Introduction to machine learning

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Course information

- Instructor - Victor Vladimirovich Kitov
- Tasks of the course
- Structure:
  - lectures, seminars
  - assignements: theoretical, labs, competitions
  - exam
- Tools
  - python
  - ipython notebook
  - numpy, scipy, pandas
  - matplotlib, seaborn
  - scikit-learn.

Recommended materials

- Лекции К.В.Воронцова (видео-лекции и материалы на `machinelearning.ru`)
- **The Elements of Statistical Learning: Data Mining, Inference, and Prediction.** Trevor Hastie, Robert Tibshirani, Jerome Friedman, 2nd Edition, Springer, 2009. `http://statweb.stanford.edu/~tibs/ElemStatLearn/`.
- **Statistical Pattern Recognition.** 3rd Edition, Andrew R. Webb, Keith D. Copsey, John Wiley & Sons Ltd., 2011.

- Any additional public sources:
  - wikipedia, articles, tutorials, video-lectures.
- Practical questions:
  - stackoverflow.com, sklearn documentation, kaggle forums.

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Formal definitions of machine learning

- Machine learning is a field of study that gives computers the ability to learn without being explicitly programmed.
- A computer program is said to learn from **experience E** with respect to some **class of tasks T** and **performance measure P**, if its performance P at tasks in T improves with experience E.
- Examples from text analysis: spell checker, spam filtering, POS tagger.

Major niches of ML

- dealing with huge datasets with many attributes (text categorization)
- hard to formulate explicit rules (image recognition)
- further adaptation to usage conditions is required (voice detection)
- fast adaptation to changing conditions (stock prices prediction)

Examples of ML applications

- WEB
  - Web-page ranking
  - Spam filtering
    - e-mails
    - search results
- Networks monitoring
  - Intrusion detection
  - Anomaly detection
- Business
  - Fraud detection
  - Churn prediction
  - Credit scoring
  - Stock prices / risks forecsting

Examples of ML applications

- Texts
  - Document classification
  - POS tagging, semantic parsing,
  - named entities detection
  - sentimental analysis
  - automatic summarization
- Images
  - Handwriting recognition
  - Face detection, pose detection
  - Person identification
  - Image classification
  - Image segmentation
  - Adding artistic style
- Other
  - Target detection / classification
  - Particle classification

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General problem statement

- Set of objects O
- Each object is described by a vector of known characteristics $\mathbf{x} \in \mathcal{X}$ and predicted characteristics $y \in \mathcal{Y}$.

$$o \in O \longrightarrow (\mathbf{x}, y)$$

- Usually $\mathcal{X} = \mathbb{R}^D$, $\mathcal{Y}$ - a scalar, but they may be any structural descriptors of objects in general.

General problem statement

- Task: find a mapping f, which could accurately approximate $\mathcal{X} \to \mathcal{Y}$.
  - using a finite «training» set of objects with known (x, y).
  - to apply on a set of objects of interest
- Questions solved in ML:
  - how to select object descriptors - features
  - in what sense a mapping f should approximate true relationship
  - how to construct f

Variants of problem statement

- For each new object x need to associate y.
- What is known:
  - $(x_1, y_1), (x_2, y_2), ...(x_N, y_N)$ - supervised learning:
  - $x_1, x_2, ...x_N$ - unsupervised learning
    - dimensionality reduction
    - clustering
  - $(x_1, y_1), (x_2, y_2), ...(x_N, y_N), x_{N+1}x_{N+2}, ...x_{N+M}$ - semi-supervised learning.
- If predicted objects $x'_1, x'_2, ...x'_K$ for which y is forecasted, are known in advance, then this is «transductive» learning.

Example of supervised classification

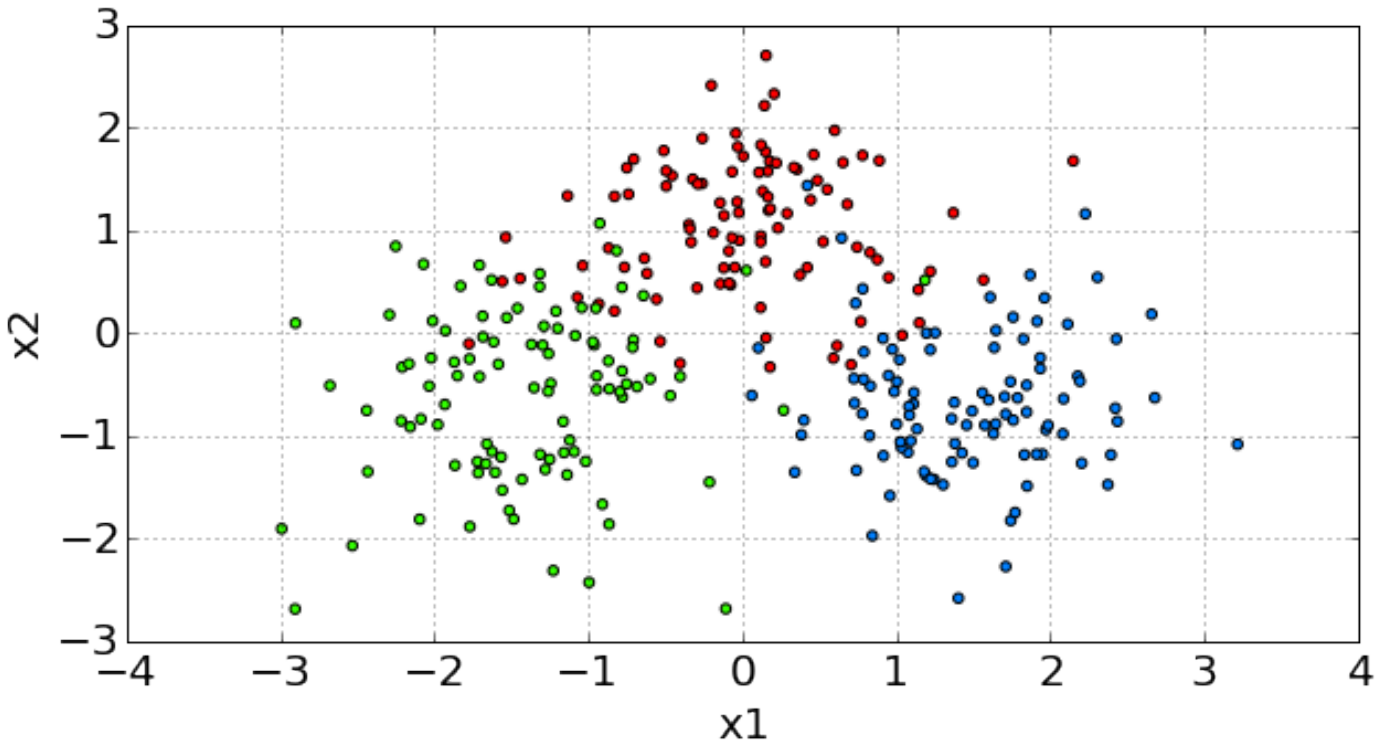

Figure: Supervised learning: $x = (x_1, x_2)$, y is shown with color

Example of semi-supervised classification

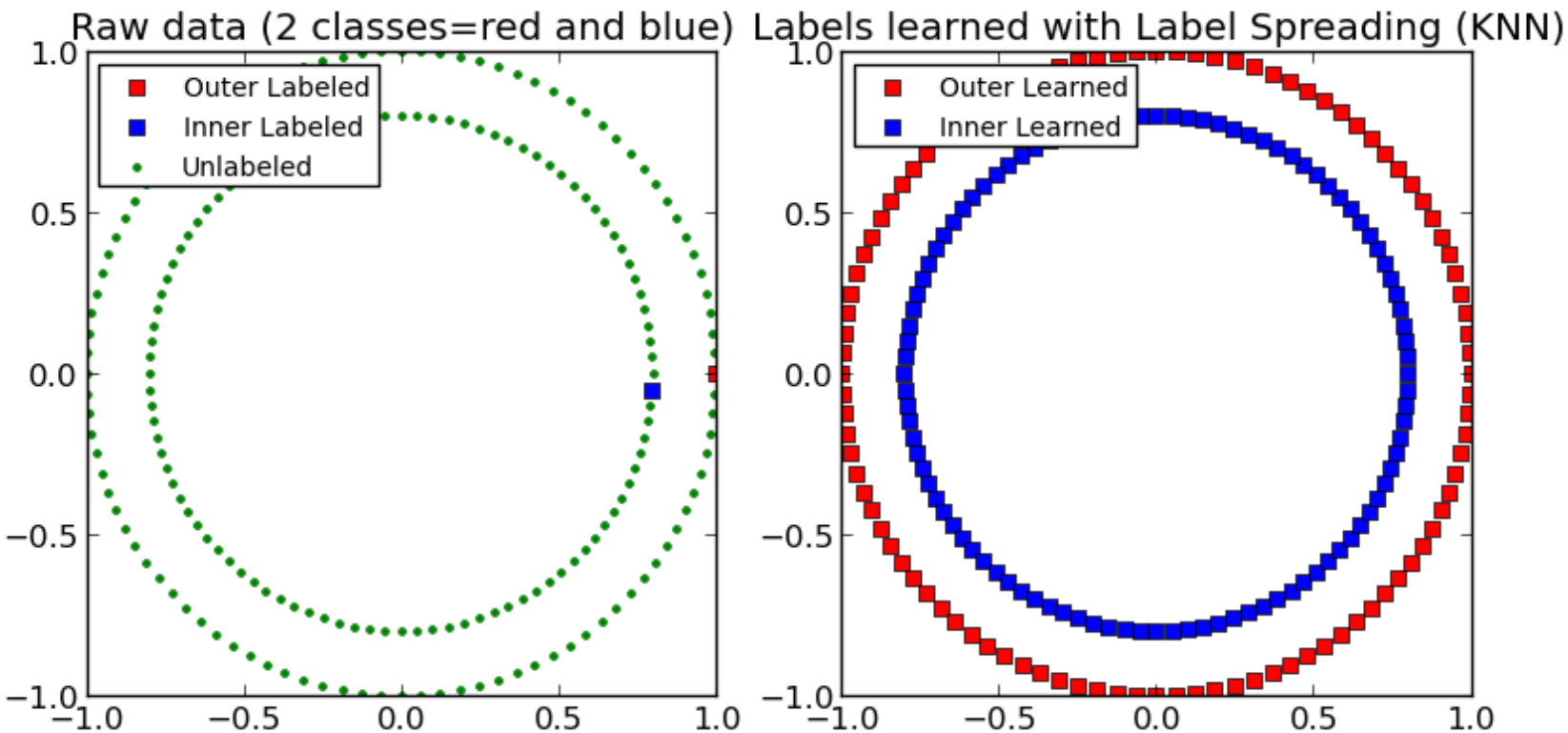

Figure: Semi-supervised learning.

Example of clustering (unsupervised)

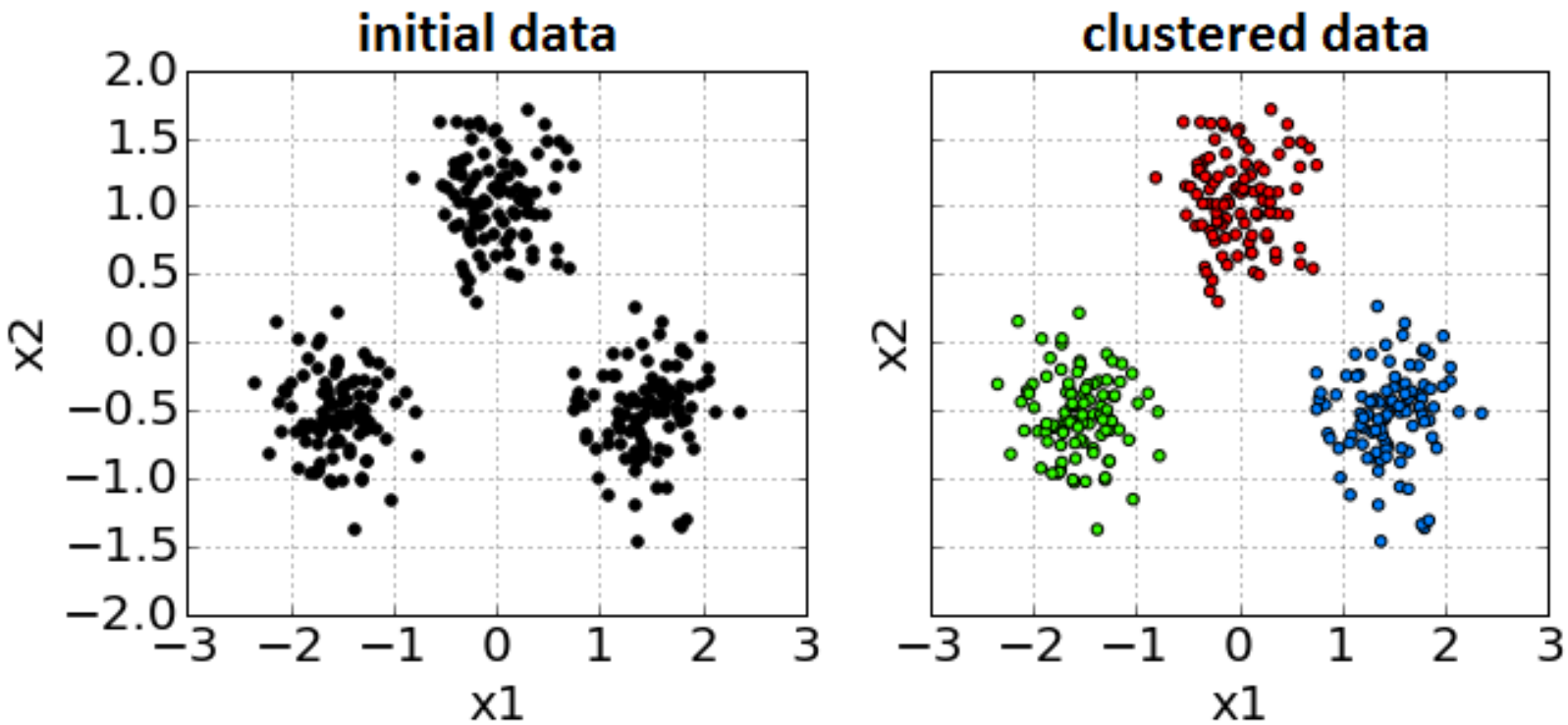

Figure: Unsupervised learning: clustering

Dimensionality reduction (unsupervised)

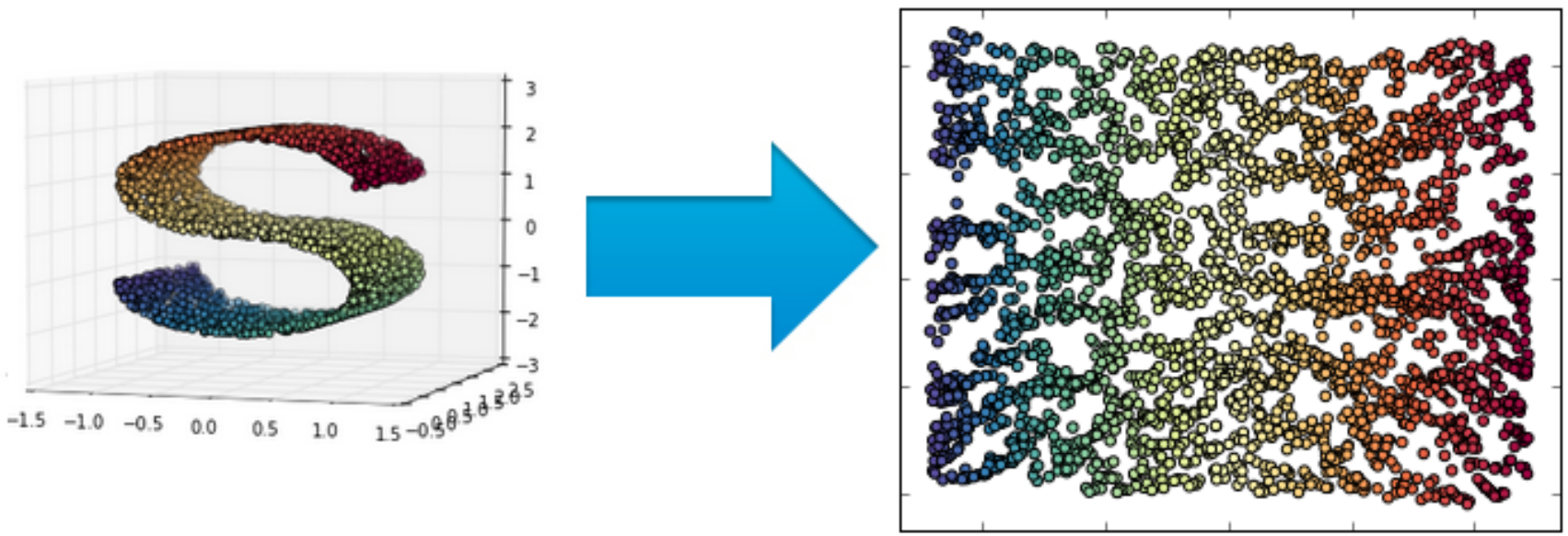

Figure: Unsupervised learning: dimensionality reduction

Generative and discriminative models[1]

Generative model

Full distribution $p(x, y)$ is modeled.

- Can generate new observations (x, y)

$$\begin{aligned}\widehat{y}(x) &= \arg\max_y p(y|x) = \arg\max_y \frac{p(x,y)}{p(x)} = \arg\max_y p(y)p(x|y) \\ &= \arg\max_y \{\log p(y) + \log p(x|y)\}\end{aligned}$$

Discriminative model

- **Discriminative with probability**: only $p(y|x)$ is modeled
- **Reduced discriminative**: only $y = f(x)$ is modeled.

[1] Which is more general problem statement and which - more specific?

Generative and discriminative - discussion

- **Disadvantages of generative models:**
  - Discriminative models are more general
  - $p(x|y)$ may be inaccurate in high dimensional spaces

Generative and discriminative - discussion

- **Disadvantages of generative models:**
  - Discriminative models are more general
  - $p(x|y)$ may be inaccurate in high dimensional spaces
- **Advantages of generative models:**
  - Generative models can be adjusted to varying $p(y)$
  - Naturally adjust to missing features (by marginalization)
  - Easily detect outliers (small $p(x)$)

Types of features

- Full object description $\mathbf{x} \in \mathcal{X}$ consists of individual features $x_i \in \mathcal{X}_i$
- Types of feature:
  - $\mathcal{X}_i = \{0, 1\}$ - binary feature
  - $|\mathcal{X}_i| < \infty$ - discrete (nominal) feature
  - $|\mathcal{X}_i| < \infty$ and $\mathcal{X}_i$ is ordered - ordinal feature
  - $\mathcal{X}_i = \mathbb{R}$ - real feature

Types of target variable

- Types of target variable:
  - $\mathcal{Y} = \mathbb{R}$ - regression (in supervised learning)
  - $\mathcal{Y} = \mathbb{R}^M$ - vector regression (in supervised learning) or feature extraction (in unsupervised learning)
  - $\mathcal{Y} = \{\omega_1, \omega_2, ...\omega_C\}$ - classification (in supervised learning) or clustering (in unsupervised learning).
    - C=2: binary classification, encoding - $\mathcal{Y} = \{+1, -1\}$ or $\mathcal{Y} = \{0, 1\}$.
    - C>2: multiclass classification
  - $\mathcal{Y}$-set of all sets of $\{\omega_1, \omega_2, ...\omega_C\}$ - labeling
    - $\mathcal{Y} = \{y \in \mathbb{R}^C : y_i \in \{0, 1\}\}$, $y_i = 1 \Leftrightarrow$object is associated with ω_i.

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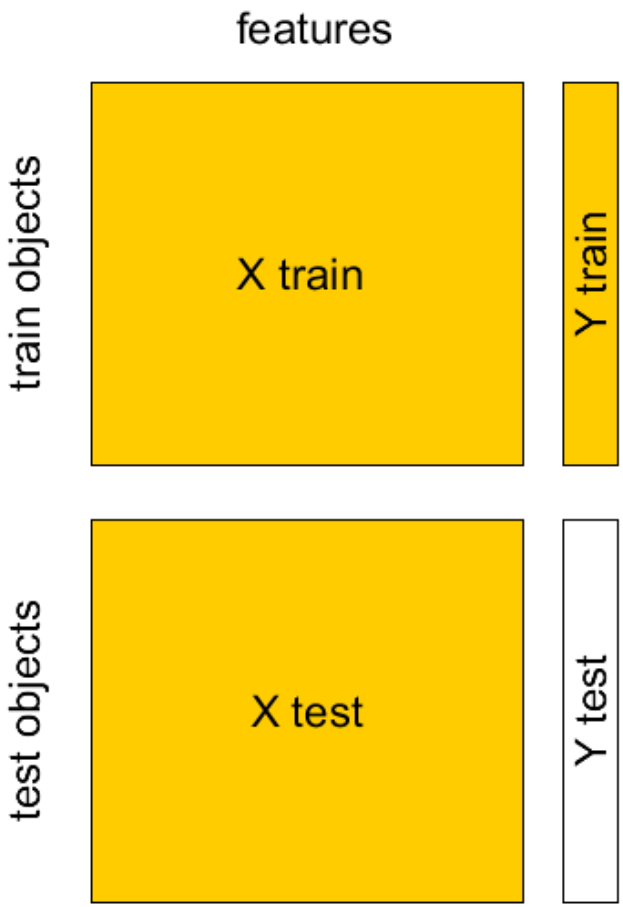
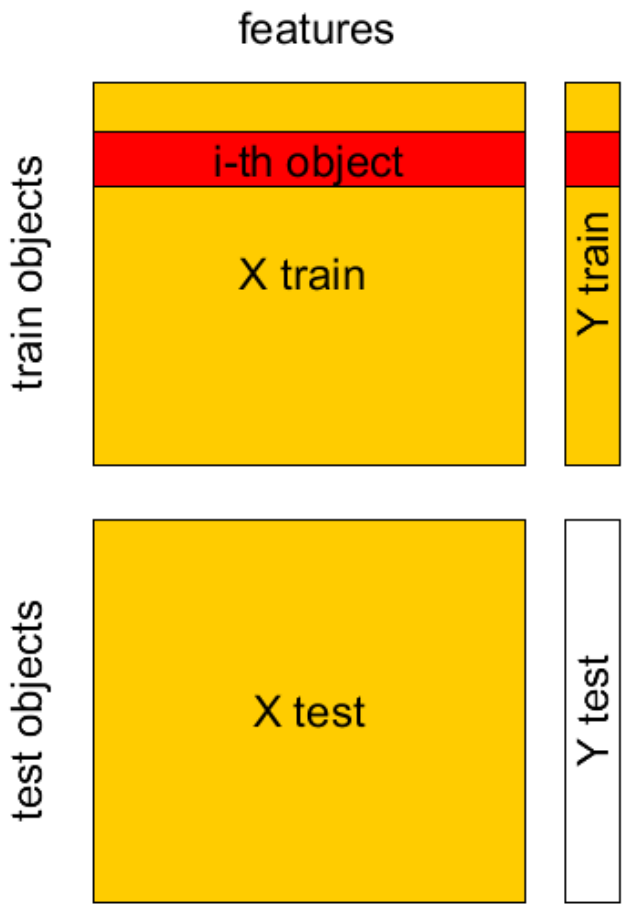
Training set

- **Training set:** $X \in \mathbb{R}^{N \times D}$ - **design matrix**, $Y \in \mathbb{R}^{N}$- predicted outputs (target values)
- Using X, Y the task is to estimate unknown parameters $\widehat{\theta}$ of mapping $\widehat{y} = f_{\theta}(x)$ so that it will approximate true relationship $y = y(x)$
- It is assumed that $z_n = (x_n, y_n)$ for $n = 1, 2, ...N$ - are independent and identically distributed random variables (i.i.d).
- Two steps of ML:
  - **training**
  - **application**

Train set, test set

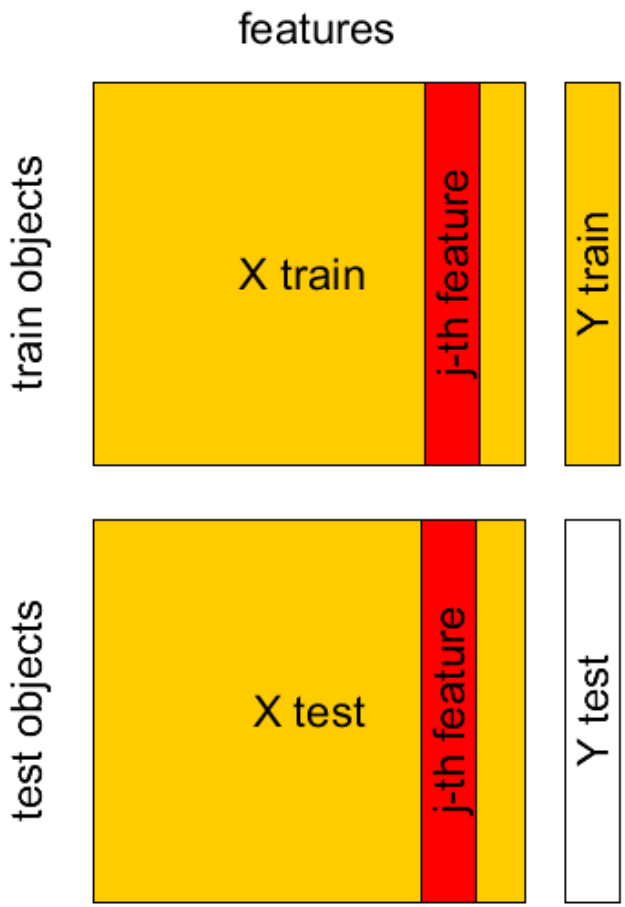


Train set, test set



N - number of objects for which targets (Y) are known.

Train set, test set



D - number of features (advanced case: variable feature count).

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Function class. Linear example.

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  - regression:

$$f(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2 + ... + \theta_D x^D$$

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  - regression:

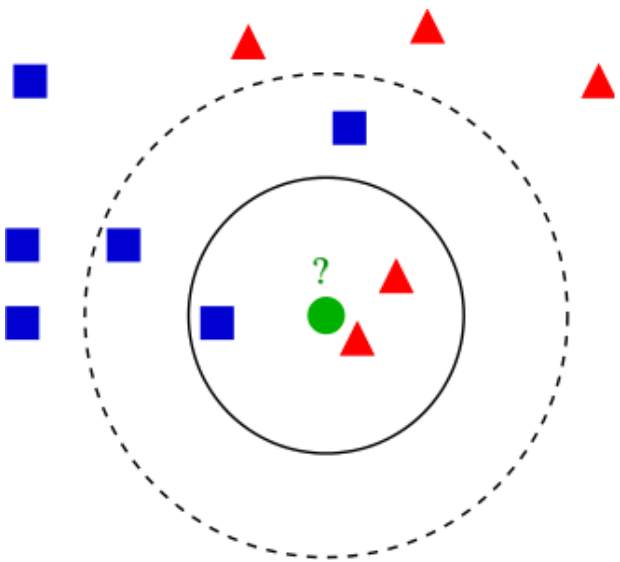
$$f(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2 + ... + \theta_D x^D$$

  - binary classification $y \in \{+1, -1\}$:

$$f(x) = \text{sign}\{\theta_0 + \theta_1 x^1 + \theta_2 x^2 + ... + \theta_D x^D\},$$

Function class. K-NN example.

Figure: Classification:



Function class. K-NN example.

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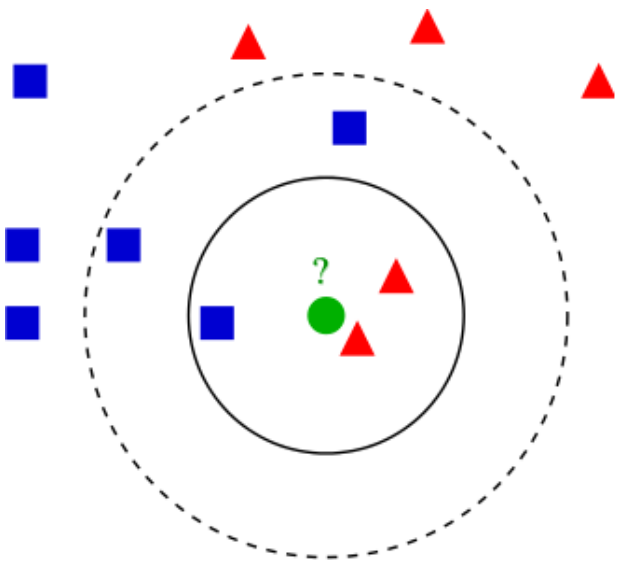
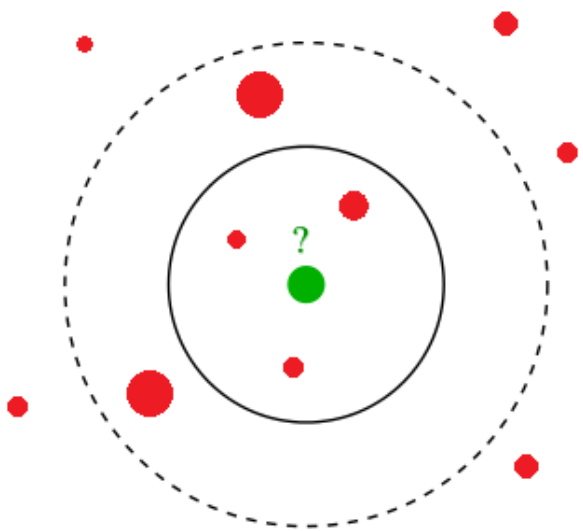


Figure: Regression:



Function class. K-NN example.

- denote for each x:
  - $i(x,k)$ - index of the k-th most close object to x
  - $I(x,K)$ - set of indexes of K nearest neighbours.
- regression:

$$f(x) = \frac{1}{K}\left(y_{i(x,1)} + \ldots + y_{i(x,K)}\right)$$

- classification:

$$f(x) = argmax\left\{\sum_{i\in I(x,K)} \mathbb{I}[y_i = 1], \ldots \sum_{i\in I(x,K)} \mathbb{I}[y_i = C],\right\}$$

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Score versus loss

- In machine learning predictions, functions, objects can be assigned:
  - **score, rating** - this should be maximized
  - **loss, cost** - this should be minimized[2]

[2] how can one convert score↔loss?

Loss function $\mathcal{L}(\widehat{y}, y)$[3]

- Examples:
  - **classification:**
    - misclassification rate

$$\mathcal{L}(\widehat{y}, y) = \mathbb{I}[\widehat{y} \neq y]$$

  - **regression:**
    - MAE (mean absolute error):

$$\mathcal{L}(\widehat{y}, y) = |\widehat{y} - y|$$

    - MSE (mean squared error):

$$\mathcal{L}(\widehat{y}, y) = (\widehat{y} - y)^2$$

[3] Selecting loss is not trivial. Consider demand forecasting.

Empirical risk

- Want to minimize:

$$\int\int \mathcal{L}(f_\theta(x), y)p(x, y)dxdy \to \min_\theta$$

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- Empirical risk:

$$L(\theta|X, Y) = \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}(f_\theta(x_n),\ y_n)$$

- Method of empirical risk minimization:

$$\widehat{\theta} = \arg\min_\theta L(\theta|X, Y)$$

Estimation of empirical risk

- Generally it holds that:

$$L(\widehat{\theta}|X,Y) < L(\widehat{\theta}|X',Y')$$

where X, Y is the training sample and X', Y' is the new data.

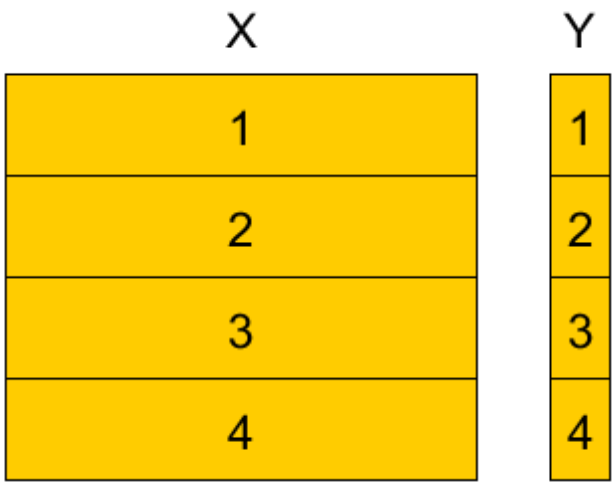
Estimation of empirical risk

- Generally it holds that:

$$L(\widehat{\theta}|X,Y) < L(\widehat{\theta}|X',Y')$$

  where X, Y is the training sample and X', Y' is the new data.
- $L(\widehat{\theta}|X',Y')$ can be estimated using :
  - separate **validation set**
  - **cross-validation**
  - **leave-one-out** method

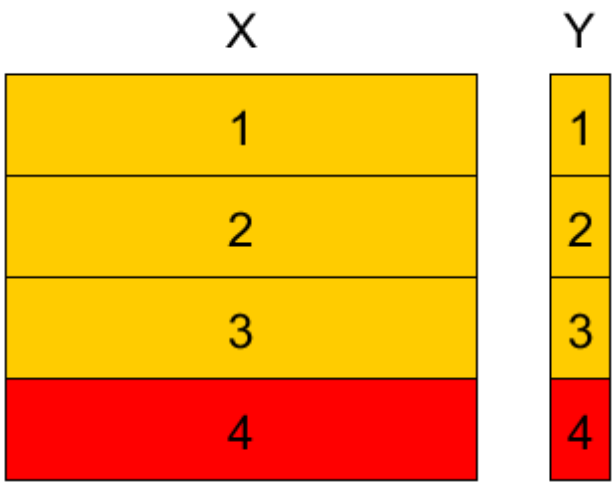
4-fold cross validation example



Divide training set into K parts, referred as «folds» (here $K = 4$).
Variants:

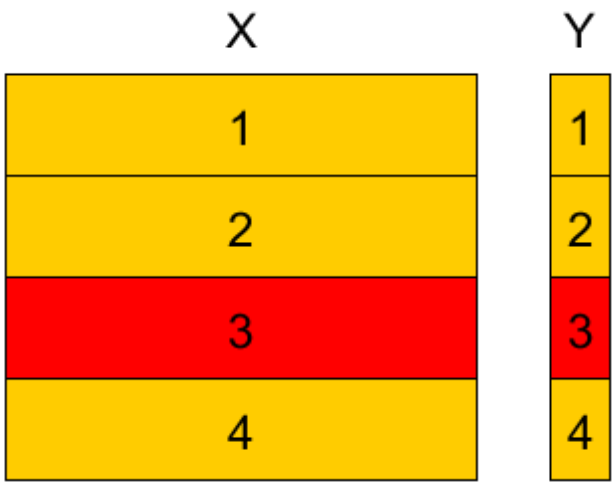
- randomly
- randomly with stratification (w.r.t target value or feature value).

4-fold cross validation example



Use folds 1,2,3 for model estimation and fold 4 for model evaluation.

4-fold cross validation example

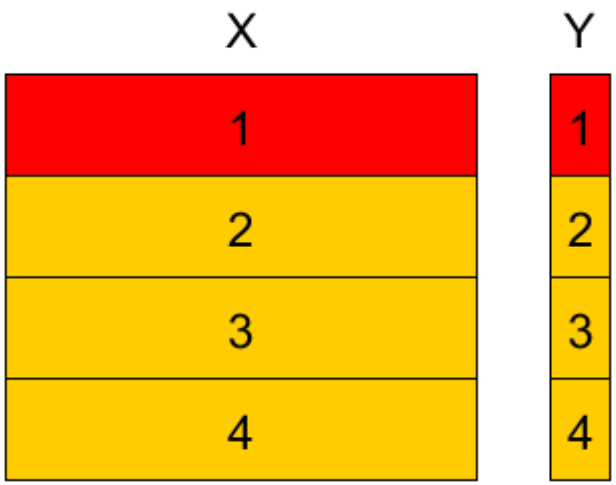


Use folds 1,2,4 for model estimation and fold 3 for model evaluation.

4-fold cross validation example

Use folds 1,3,4 for model estimation and fold 2 for model evaluation.

4-fold cross validation example



Use folds 2,3,4 for model estimation and fold 1 for model evaluation.

4-fold cross validation example

- Denote
  - $k(n)$ - fold to which observation (x_n, y_n) belongs to: $n \in I_k$.
  - $\widehat{\theta}^{-k}$ - parameter estimation using observations from all folds except fold k.

[4] will samples be correlated?

4-fold cross validation example

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Cross-validation empirical risk estimation

$$\widehat{L}_{total} = \frac{1}{N}\sum_{n=1}^{N} \mathcal{L}(f_{\widehat{\theta}^{-k(n)}}(x_n),\, y_n)$$

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Cross-validation empirical risk estimation

$$\widehat{L}_{total} = \frac{1}{N}\sum_{n=1}^{N}\mathcal{L}(f_{\widehat{\theta}^{-k(n)}}(x_n),\, y_n)$$

- For K-fold CV we have:
  - K parameters $\widehat{\theta}^{-1}, ...\widehat{\theta}^{-K}$
  - K models $f_{\widehat{\theta}^{-1}}(x), ...f_{\widehat{\theta}^{-K}}(x)$.
    - can use ensembles
  - K estimations of empirical risk:
    $\widehat{L}_k = \frac{1}{|I_k|}\sum_{n\in I_k}\mathcal{L}(f_{\widehat{\theta}^{-k}}(x_n),\, y_n),\ k = 1, 2, ...K.$
    - can estimate variance & use statistics![4]

[4] will samples be correlated?

Comments on cross-validation

- When number of folds K is equal to number of objects N, this is called **leave-one-out method**.
- Cross-validation uses the i.i.d.[5] property of observations
- Stratification by target helps for imbalanced/rare classes.

[5] i.i.d.=independent and identically distributed

Cross-validation vs. A/B testing

- A/B testing:
  1. divide objects randomly into two groups - A and B.
  2. apply model 1 to A
  3. apply model 2 to B
  4. compare final results

[6] may final business quality be high when forecasting quality is low?

Cross-validation vs. A/B testing

- A/B testing:
  1. divide objects randomly into two groups - A and B.
  2. apply model 1 to A
  3. apply model 2 to B
  4. compare final results

Table: Comparison of cross-validation and A/B test:

cross-validation	A/B test
evaluates forecasting quality	evaluates final business quality[6] (may evaluate forecasting quality as well)
uses available data, only computational costs	requires time and resources for collecting & evaluating feedback from objects of groups A and B

[6] may final business quality be high when forecasting quality is low?

Hyperparameters selection

- Using CV we can select hyperparameters of the model[7]:
  - regression: # of features d, e.g. $x, x^2, ...x^d$
  - K-NN: number of neighbors K

[7] can we use CV loss in this case as estimation for future losses?

Model complexity vs. data complexity

Too simple (underfitted) model

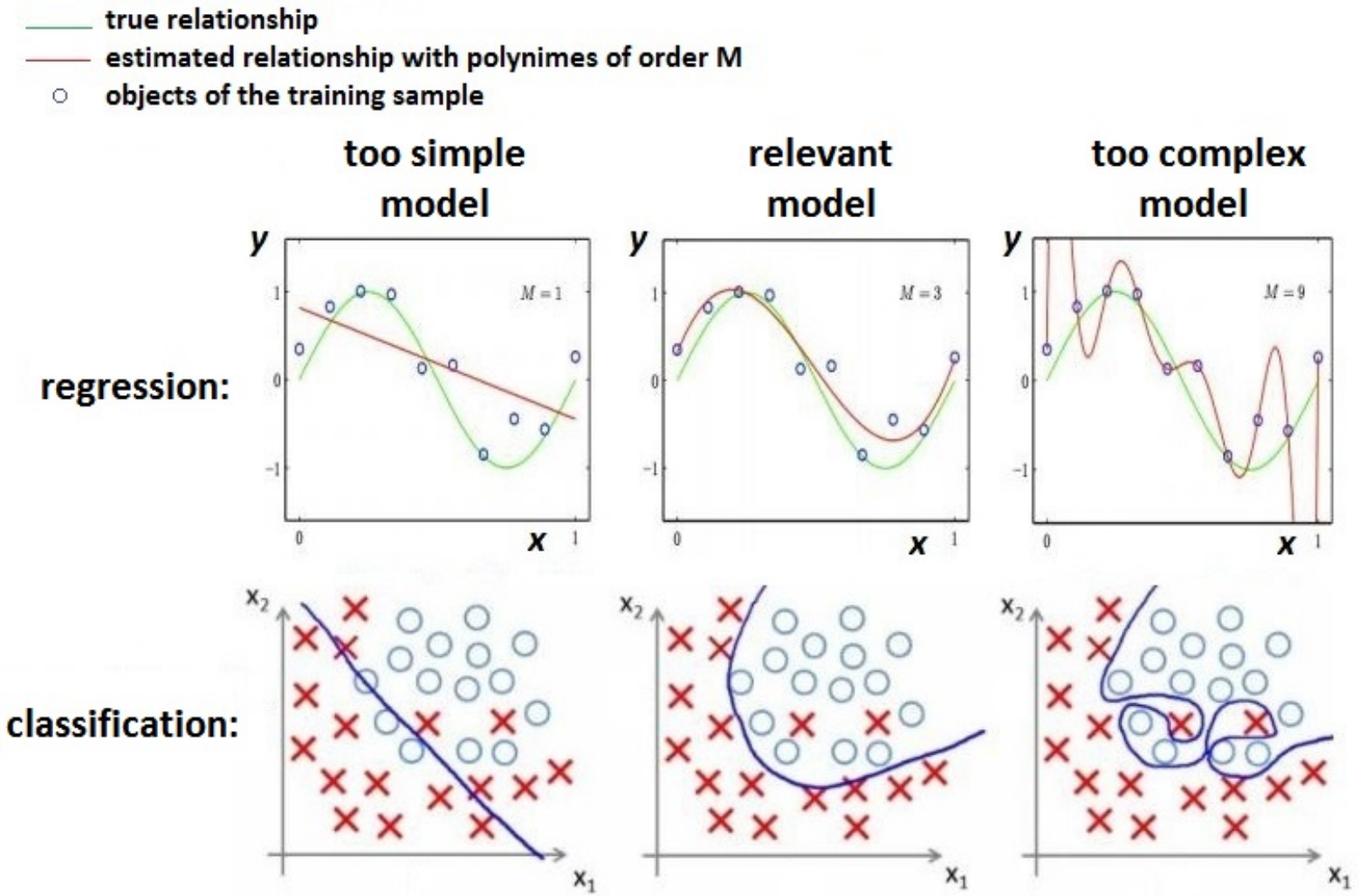
Model that oversimplifies true relationship $\mathcal{X} \to \mathcal{Y}$.

Too complex (overfitted) model

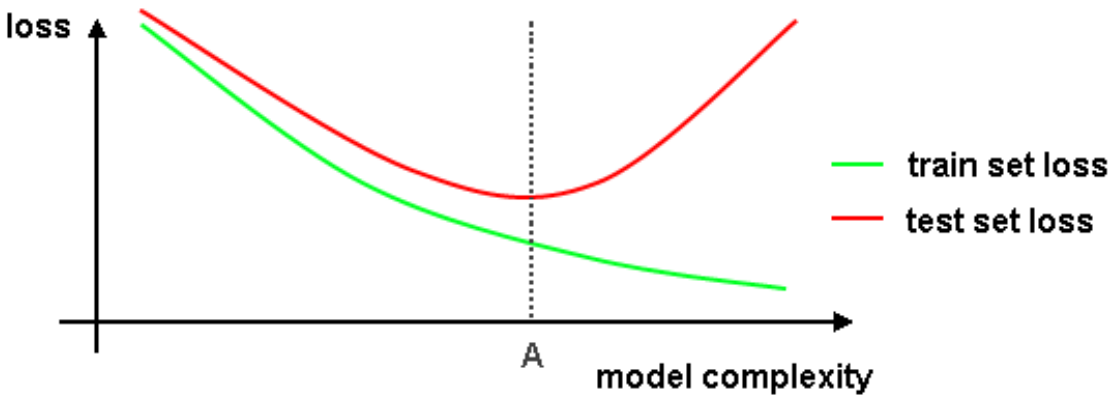
Model that is too tuned on particular peculiarities (noise) of the training set instead of the true relationship $\mathcal{X} \to \mathcal{Y}$.

Pay attention to difference between overfitting and overfitted model. Overfitting is a typical situation when expected loss on training set is lower than expected loss on testing set. Since this is typical, all models are overfitted more (complex ones) or less (simple ones).

Examples of overfitted/underfitted models



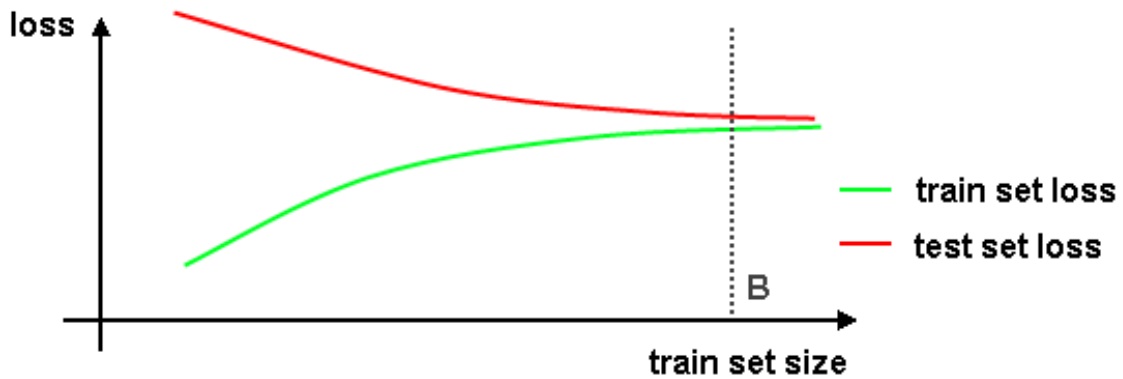
Loss vs. model complexity



Comments:

- expected loss on test set is always higher than on train set.
- left to A: model too simple, underfitting, high bias
- right to A: model too complex, overfitting, high variance

Loss vs. train set size



Comments:

- expected loss on test set is always higher than on train set.
- right to B there is no need to further increase training set size
  - useful to limit training set size when model fitting is time consuming

Cost matrix[8]

For classification in case we output final class predictions $\widehat{y}$ (not probabilities) $\mathcal{L}(y, \widehat{y})$ becomes a matrix:

		predicted classes		
		$\widehat{y}=1$	$\cdots$	$\widehat{y}=C$
true classes	$y=1$	λ_{11}	$\cdots$	λ_{1C}
	$\cdots$	$\cdots$	$\cdots$	$\cdots$
	$y=C$	λ_{C1}	$\cdots$	λ_{CC}

[8] propose some sample cost matrix for binary classification predicting illness

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Discriminant functions[9]

- Discriminant functions is the most general way to describe each classifier.
- Each classifier implies a particular set of discriminant functions.

Discriminant functions

- a set of C functions $g_y(x)$, $y = 1, 2...C$.
- $g_y(x)$ measures the score of class y, given object x.

Usage

Assign x to class having maximum discriminant function value:

$$\widehat{c} = \arg\max_c g_c(x)$$

[9] For fixed classifier are they uniquely defined?

Examples[10]

- K-NN:

$$g_f(x) = \sum_{k=1}^{K} \mathbb{I}[y_{i(k)} = f]$$

- Linear classifier:

$$g_f(x) = \langle w_f, x \rangle$$

- Nearest centroid:

$$g_f(x) = \rho(x, \mu_f)$$

- Maximum posterior probability classifier:

$$g_f(x) = p(y = f|x)$$

[10] Provide discriminant functions for classifier minimizing expected cost according to given cost matrix.

Binary classification

- For two class case $y \in \{-1, +1\}$ we may define a single discriminant function $g(x) = g_{+1}(x) - g_{-1}(x)$ such that

$$\widehat{y}(x) = \begin{cases} +1, & g(x) \geq 0, \\ -1 & g(x) < 0. \end{cases}$$

- Compact notation: $\widehat{y}(x) = \text{sign}[g(x)]$
- Boundary between classes:

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- Compact notation: $\widehat{y}(x) = \text{sign}[g(x)]$
- Boundary between classes: $\{x : \ g(x) = 0\}$.

Binary classification: probability calibration

- $g(x)$ - score of positive class, $p(y=+1|x)$[11]-?

[11] does this apply to K-NN? How to smooth probabilities of K-NN for small K?

Binary classification: probability calibration

- $g(x)$ - score of positive class, $p(y=+1|x)$[11]-?
- Platt scaling: $p(y=+1|x)=\sigma\left(\theta_0+\theta_1 g(x)\right)$,
  - $\sigma(u)=\frac{1}{1+e^{-u}}$

[11] does this apply to K-NN? How to smooth probabilities of K-NN for small K?

Binary classification: probability calibration[12]

- Using the property $1 - \sigma(z) = \sigma(-z)$:

$$p(y = 1|x) = \sigma\left(\theta_0 + \theta_1 g(x)\right)$$
$$p(y = -1|x) = 1 - \sigma(\theta_0 + \theta_1 g(x)) = \sigma\left(-\theta_0 - \theta_1 g(x)\right)$$

- Thus $p(y|x) = \sigma\left(y(\theta_0 + \theta_1 g(x))\right)$
- Estimate θ_0, θ_1 using maximum likelihood:

$$\prod_{n=1}^{N} \sigma\left(y_n(\theta_0 + \theta_1 g(x_n))\right) \to \max_{\theta_0,\theta_1}$$

[12] extend this reasoning to multiclass case

Margin definition

- Consider the training set: $(x_1, y_1), (x_2, y_2), ...(x_N, y_N)$, where y_i is the correct class for object x_i, and $\mathbf{Y} = \{1, 2, ...C\}$ - is the set of all classes.
- Define the margin:

$$M(x_i, y_i) = g_{y_i}(x_i) - \max_{y \in \mathbf{Y} \setminus \{\mathbf{y_i}\}} g_y(x_i)$$

  - margin is negative <=> object x_i was incorrectly classified
  - the value of margin shows how much the classifier is inclined to vote for class y_i

Margin for binary classification

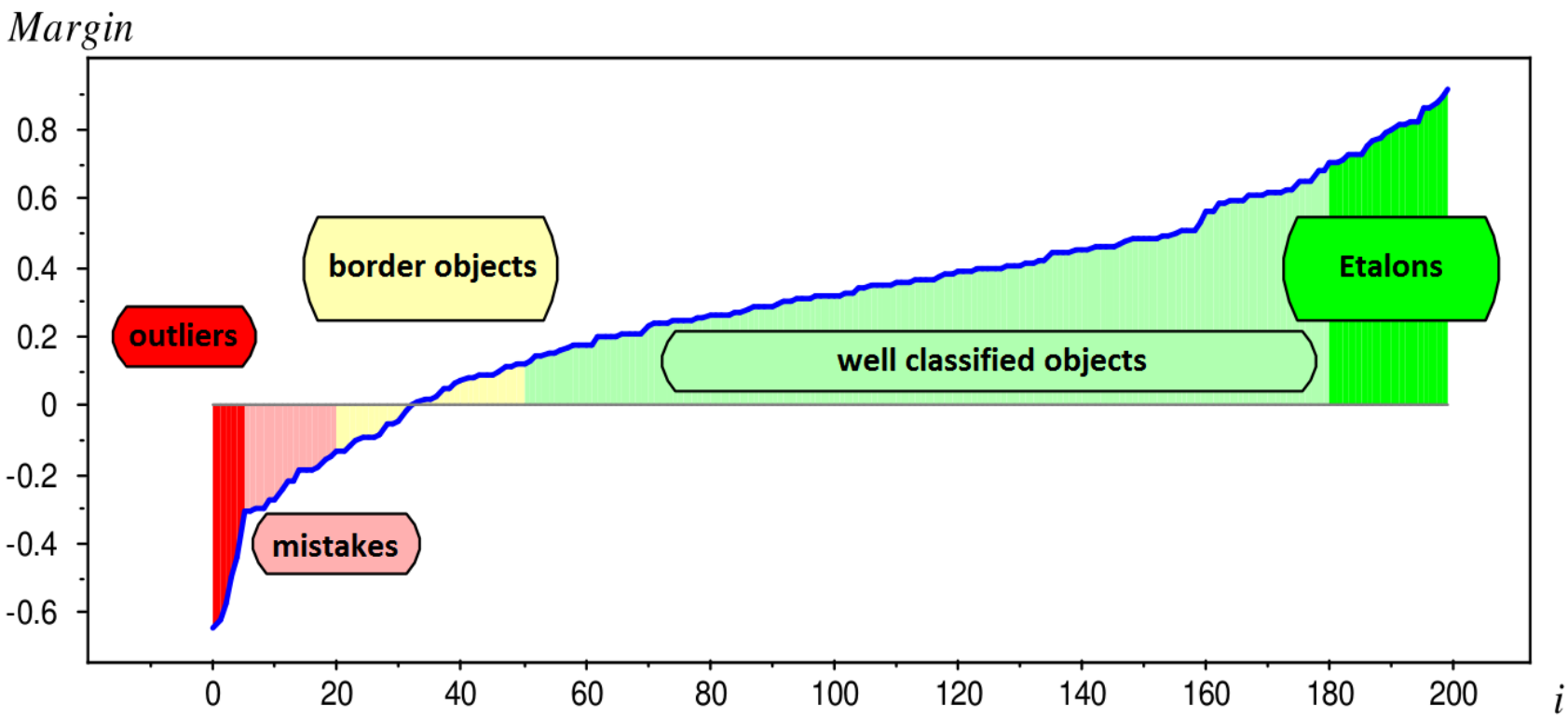
Consider

- $y \in \{+1, -1\}$
- $g(x) = g_{+1}(x) - g_{-1}(x)$ - score of positive class versus negative.
- $\widehat{y}(x) = \text{sign}\, g(x)$

Then

$$M(x, y) = g_y(x) - g_{-y}(x) = y\left(g_{+1}(x) - g_{-1}(x)\right) = yg(x)$$

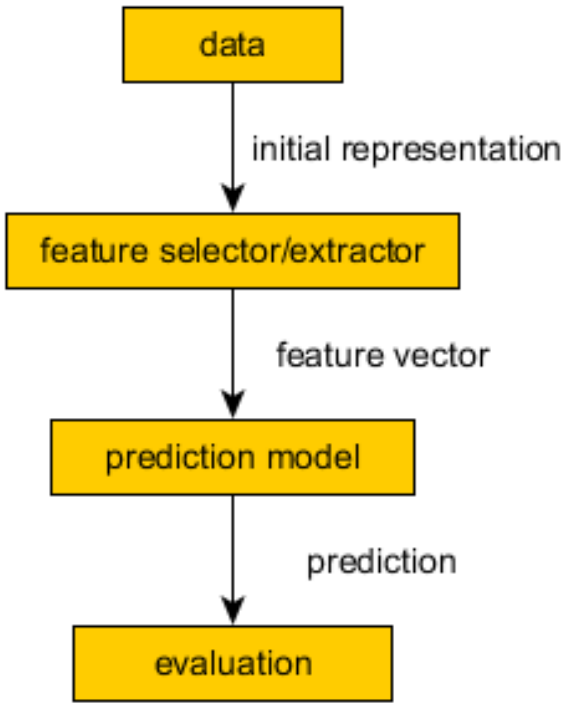
Categorization of objects based on margin



Good classifier should:

- minimize the number of negative margin region
- classify correctly with high margin

General modelling pipeline



If evaluation gives poor results we may return to each of preceding stages.

Connection of ML with other fields

- Pattern recognition
  - recognize patterns and regularities in the data
- Computer science
- Artificial intelligence
  - create devices capable of intelligent behavior
- Time-series analysis
- Theory of probability, statistics
  - when relies upon probabilistic models
- Optimization methods
- Theory of algorithms

Notation used in the course

- If this corresponds the context and there are no redefinitions, then:
  - x - vector of known input characteristics of an object
  - y - predicted target characteristics of an object specified by x
  - x_i - i-th object of a set, y_i - corresponding target characteristic
  - x^k - k-th feature of object specified by x
  - x_i^k - k-th feature of object specified by x_i
  - D - dimensionality of the feature space: $x \in \mathbb{R}^D$
  - N - the number of objects in the training set
  - X - design matrix, $X \in \mathbb{R}^{N \times D}$
  - $Y \in \mathbb{R}^N$ - target characteristics of a training set
  - $\mathcal{L}(\widehat{y}, y)$ - loss function, where y is the true value and $\widehat{y}$ is the predicted value.
  - $\{\omega_1, \omega_2, ...\omega_C\}$ - possible classes, C - total number of classes.
  - $\widehat{z}$ defines an estimate of z, based on the training set: for example, $\widehat{\theta}$ is the estimate of θ, $\widehat{y}$ is the estimate of y, etc.
- All vectors are vectors-columns.