

Introduction to machine learning

Victor Kitov

v.v.kitov@yandex.ru

Yandex School of Data Analysis



Course information

- Lectures - Victor Kitov
- Seminarists - Alex Rogozhikov, Tatiana Likhomanenko
- Structure:
 - lectures, seminars
 - assignments: theoretical, labs, competitions
 - exam
- Tools
 - python
 - ipython notebook
 - numpy, scipy, pandas
 - matplotlib, seaborn
 - scikit-learn.

Recommended materials

- **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](https://scikitlearn.org) documentation, [kaggle](https://www.kaggle.com) forums.

Table of Contents

- 1 Tasks solved by machine learning
- 2 Problem statement
- 3 Training / testing set.
- 4 Function class
- 5 Function estimation

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 forecasting

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

Table of Contents

- 1 Tasks solved by machine learning
- 2 Problem statement**
- 3 Training / testing set.
- 4 Function class
- 5 Function estimation

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.

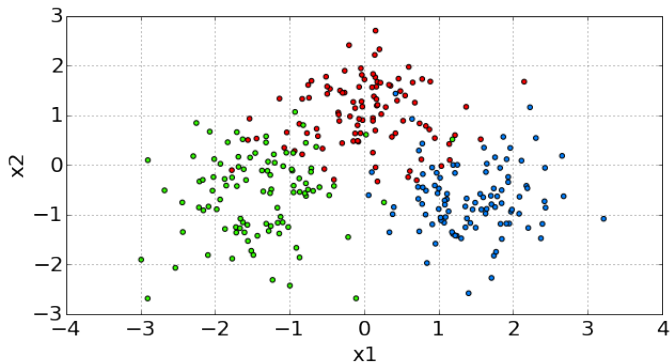
General problem statement

- Task: find a mapping f , which could accurately approximate $\mathcal{X} \rightarrow \mathcal{Y}$.
 - 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

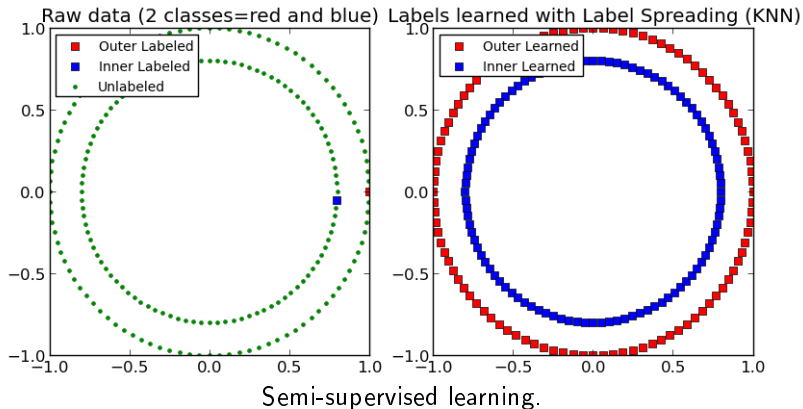
- For each new object x need to associate y .
- What is known:
 - $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$ - supervised learning:
 - x_1, x_2, \dots, x_N - unsupervised learning
 - dimensionality reduction
 - clustering
 - $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N), x_{N+1}, x_{N+2}, \dots, x_{N+M}$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

Example of supervised classification

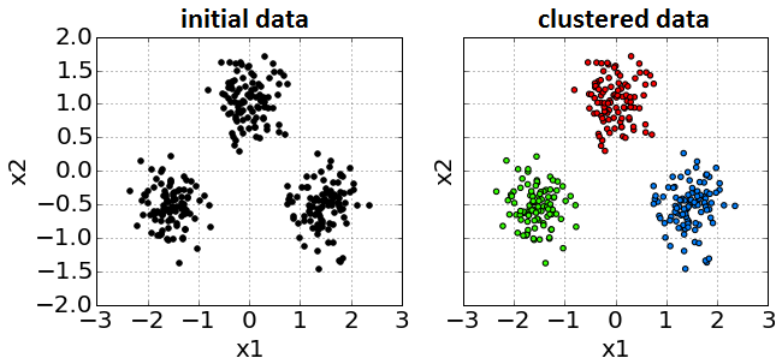


Supervised learning: $x = (x_1, x_2)$, y is shown with color

Example of semi-supervised classification

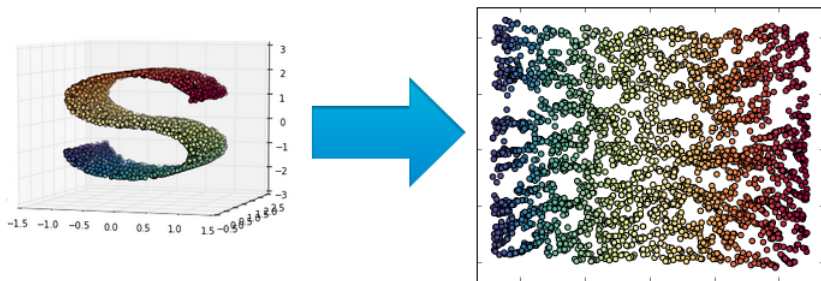


Example of clustering (unsupervised)



Unsupervised learning: clustering

Dimensionality reduction (unsupervised)



Unsupervised learning: dimensionality reduction

Generative and discriminative models¹

Generative model

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

- Can generate new observations (x, y)

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

Discriminative model

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

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

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)
 - $\mathcal{Y} = \{\omega_1, \omega_2, \dots, \omega_C\}$ - 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 $\{\omega_1, \omega_2, \dots, \omega_C\}$ - labeling
 - $\mathcal{Y} = \{y \in \mathbb{R}^C : y_i \in \{0, 1\}\}$, $y_i = 1 \Leftrightarrow$ object is associated with ω_i .

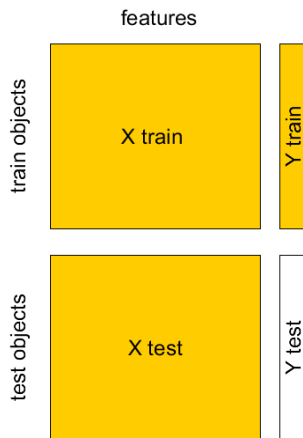
Table of Contents

- 1 Tasks solved by machine learning
- 2 Problem statement
- 3 Training / testing set.
- 4 Function class
- 5 Function estimation

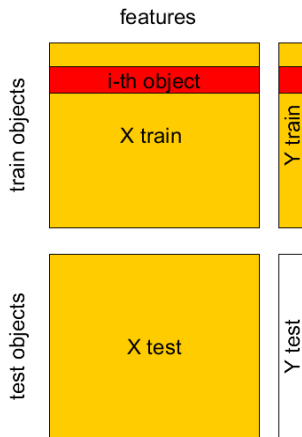
Training set

- **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 $\hat{\theta}$ of mapping $\hat{y} = f_{\theta}(x)$ so that it will approximate true relationship $y = y(x)$
- It is assumed that $z_n = (x_n, y_n)$ for $n = 1, 2, \dots, N$ - 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).

Table of Contents

- 1 Tasks solved by machine learning
- 2 Problem statement
- 3 Training / testing set.
- 4 Function class**
- 5 Function estimation

Function class. Linear example.

- **Function class** - parametrized set of functions $F = \{f_\theta, \theta \in \Theta\}$, from which the true relationship $\mathcal{X} \rightarrow \mathcal{Y}$ is approximated.

Function class. Linear example.

- **Function class** - parametrized set of functions $F = \{f_\theta, \theta \in \Theta\}$, from which the true relationship $\mathcal{X} \rightarrow \mathcal{Y}$ is approximated.
- Examples of linear class functions:
 - regression:

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

Function class. Linear example.

- **Function class** - parametrized set of functions $F = \{f_\theta, \theta \in \Theta\}$, from which the true relationship $\mathcal{X} \rightarrow \mathcal{Y}$ is approximated.
- Examples of linear class functions:
 - regression:

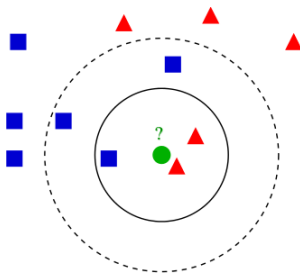
$$f(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2 + \dots + \theta_D x^D$$

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

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

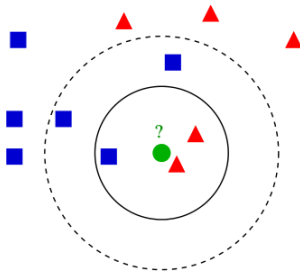
Function class. K-NN example.

Classification:

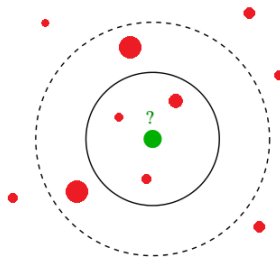


Function class. K-NN example.

Classification:



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:

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

- classification:

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

Table of Contents

- 1 Tasks solved by machine learning
- 2 Problem statement
- 3 Training / testing set.
- 4 Function class
- 5 Function estimation**

Score versus loss

- In machine learning predictions, functions, objects can be assigned:
 - **score, rating** - this should be maximized
 - **loss, cost** - this should be minimized²

²how can one convert score \leftrightarrow loss?

Loss function $\mathcal{L}(\hat{y}, y)$ ³

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

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

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

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

- MSE (mean squared error):

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

³Selecting loss is not trivial. Consider demand forecasting.

Empirical risk

- Want to minimize:

$$\int \int \mathcal{L}(f_{\theta}(x), y) p(x, y) dx dy \rightarrow \min_{\theta}$$

Empirical risk

- Want to minimize:

$$\int \int \mathcal{L}(f_{\theta}(x), y) p(x, y) dx dy \rightarrow \min_{\theta}$$

- 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:

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

Estimation of empirical risk

- Generally it holds that:

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

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

Estimation of empirical risk

- Generally it holds that:

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

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

- $L(\hat{\theta}|X', Y')$ can be estimated using :
 - separate **validation set**
 - **cross-validation**
 - **leave-one-out** method

4-fold cross validation example

X	Y
1	1
2	2
3	3
4	4

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

X	Y
1	1
2	2
3	3
4	4

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

4-fold cross validation example

X	Y
1	1
2	2
3	3
4	4

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

4-fold cross validation example

X	Y
1	1
2	2
3	3
4	4

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

4-fold cross validation example

X	Y
1	1
2	2
3	3
4	4

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: $n \in I_k$.
 - $\hat{\theta}^{-k}$ - parameter estimation using observations from all folds except fold k .

⁴will samples be correlated?

4-fold cross validation example

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

Cross-validation empirical risk estimation

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

⁴will samples be correlated?

4-fold cross validation example

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

Cross-validation empirical risk estimation

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

- For K -fold CV we have:
 - K parameters $\hat{\theta}^{-1}, \dots, \hat{\theta}^{-K}$
 - K models $f_{\hat{\theta}^{-1}}(x), \dots, f_{\hat{\theta}^{-K}}(x)$.
 - can use ensembles
 - K estimations of empirical risk:

$$\hat{L}_k = \frac{1}{|I_k|} \sum_{n \in I_k} \mathcal{L}(f_{\hat{\theta}^{-k}}(x_n), y_n), \quad k = 1, 2, \dots, K.$$
 - can estimate variance & use statistics!⁴

⁴will 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.

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

Hyperparameters selection

- Using CV we can select hyperparameters of the model⁶:
 - regression: # of features d , e.g. $x, x^2, \dots x^d$
 - K-NN: number of neighbors K

⁶can 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 $\mathcal{X} \rightarrow \mathcal{Y}$.

Too complex (overfitted) model

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

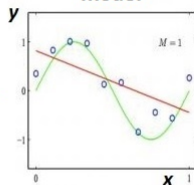
Pay attention to difference between overfitting and overfitted model. Overfitting is a typical situation when expected loss on training set is lower than expected loss on testing set. Since this is typical, all models are overfitted more (complex ones) or less (simple ones).

Examples of overfitted/underfitted models

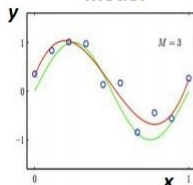
- true relationship
- estimated relationship with polynimes of order M
- objects of the training sample

regression:

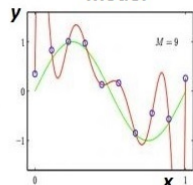
too simple model



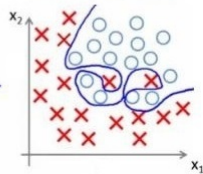
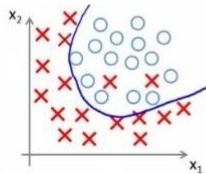
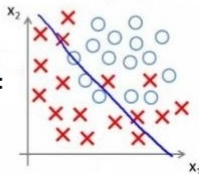
relevant model



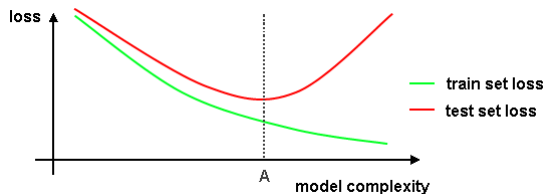
too complex model



classification:



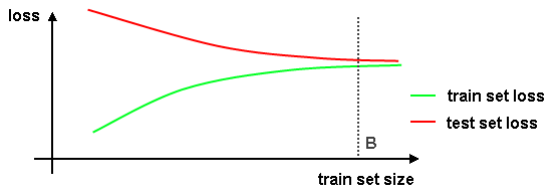
Loss vs. model complexity



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

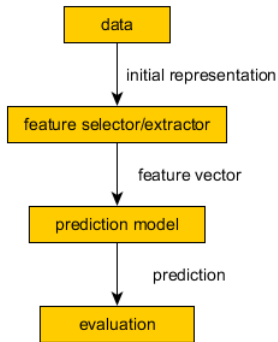
Loss vs. train set size



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

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 course⁷

- 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
- \hat{z} defines an estimate of z , based on the training set: for example, $\hat{\theta}$ is the estimate of θ , \hat{y} is the estimate of y , etc.
- r.v.=random variable, w.r.t.=with respect to, e.g.=for example.

⁷If this corresponds the context and there are no redefinitions

Notation used in the course

- $\mathcal{L}(\hat{y}, y)$ - loss function, where y is the true value and \hat{y} is the predicted value.
- $L(\theta) = \sum_{n=1}^N \mathcal{L}(f_{\theta}(x_n), y_n)$ total loss on the training set.
- $\{\omega_1, \omega_2, \dots, \omega_C\}$ - possible classes, C - total number of classes.
- $[x]_+ = \max\{x, 0\}$
- $\mathbb{I}[\text{condition}] = \begin{cases} 1, & \text{if condition is satisfied} \\ 0, & \text{if condition is not satisfied} \end{cases}$
- $\text{sign}(x) = \begin{cases} 1, & x \geq 0 \\ -1, & x < 0 \end{cases}$
- All vectors are vectors-columns, e.g. if $x \in \mathbb{R}^D$ its dimensions are $D \times 1$.
- $A \succcurlyeq 0$ means that A is a square positive semi-definite matrix
- $A \succ 0$ means that A is a square positive definite matrix