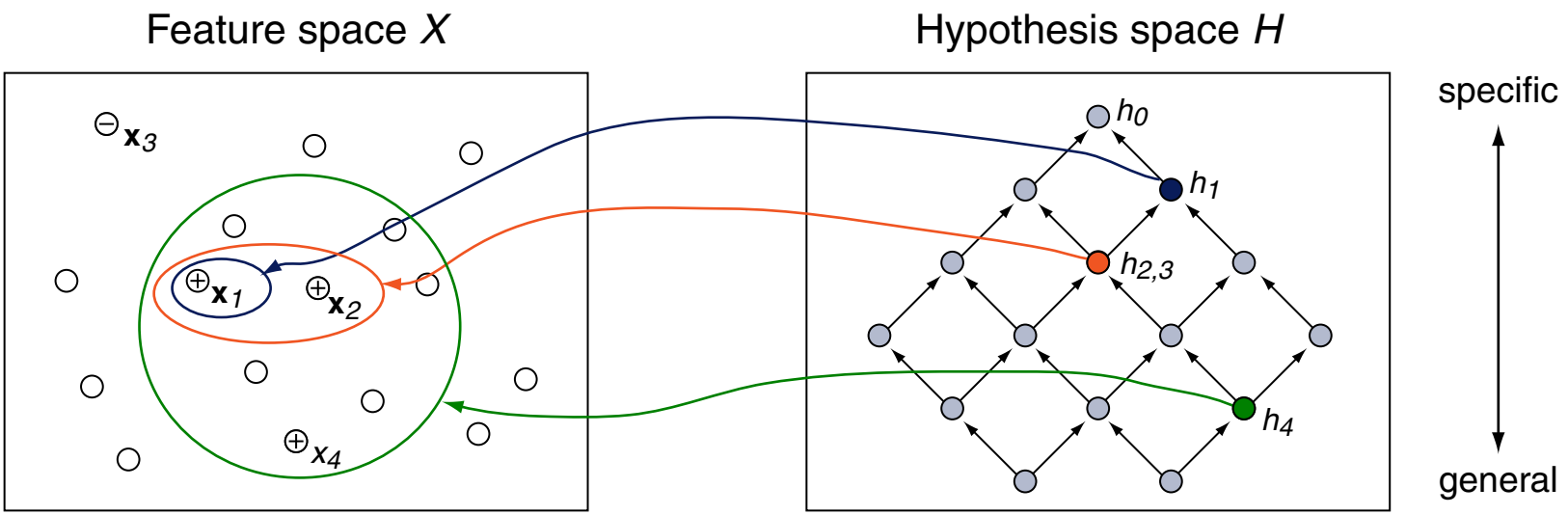
Concept Learning: Search in Hypothesis Space

Find-S Algorithm

See the example set D for the concept *EnjoySport*.



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$\mathbf{x}_1 = (\textit{sunny, warm, normal, strong, warm, same})$ $h_1 = \langle \textit{sunny, warm, normal, strong, warm, same} \rangle$

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Concept Learning: Search in Hypothesis Space

Discussion of the Find-S Algorithm

1. Did we learn the only concept—or are there others?
2. Why should one pursuit the maximally specific hypothesis?
3. What if several maximally specific hypotheses exist?
4. Inconsistencies in the example set D remain undetected.
5. An inappropriate hypothesis structure or space H remains undetected.

Concept Learning: Search in Version Space

Definition 5 (Version Space)

The version space $V_{H,D}$ of an hypothesis space H and a example set D is comprised of all hypotheses $h \in H$ that are consistent with a set D of examples:

$$V_{H,D} = \{h \mid h \in H \ \wedge \ (\ \forall(\mathbf{x}, c(\mathbf{x})) \in D : \ h(\mathbf{x}) = c(\mathbf{x})\ )\ \}$$

Concept Learning: Search in Version Space

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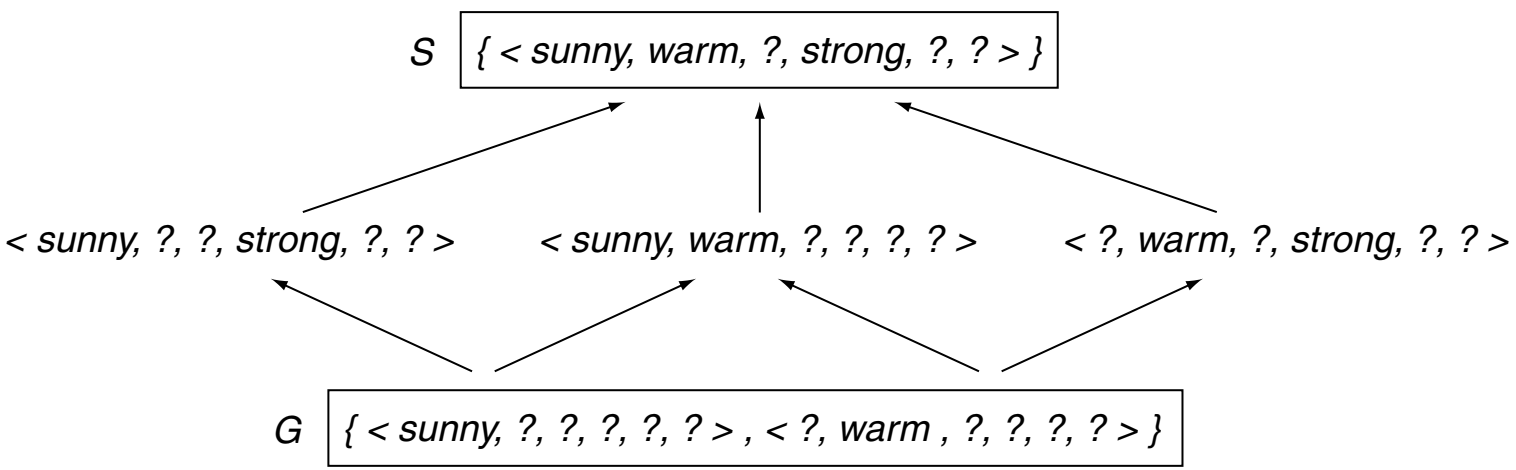
Illustration of $V_{H,D}$ for the example set D:



Remarks:

- The term “version space” reflects the fact that $V_{H,D}$ represents the set of all consistent versions of the target concept that are encoded in D.
- A naive approach for the construction of the version space is the following: (1) enumeration of all members of H, and, (2) elimination of those $h \in H$ for which $h(\mathbf{x}) \neq c(\mathbf{x})$ holds. This approach presumes a finite hypothesis space H and is feasible only for toy problems.

Concept Learning: Search in Version Space

Definition 6 (Boundary Sets of a Version Space)

Let H be hypothesis space and let D be set of examples. Then, based on the $\geq_g$-relation, the set of maximally general hypotheses, G, is defined as follows:

$$\{g \mid g \in H \ \wedge \ \textit{consistent}(g, D) \ \wedge \ (\nexists g' : g' \in H \ \wedge \ g' >_g g \ \wedge \ \textit{consistent}(g', D))\}$$

Similarly, the set of maximally specific (i.e., minimally general) hypotheses, S, is defined as follows:

$$\{s \mid s \in H \ \wedge \ \textit{consistent}(s, D) \ \wedge \ (\nexists s' : s' \in H \ \wedge \ s >_g s' \ \wedge \ \textit{consistent}(s', D))\}$$

Concept Learning: Search in Version Space

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Theorem 7 (Version Space Representation)

Let X be a feature space and let H be a set of boolean-valued functions with domain X. Moreover, let $c : X \to \{0, 1\}$ be a target concept and let D be a set of examples of the form $(\mathbf{x}, c(\mathbf{x}))$. Then, based on the $\geq_g$-relation, each member of the version space $V_{H,D}$ lies in between two members of G and S respectively:

$$V_{H,D} = \{h \mid h \in H \ \wedge \ (\ \exists g \in G \ \ \exists s \in S : \ g \geq_g h \geq_g s \ ) \}$$

Concept Learning: Search in Version Space

Candidate Elimination Algorithm [Mitchell 1997]

1. Initialization: $G = \{g_0\},\ S = \{s_0\}$
2. If $\mathbf{x}$ is a positive example
   - Remove from G any hypothesis that is not consistent with $\mathbf{x}$
   - For each hypothesis s in S that is not consistent with $\mathbf{x}$
     - Remove s from S
     - Add to S all minimal generalizations h of s such that
       1. h is consistent with $\mathbf{x}$ and
       2. some member of G is more general than h
     - Remove from S any hypothesis that is less specific than another hypothesis in S

Concept Learning: Search in Version Space

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       2. some member of G is more general than h
     - Remove from S any hypothesis that is less specific than another hypothesis in S
3. If $\mathbf{x}$ is a negative example
   - Remove from S any hypothesis that is not consistent with $\mathbf{x}$
   - For each hypothesis g in G that is not consistent with $\mathbf{x}$
     - Remove g from G
     - Add to G all minimal specializations h of g such that
       1. h is consistent with $\mathbf{x}$ and
       2. some member of S is more specific than h
     - Remove from G any hypothesis that is less general than another hypothesis in G

Remarks:

- The basic idea of Candidate Elimination is as follows.
  - A maximally specific hypothesis $s \in S$ restricts the positive examples in first instance. Hence, s must be relaxed (= generalized) with regard to each positive example that is not consistent with s.
  - Conversely, a maximally general hypothesis $g \in G$ tolerates the negative examples in first instance. Hence, g must be constrained (= specialized) with regard to each negative example that is not consistent with g.

Concept Learning: Search in Version Space

Candidate Elimination Algorithm (pseudo code)

1. $G = \{g_0\}$ // G is the set of maximally general hypothesis in H.
   $S = \{s_0\}$ // S is the set of maximally specific hypothesis in H.
2. **FOREACH** $(\mathbf{x}, c(\mathbf{x})) \in D$ **DO**
   IF $c(\mathbf{x}) = 1$ **THEN** // $\mathbf{x}$ is a positive example.
   FOREACH $g \in G$ **DO IF** $g(\mathbf{x}) \neq 1$ **THEN** $G = G \setminus \{g\}$ **ENDDO**
   FOREACH $s \in S$ **DO**
   IF $s(\mathbf{x}) \neq 1$ **THEN**
   $S = S \setminus \{s\}$, $S^+ = \mathit{min\_generalizations}(s, \mathbf{x})$
   FOREACH $s \in S^+$ **DO IF** $(\exists g \in G : g \geq_g s)$ **THEN** $S = S \cup \{s\}$ **ENDDO**
   FOREACH $s \in S$ **DO IF** $(\exists s' \in S : s' \neq s \wedge s \geq_g s')$ **THEN** $S = S \setminus \{s\}$ **ENDDO**
   ENDDO
   ELSE // $\mathbf{x}$ is a negative example.
   ENDIF
   ENDDO
3. *return*(G, S)

Concept Learning: Search in Version Space

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   FOREACH $s \in S$ **DO IF** $(\exists s' \in S : s' \neq s \wedge s \geq_g s')$ **THEN** $S = S \setminus \{s\}$ **ENDDO**
   ENDDO
   ELSE // $\mathbf{x}$ is a negative example.
   FOREACH $s \in S$ **DO IF** $s(\mathbf{x}) \neq 0$ **THEN** $S = S \setminus \{s\}$ **ENDDO**
   FOREACH $g \in G$ **DO**
   IF $g(\mathbf{x}) \neq 0$ **THEN**
   $G = G \setminus \{g\}$, $G^- = \mathit{min\_specializations}(g, \mathbf{x})$
   FOREACH $g \in G^-$ **DO IF** $(\exists s \in S : g \geq_g s)$ **THEN** $G = G \cup \{g\}$ **ENDDO**
   FOREACH $g \in G$ **DO IF** $(\exists g' \in G : g' \neq g \wedge g' \geq_g g)$ **THEN** $G = G \setminus \{g\}$ **ENDDO**
   ENDDO
   ENDIF
   ENDDO
3. *return*(G, S)

Concept Learning: Search in Version Space

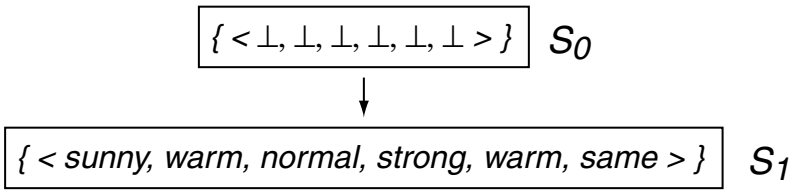
Candidate Elimination Algorithm (illustration)

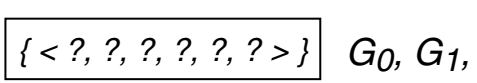
$\{ < \bot, \bot, \bot, \bot, \bot, \bot > \}$ S_0

$\{ < ?, ?, ?, ?, ?, ? > \}$ G_0,

Concept Learning: Search in Version Space

Candidate Elimination Algorithm (illustration)

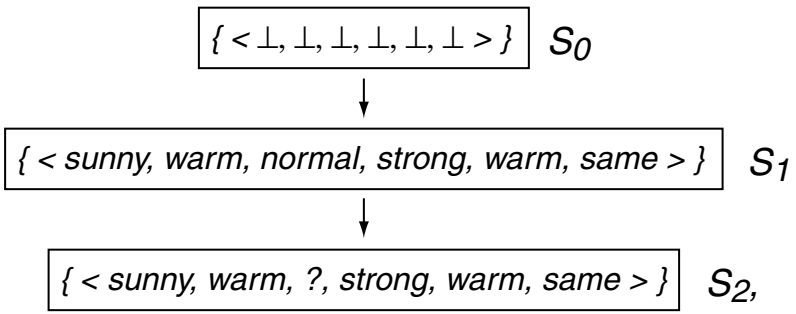




$\mathbf{x}_1 = (\textit{sunny, warm, normal, strong, warm, same})$ $\quad\quad$ $\textit{EnjoySport}(\mathbf{x}_1) = 1$

Concept Learning: Search in Version Space

Candidate Elimination Algorithm (illustration)



{ < ?, ?, ?, ?, ?, ? > } G_0, G_1, G_2

$\mathbf{x}_1 = (\textit{sunny, warm, normal, strong, warm, same})$ $\quad$ $\textit{EnjoySport}(\mathbf{x}_1) = 1$

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Concept Learning: Search in Version Space

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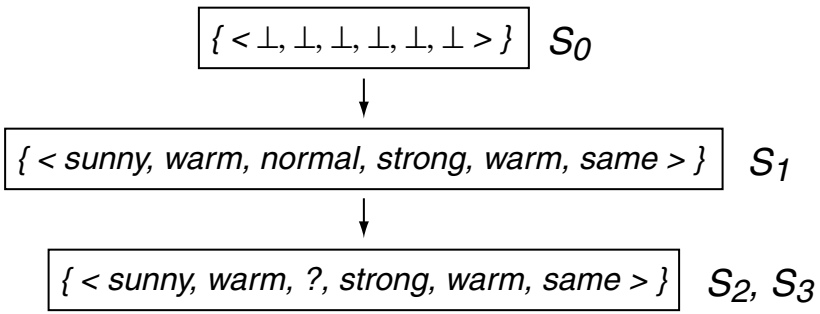
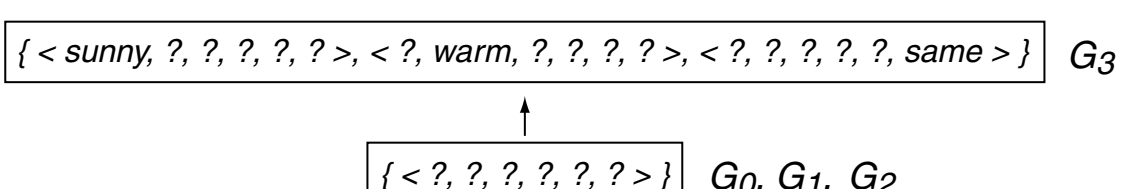




$\mathbf{x}_1 = (\textit{sunny, warm, normal, strong, warm, same})$ $\quad$ $\textit{EnjoySport}(\mathbf{x}_1) = 1$

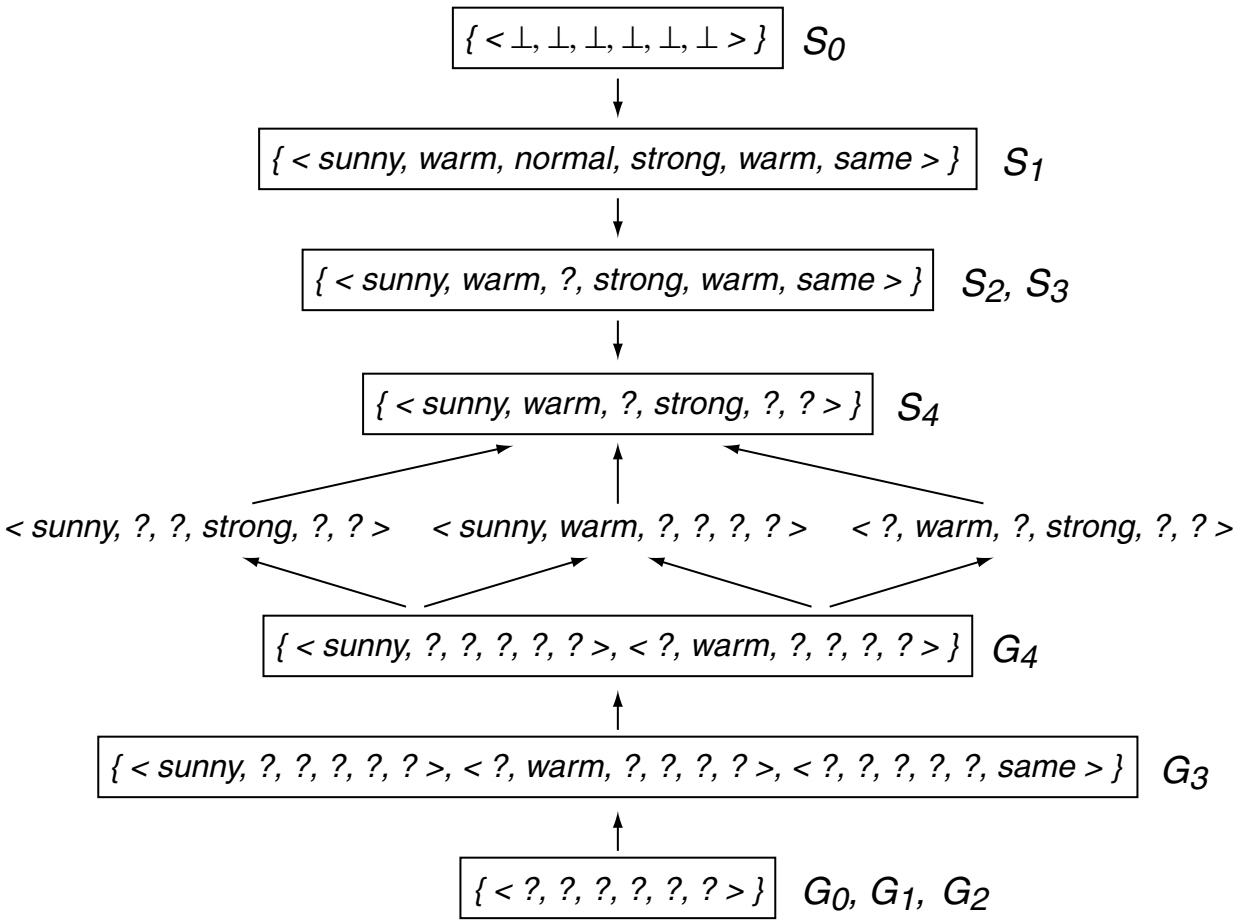
$\mathbf{x}_2 = (\textit{sunny, warm, high, strong, warm, same})$ $\quad$ $\textit{EnjoySport}(\mathbf{x}_2) = 1$

$\mathbf{x}_3 = (\textit{rainy, cold, high, strong, warm, change})$ $\quad$ $\textit{EnjoySport}(\mathbf{x}_3) = 0$

[Feature domains] [Algorithm]

Concept Learning: Search in Version Space

Candidate Elimination Algorithm (illustration)



$\mathbf{x}_1 = (\textit{sunny, warm, normal, strong, warm, same})$ $\quad$ $\textit{EnjoySport}(\mathbf{x}_1) = 1$

$\mathbf{x}_2 = (\textit{sunny, warm, high, strong, warm, same})$ $\quad$ $\textit{EnjoySport}(\mathbf{x}_2) = 1$

$\mathbf{x}_3 = (\textit{rainy, cold, high, strong, warm, change})$ $\quad$ $\textit{EnjoySport}(\mathbf{x}_3) = 0$

$\mathbf{x}_4 = (\textit{sunny, warm, high, strong, cool, change})$ $\quad$ $\textit{EnjoySport}(\mathbf{x}_4) = 1$

[Feature domains] [Algorithm]

Concept Learning: Search in Version Space

Discussion of the Candidate Elimination Algorithm

1. What about selecting examples from D according to a certain strategy?
   Keyword: active learning

2. What are partially learned concepts and how to exploit them?
   Keyword: ensemble classification

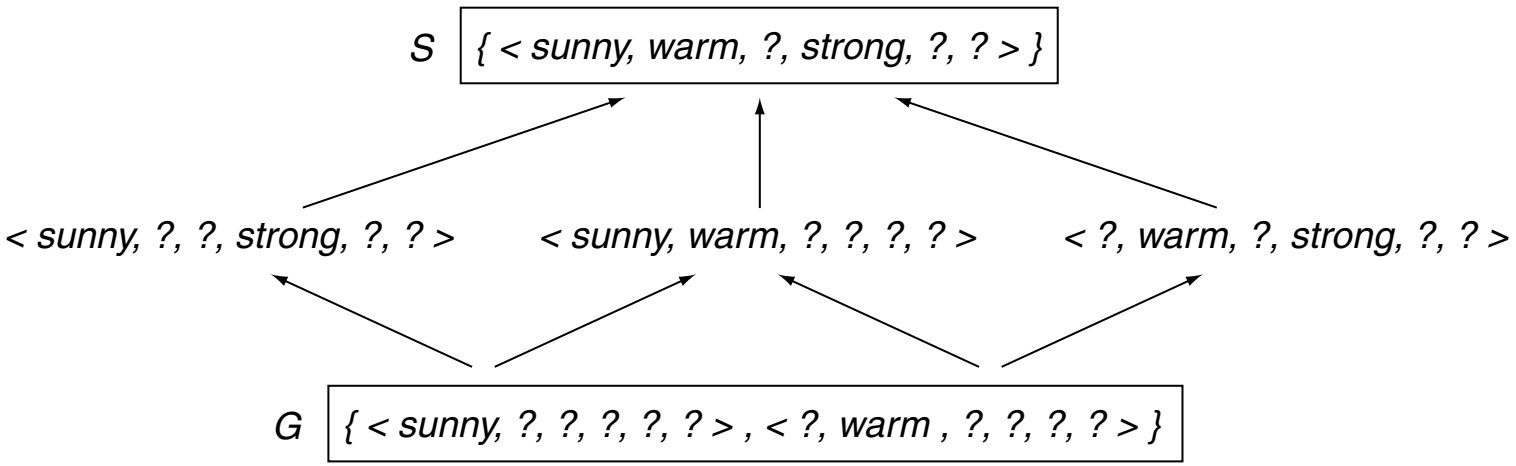
3. The version space as defined here is “biased”. What does this mean?

4. Will Candidate Elimination converge towards the correct hypothesis?

5. When does one end up with an empty version space?

Concept Learning: Search in Version Space

Question 1: Selecting Examples from D

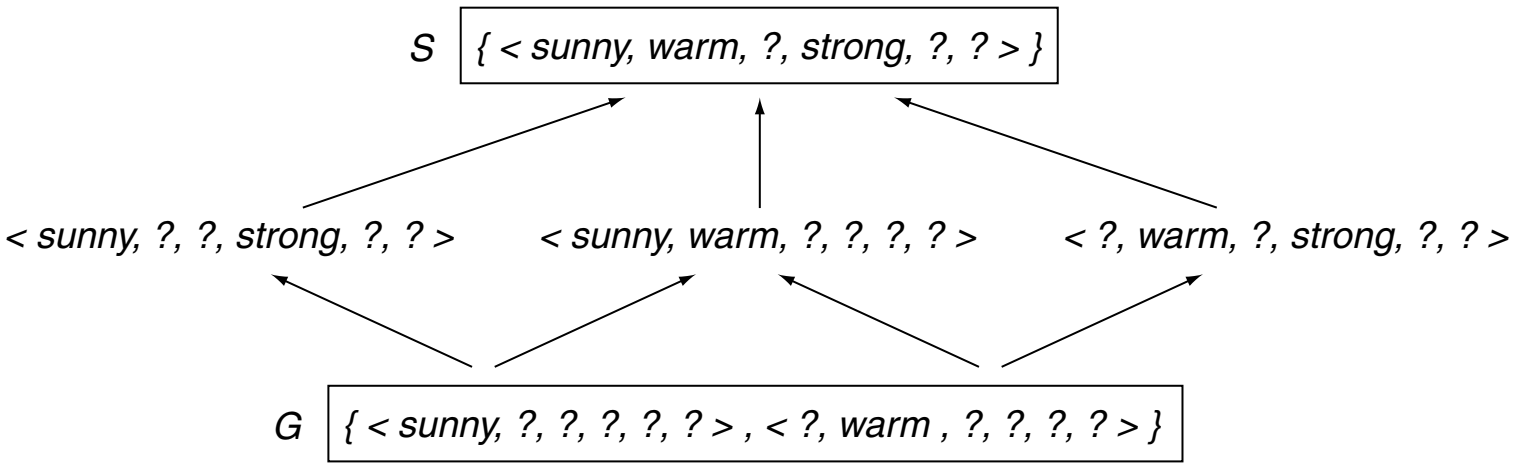


New example:

$\mathbf{x}_7 = (\textit{sunny, warm, normal, light, warm, same})$

Concept Learning: Search in Version Space

Question 1: Selecting Examples from D



New example:

$\mathbf{x}_7 = (\textit{sunny, warm, normal, light, warm, same})$

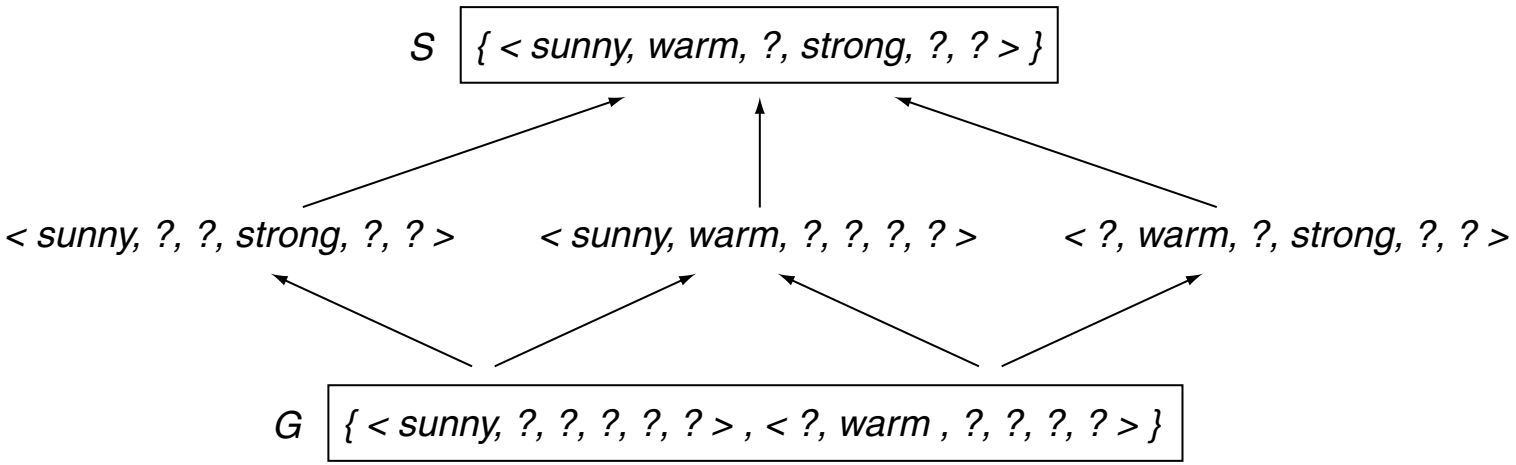
Discussion:

Irrespective the value of $c(\mathbf{x}_7)$, the example $(\mathbf{x}_7, c(\mathbf{x}_7))$ will be consistent with three of the six hypotheses. It follows:

- If $\textit{EnjoySport}(\mathbf{x}_7) = 1$ S can be further generalized.
- If $\textit{EnjoySport}(\mathbf{x}_7) = 0$ G can be further specialized.

Concept Learning: Search in Version Space

Question 2: Partially Learned Concepts

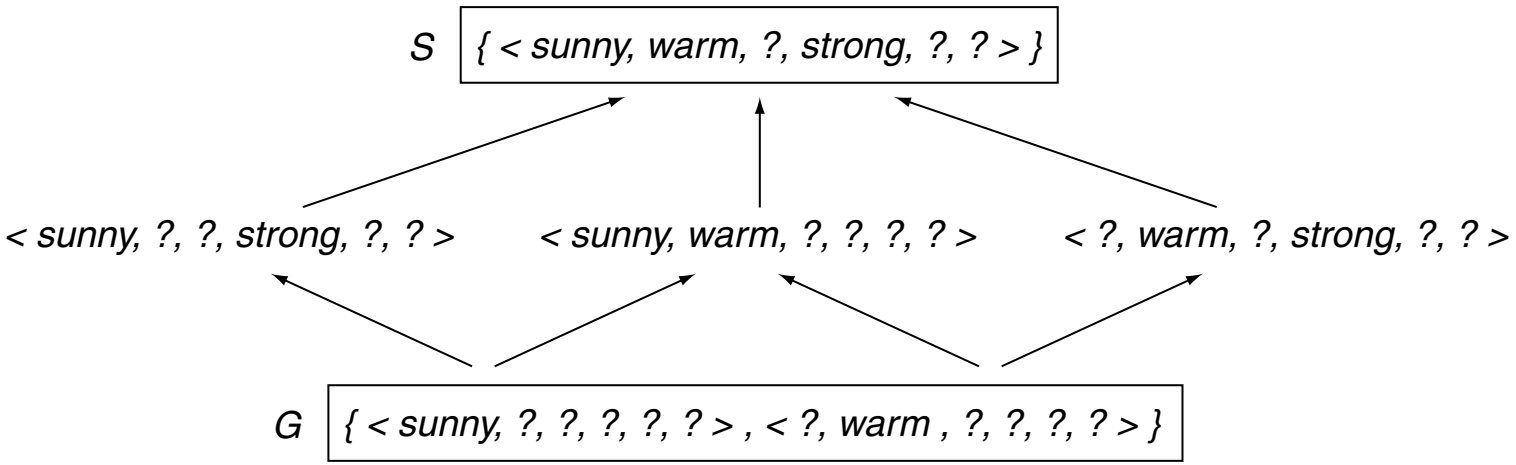


Classify examples using the shown version space:

Example	Sky	Temperature	Humidity	Wind	Water	Forecast	EnjoySport
5	sunny	warm	normal	strong	cool	change	
6	rainy	cold	normal	light	warm	same	
7	sunny	warm	normal	light	warm	same	
8	sunny	cold	normal	strong	warm	same	

Concept Learning: Search in Version Space

Question 2: Partially Learned Concepts



Classify examples using the shown version space:

Example	Sky	Temperature	Humidity	Wind	Water	Forecast	EnjoySport
5	sunny	warm	normal	strong	cool	change	6+ : 0–
6	rainy	cold	normal	light	warm	same	
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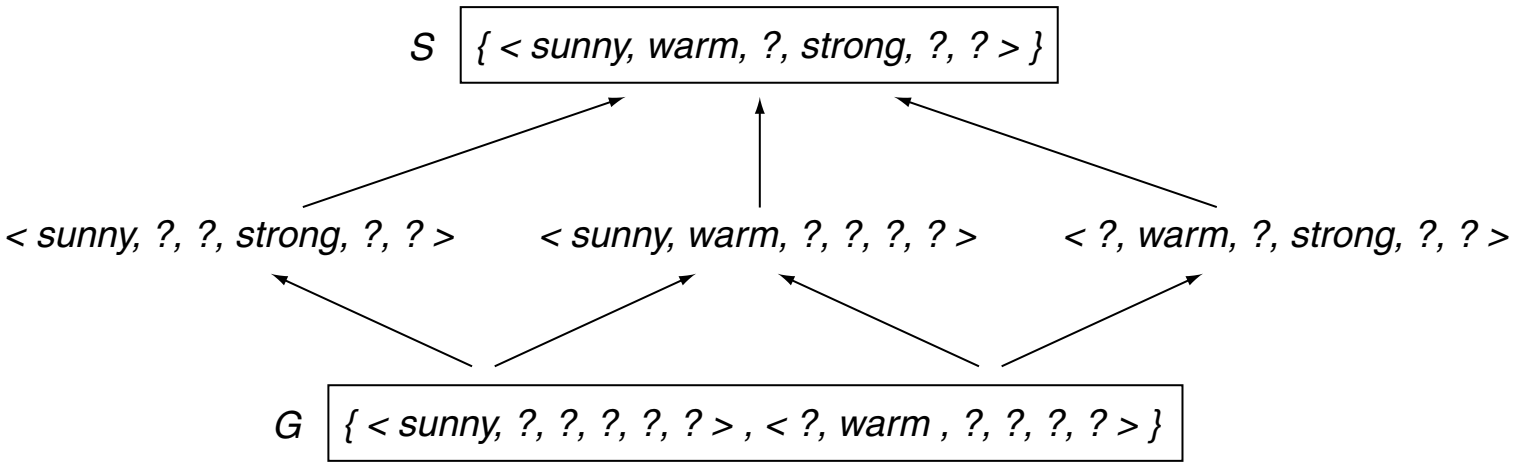
Concept Learning: Search in Version Space

Question 2: Partially Learned Concepts



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Concept Learning: Search in Version Space

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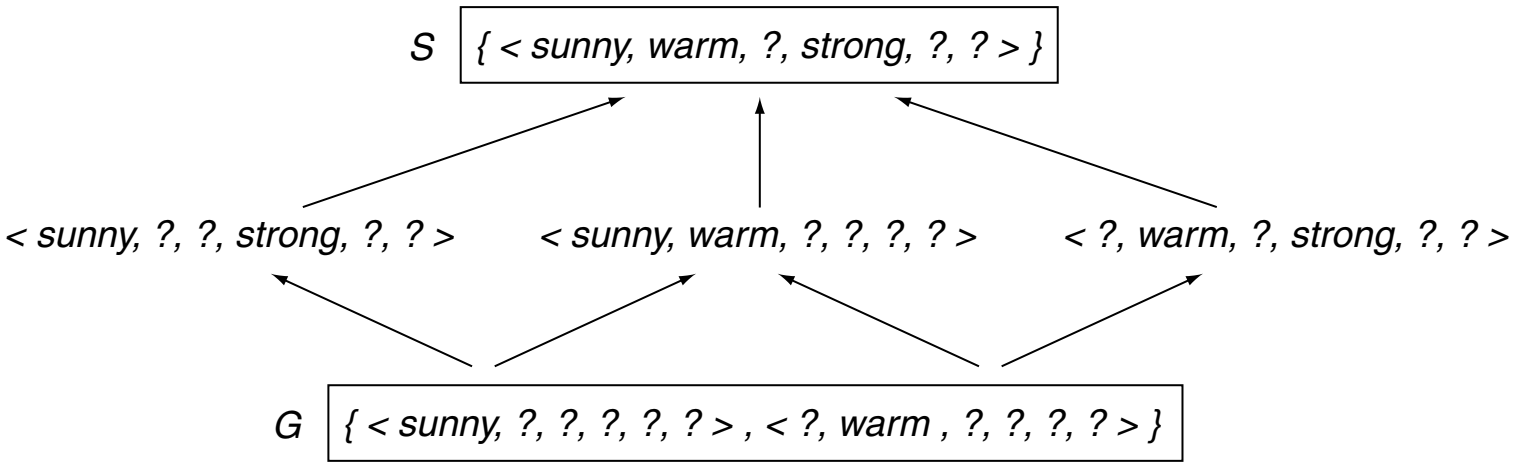

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7	sunny	warm	normal	light	warm	same	3+ : 3–
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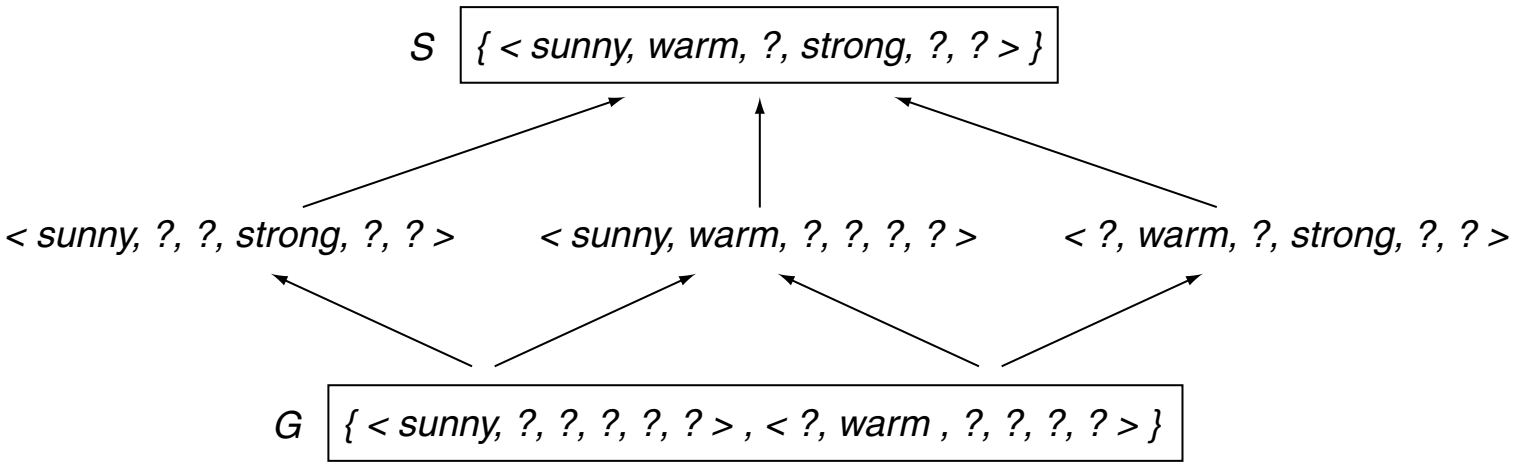
Concept Learning: Search in Version Space

Question 2: Partially Learned Concepts



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8	sunny	cold	normal	strong	warm	same	2+ : 4–

Concept Learning: Search in Version Space

Question 3: Inductive Bias

A different set of examples D' :

Example	Sky	Temperature	Humidity	Wind	Water	Forecast	EnjoySport
9	sunny	warm	normal	strong	cool	change	yes
10	sunny	warm	normal	light	warm	same	yes

➜ $S = \{ \langle \textit{sunny, warm, normal, ?, ?, ?} \rangle \}$

Concept Learning: Search in Version Space

Question 3: Inductive Bias

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Example	Sky	Temperature	Humidity	Wind	Water	Forecast	EnjoySport
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➜ $S = \{ \langle \textit{sunny, warm, normal, ?, ?, ?} \rangle \}$

In particular, Example $\mathbf{x}_1$ is correctly classified as positive [Example set D] :

$$\mathbf{x}_1 = (\textit{sunny, warm, normal, strong, warm, same})$$

Discussion:

- What if $\mathbf{x}_1$ were a negative example?
- What assumptions about the target concept are met a-priori by the learner?

Concept Learning: Search in Version Space

Question 3: Inductive Bias (continued)

A different set of examples D'' :

Example	Sky	Temperature	Humidity	Wind	Water	Forecast	EnjoySport
9	sunny	warm	normal	strong	cool	change	yes
11	cloudy	warm	normal	strong	cool	change	yes

➜ $S = \{ \langle$ *?, warm, normal, strong, cool, change* $\rangle \}$

Concept Learning: Search in Version Space

Question 3: Inductive Bias (continued)

A different set of examples D'' :

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9	sunny	warm	normal	strong	cool	change	yes
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➜ $S = \{ \langle$ *?, warm, normal, strong, cool, change* $\rangle \}$

⋮

12	rainy	warm	normal	strong	cool	change	no

➜ $S = \{ \}$

Concept Learning: Search in Version Space

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⋮

12	rainy	warm	normal	strong	cool	change	no

➜ $S = \{ \}$

Discussion:

The hypothesis space H may be designed to contain more complex concepts, e.g. including: $\langle$ *sunny, ?, ?, ?, ?, ?* $\rangle \vee \langle$ *cloudy, ?, ?, ?, ?, ?* $\rangle$.

Concept Learning: Search in Version Space

Question 3: Inductive Bias (continued)

- In a binary classification problem the unrestricted (= unbiased) hypothesis space contains $|\mathcal{P}(X)| \equiv 2^{|X|}$ elements.
- A learning algorithm that considers all possible hypotheses as equally likely makes no a-priori assumption with regard to the target concept.
- A learning algorithm without a-priori assumptions has no "inductive bias".

> *"The policy by which a* [learning] *algorithm generalizes from observed training examples to classify unseen instances is its inductive bias.* [. . .] *Inductive bias is the set of assumptions that, together with the training data, deductively justify the classification by the learner to future instances."*
>
> [p.63, Mitchell 1997]

Concept Learning: Search in Version Space

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>
> [p.63, Mitchell 1997]

➜ A learning algorithm without inductive bias has no directive to classify unseen examples. Put another way: the learner cannot *generalize*.

➜ A learning algorithm without inductive bias will only *memorize*.

Which algorithm (Find-S, Candidate Elimination) has a stronger inductive bias?

Chapter ML:II (continued)

II. Machine Learning Basics

- On Data
- Regression
- Concept Learning: Search in Hypothesis Space
- Concept Learning: Search in Version Space
- Measuring Performance

Measuring Performance

True Misclassification Rate

Definition 8 (True Misclassification Rate)

Let X be a feature space with a finite number of elements. Moreover, let C be a set of classes, let $y : X \to C$ be a classifier, and let c be the target concept to be learned. Then the true misclassification rate, denoted as $Err^*(y)$, is defined as follows:

$$Err^*(y) = \frac{|\{\mathbf{x} \in X : c(\mathbf{x}) \neq y(\mathbf{x})\}|}{|X|}$$

Measuring Performance

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Problem:

- Usually the *total function* c is unknown.

Solution:

- Estimation of $Err^*(y)$ with $Err(y, D_s)$, i.e., evaluating y on a subset $D_s \subseteq D$ of carefully chosen examples D. Recall that for the feature vectors in D the target concept c is known.

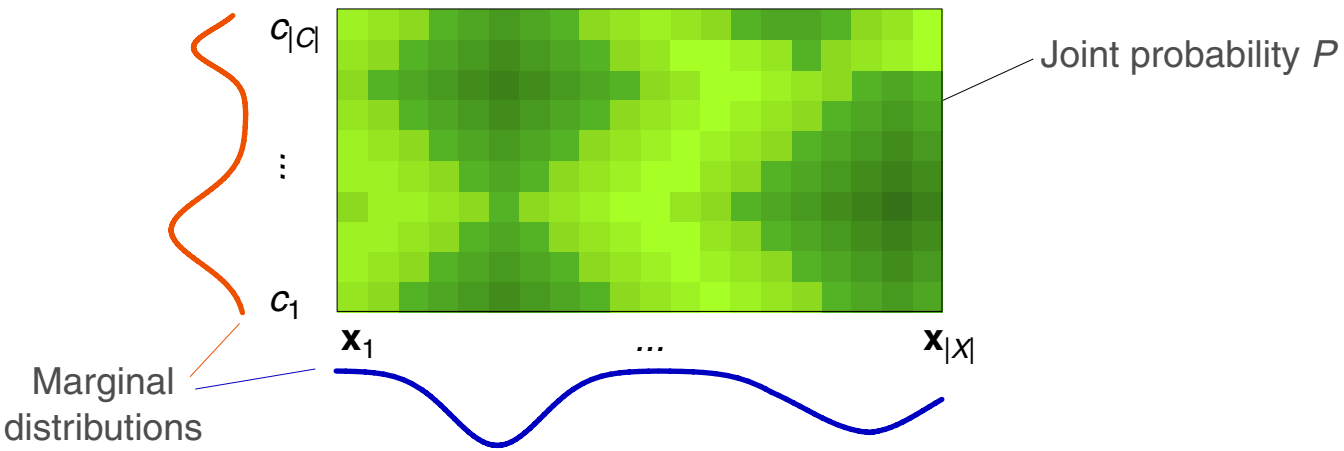
Remarks:

- Instead of the term “true misclassification rate” we may also use the term “true misclassification error” or simply “true error”.
- The English word “rate” can be used to denote both the mathematical concept of a flow quantity (a change of a quantity per time unit) as well as the mathematical concept of a *portion*, a *percentage*, or a *ratio*, which has a stationary (= time-independent) semantics. This latter semantics is meant here when talking about the misclassification rate.
- Unfortunately, the German word “Rate” is often (mis)used to denote the mathematical concept of a portion, a percentage, or a ratio. Taking a precise mathematical standpoint, the correct German words are “Anteil” or “Quote”. I.e., a semantically correct translation of misclassification rate is “Missklassifikationsanteil”, and not “Missklassifikationsrate”.

Measuring Performance

True Misclassification Rate: Probabilistic Foundation

Let X and C be defined as before. Moreover, let P be a probability measure on $X \times C$. Then $P(\mathbf{x}, c)$ (precisely: $P(\mathcal{H} = \mathbf{x}, \mathcal{C} = c)$) denotes the probability that feature vector $\mathbf{x} \in X$ belongs to class $c \in C$. Illustration:



Measuring Performance

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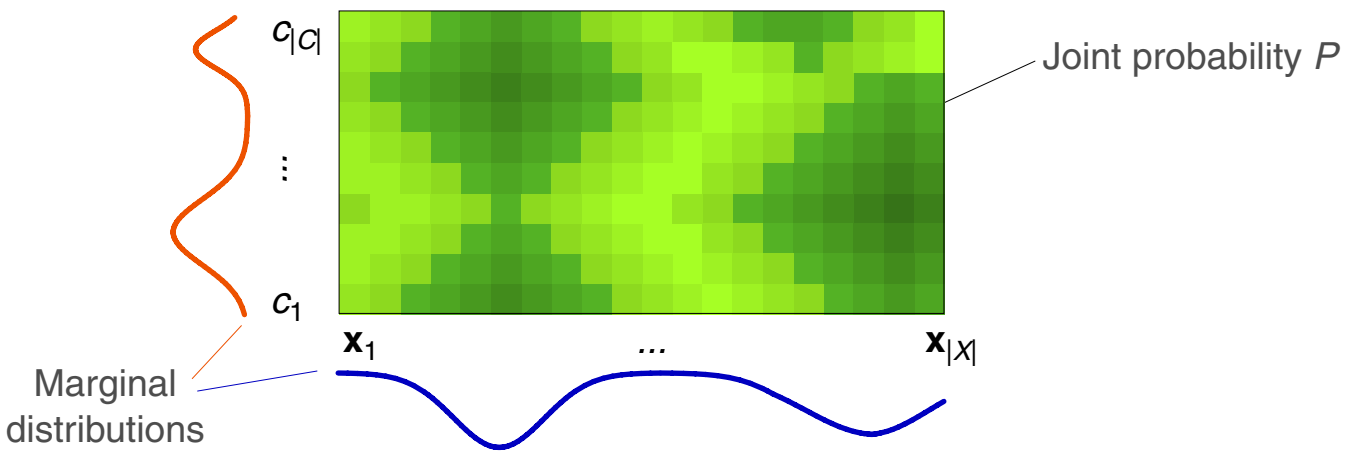

$$Err^*(y) = \sum_{\mathbf{x} \in X} \sum_{c \in C} P(\mathbf{x}, c) \cdot I(y(\mathbf{x}), c), \quad \text{with } I(y(\mathbf{x}), c) = \begin{cases} 0 & \text{if } y(\mathbf{x}) = c \\ 1 & \text{otherwise} \end{cases}$$

Measuring Performance

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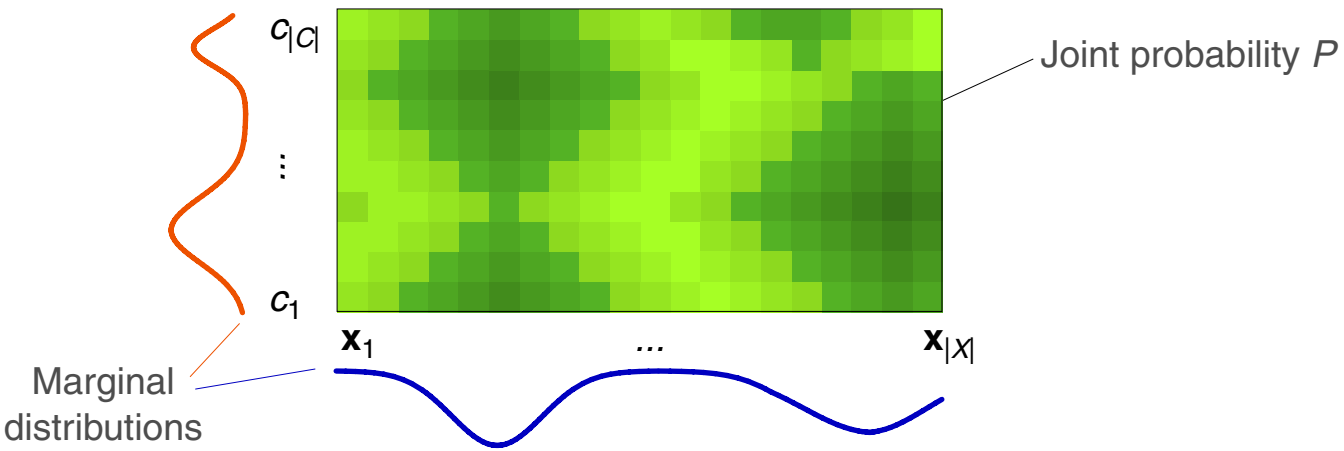

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$D = \{(\mathbf{x}_1, c_1)), \ldots, (\mathbf{x}_n, c_n))\} \subseteq X \times C$ is a set of examples whose elements are drawn independently and according to the same P.

Remarks:

- See the definition of a probability measure in [ML:IV Probability Basics].
- $\mathcal{H}$ and $\mathcal{C}$ are random variables with domains X and C respectively.
- Let A and B denote two events, e.g., $A =$ "$\mathcal{H} = \mathbf{x}$" and $B =$ "$\mathcal{C} = c$". Then the following expressions are syntactic variants, i.e., they are semantically equivalent: $P(A, B)$, $P(A \text{ and } B)$, $P(A \wedge B)$.
- The function $c(\mathbf{x})$ has been modeled as random variable, $\mathcal{C}$, since in the real world the classification of a feature vector $\mathbf{x}$ may not be deterministic but the result of a random process. Keyword: label noise.
- The elements in D are considered as random variables that are both independent of each other and identically distributed. This property of a set of random variables is abbreviated with "i.i.d."
- If the elements in D or D_s were not chosen according to P, then $\mathit{Err}(y, D_s)$ could not be used as an estimation of $\mathit{Err}^*(y)$. Keyword: sample selection bias

Measuring Performance

Training Error [True Misclassification Rate]

- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.
- $D_{tr} = D$ is the training set.
- $y : X \to C$ is a classifier learned on the basis of D_{tr}.

Training error = misclassification rate with respect to D_{tr} :

$$\mathit{Err}(y, D_{tr}) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D_{tr} : c(\mathbf{x}) \neq y(\mathbf{x})\}|}{|D_{tr}|}$$

Measuring Performance

Training Error [True Misclassification Rate]

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Problems:

- $\mathit{Err}(y, D_{tr})$ is based on examples that are also exploited to learn y.

➜ $\mathit{Err}(y, D_{tr})$ quantifies memorization but not the generalization capability of y.

➜ $\mathit{Err}(y, D_{tr})$ is an optimistic estimation, i.e., it is constantly lower compared to the error incurred when applying y in the wild.

Measuring Performance

Holdout Estimation (2-Fold Cross-Validation) [True Misclassification Rate]

- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.
- $D_{tr} \subset D$ is the training set.
- $y : X \to C$ is a classifier learned on the basis of D_{tr}.
- $D_{ts} \subset D$ with $D_{ts} \cap D_{tr} = \emptyset$ is a test set.

Holdout estimation = misclassification rate with respect to D_{ts} :

$$\mathit{Err}(y, D_{ts}) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D_{ts} : c(\mathbf{x}) \neq y(\mathbf{x})\}|}{|D_{ts}|}$$

Measuring Performance

Holdout Estimation (2-Fold Cross-Validation) [True Misclassification Rate]

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Holdout estimation = misclassification rate with respect to D_{ts} :

$$\mathit{Err}(y, D_{ts}) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D_{ts} : c(\mathbf{x}) \neq y(\mathbf{x})\}|}{|D_{ts}|}$$

Requirements:

- D_{tr} and D_{ts} must be drawn i.i.d.
- D_{tr} and D_{ts} should have similar sizes.

Remarks:

- A typical value for splitting D into training set D_{tr} and test set D_{ts} is 2:1.
- When splitting D into D_{tr} and D_{ts} one has to ensure that the underlying distribution is maintained. Keywords: stratification, sample selection bias

Measuring Performance

k-Fold Cross-Validation [Holdout Estimation]

- Form k test sets by splitting D into disjoint sets $D_1, \ldots, D_k$ of similar size.
- For $i = 1, \ldots, k$ do:
  1. $y_i : X \to C$ is a classifier learned on the basis of $D \setminus D_i$
  2. $\mathit{Err}(y_i, D_i) = \dfrac{|\{(\mathbf{x}, c(\mathbf{x}) \in D_i : y_i(\mathbf{x}) \neq c(\mathbf{x})\}|}{|D_i|}$

Cross-validated misclassification rate:

$$\mathit{Err}_{cv}(y, D) = \frac{1}{k} \sum_{i=1}^{k} \mathit{Err}(y_i, D_i)$$

Measuring Performance

n-Fold Cross-Validation (Leave One Out)

Special case with $k = n$:

- Determine the cross-validated misclassification rate for $D \setminus D_i$ where $D_i = \{(\mathbf{x}_i, c(\mathbf{x}_i))\},\ i \in \{1, \ldots, n\}$.

Measuring Performance

n-Fold Cross-Validation (Leave One Out)

Special case with $k = n$:

- Determine the cross-validated misclassification rate for $D \setminus D_i$ where $D_i = \{(\mathbf{x}_i, c(\mathbf{x}_i))\},\ i \in \{1, \ldots, n\}$.

Problems:

- High computational effort if D is large.
- Singleton test sets ($|D_i| = 1$) are never stratified since they contain a single class only.

Remarks:

- For large k the set $D \setminus D_i$ is of similar size as D. Hence *Err*(y_i, D_i) is close to *Err*(y, D), where y is the classifier learned on the basis of the entire set D.
- n-fold cross-validation is a special case of exhaustive cross-validation methods, which learn and test on all possible ways to divide the original sample into a training and a validation set. [Wikipedia]
- For the construction of tree classifiers, tenfold cross-validation has been reported to give good results. [Breiman]

Measuring Performance

Bootstrapping [Holdout Estimation]

Resampling the example set D:

- For $j = 1, \ldots, l$ do:
  1. Form training set D_j by drawing n examples from D with replacement.
  2. $y_j : X \to C$ is a classifier learned on the basis of D_j
  3. $\mathit{Err}(y_j, D \setminus D_j) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D \setminus D_j : y_j(\mathbf{x}) \neq c(\mathbf{x})\}|}{|D \setminus D_j|}$

Bootstrapped misclassification rate:

$$\mathit{Err}_{bt}(y, D) = \frac{1}{l} \sum_{j=1}^{l} \mathit{Err}(y_j, D \setminus D_j)$$

Remarks:

- Let $|D| = n$. The probability that an example is not considered is $(1 - 1/n)^n$. Similarly, the probability that an example is considered at least once is $1 - (1 - 1/n)^n$.
- If n is large, then $1 - (1 - 1/n)^n \approx 1 - 1/e \approx 0.632$. I.e., each training set contains about 63.2% of the examples in D.
- The classifiers $y_1, \ldots, y_l$ can be used in a combined fashion, called *ensemble*, where the class is determined by means of a majority decision:

$$y(\mathbf{x}) = \underset{c \in C}{\text{argmax}} \, |\{j \in \{1, \ldots, l\} : y_j(\mathbf{x}) = c\}|$$

- For the construction of tree classifiers, bootstrapping has been reported to improve the misclassification rate about 20% – 47% compared to a standard approach. [Breiman]

Measuring Performance

Misclassification Costs [Holdout Estimation]

Use of a cost measure for the misclassification of a feature vector $\mathbf{x}$ in class c' instead of in class c:

$$\mathit{cost}(c' \mid c) \begin{cases} \geq 0 & \text{if } c' \neq c \\ = 0 & \text{otherwise} \end{cases}$$

Estimation of $\mathit{Err}^*_{\mathit{cost}}(y)$ based on a sample $D_s \subseteq D$:

$$\mathit{Err}_{\mathit{cost}}(y, D_s) = \frac{1}{|D_s|} \cdot \sum_{(\mathbf{x}, c(\mathbf{x})) \in D_s} \mathit{cost}(y(\mathbf{x}) \mid c(\mathbf{x}))$$

Remarks:

- The misclassification rate *Err* is a special case of Err_{cost} with $cost(c' \mid c) = 1$ for $c' \neq c$.