Introduction to machine learning

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Motivation

- Beautiful math.
- Direct connection of math with practice.
    - HEP in in particular
- Machine learning partly reveals how we, humans, make decisions.
- Data scientist is a specialization in high demand.

Course information

- Instructors: Victor Kitov, Alexander Panin, Sergey Shirobokov.
- Tasks of the course
- Structure:
    - lectures, seminars
    - assignments: theoretical, labs, 2 competitions
    - exam
- Tools
    - python
    - ipython notebook
    - numpy, scipy, pandas
    - matplotlib, seaborn
    - scikit-learn.

Recommended materials

- **Data Mining: The Textbook.** Charu C. Aggarwal, Springer, 2015.
- **The Elements of Statistical Learning: Data Mining, Inference, and Prediction.** Trevor Hastie, Robert Tibshirani, Jerome Friedman, 2nd Edition, Springer, 2009.
- **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, scikit-learn documentation, kaggle forum.

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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

- Spam filtering
  - if sender belongs to black-list -> spam
  - if contains phrase 'buy now' and sender is unknown -> spam
  - ...
- Part-of-speech tagger.
  - if ends with 'ed' -> verb
  - if previous word is 'the' -> noun
  - ...
- ML finds decision rules automatically with labelled data!

Formal problem statement

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

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

- Task: find a mapping f, which could accurately approximate $\mathcal{X} \to \mathcal{Y}$.
    - using a finite **known set** of objects.
    - apply model for objects from the **test set**.
- test set way be known or not.

Specification of known/test sets

Known set:

- **supervised learning**: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), ...(\mathbf{x}_N, y_N)$
  - e.g. regression, classification.
- **unsupervised learning**: $\mathbf{x}_1, \mathbf{x}_2, ...\mathbf{x}_N$ -
  - e.g. dimensionality reduction, clustering, outlier analysis
- **semi-supervised learning**: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), ...(\mathbf{x}_N, y_N)$, $\mathbf{x}_{N+1}$, $\mathbf{x}_{N+2}, ...\mathbf{x}_{N+M}$

If test set objects $\mathbf{x}'_1$, $\mathbf{x}'_2$, $...\mathbf{x}'_K$ are known in advance, then this is **transductive learning**.

Reinforcement learning

- **Reinforcement learning** setup:
    - a set of environment and agent states S;
    - a set of actions A, of the agent
    - $P(s_{t+1} = s' | s_t = s, a_t = a)$ is the probability of transition from state s to state s' under action a.
    - $R_a(s, s')$ is the (expected) immediate reward after transition from s to s' with action a.
    - rules that describe what the agent observes
        - full / partial observability
- Well-suited to problems which include a long-term versus short-term reward trade-off
- Applications: robot control, elevator scheduling, games (chess, go), etc.

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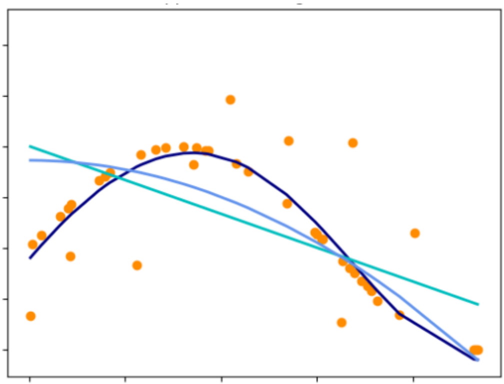
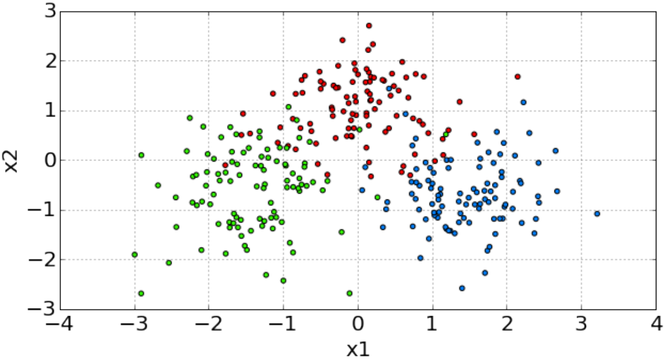
2 Visual examples
- Supervised learning
- Unsupervised learning

Regression



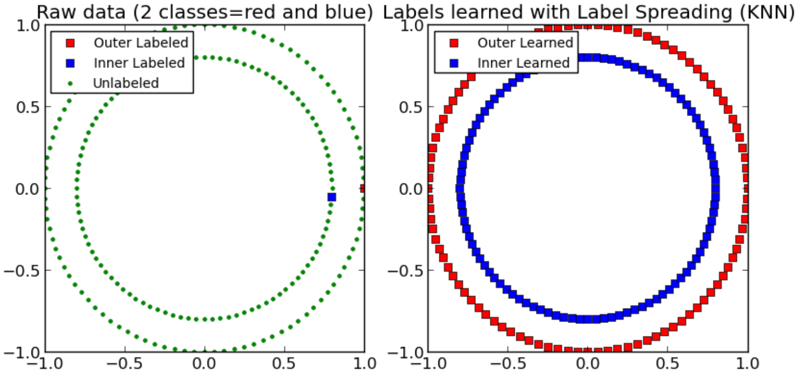
Predict $y \in \mathbb{R}$ for any x.

Classification



Predict class y shown with color for any point.

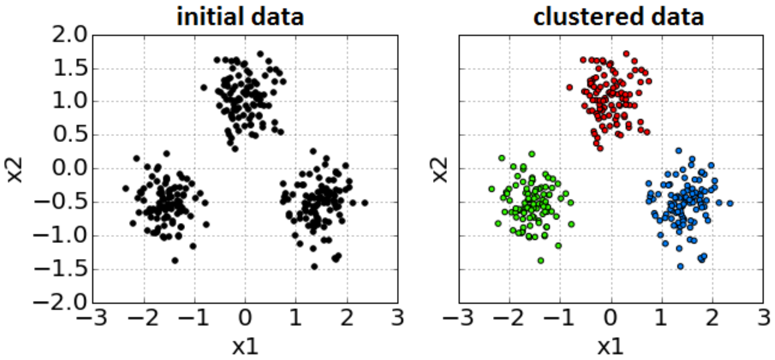
Semi-supervised classification



Semi-supervised learning.

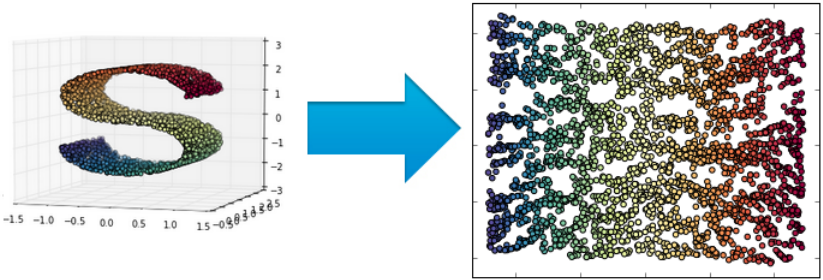
2. Visual examples
   - Supervised learning
   - Unsupervised learning

Clustering



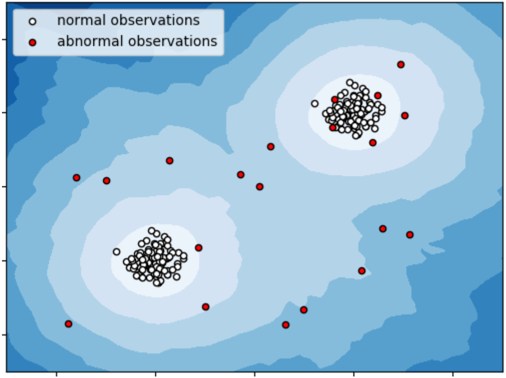
Cluster points into distinct similarity groups.

Dimensionality reduction



Reduce dimension from 3D to 2D with minimal distortion.

Outlier detection



Detect untypical observations.

General problem statement

- We want to find $f(x) : X \to Y$.
- How it may be used:
  - prediction of Y
  - qualitative analysis, understanding of $X \to Y$ dependency
  - untypical objects detection (where model fails)
- Questions solved in ML:
  - what target y we are predicting?
  - how to select object descriptors (features) x?
  - what is the kind of mapping f?
  - in what sense a mapping f should approximate true relationship?
  - how to tune f?

Types of target variable (supervised learning)[2]

- $\mathcal{Y} = \mathbb{R}$ - regression
  - e.g. flat price
- $\mathcal{Y} = \mathbb{R}^M$ - vector regression
  - e.g. stock price dynamics
- $\mathcal{Y} = \{\omega_1, \omega_2, ...\omega_C\}$ - classification.
  - C=2: binary classification.
    - e.g. spam / not spam
  - C>2: multi-class classification
    - e.g. identity recognition, activity recognition
- $\mathcal{Y}$ - set of all sets of $\{\omega_1, \omega_2, ...\omega_C\}$ - labeling.[1]
  - e.g. news categorization

[1] How to solve labeling using classification?

[2] Actually any type is possible. Listed are most common types.

Types of features[3]

- Full object description $\mathbf{x} \in \mathcal{X}$ consists of individual features $x^i \in \mathcal{X}_i$
- Types of feature (e.g. for credit scoring):
  - $\mathcal{X}_i = \{0, 1\}$ - binary feature
    - e.g. marital status
  - $|\mathcal{X}_i| < \infty$ - categorical (nominal) feature
    - e.g. occupation
  - $|\mathcal{X}_i| < \infty$ and $\mathcal{X}_i$ is ordered - ordinal feature
    - e.g.education level
  - $\mathcal{X}_i = \mathbb{R}$ - real feature
    - e.g. age

[3] Actually any type is possible. Listed are most common types.

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Function class. Linear example.

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

[4] Are discriminant functions uniquely defined for fixed mapping $X \to Y$?

Function class. Linear example.

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

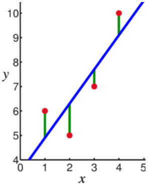
- **Regression**: $\widehat{y} = f(x|\theta)$,
- **Classification**: $\widehat{y} = f(x|\theta) = \arg\max_c \{g_c(x|\theta)\}$, $c = 1, 2, ...C$.
    - $c = 1, 2, ...C$: possible classes, $g_c(x)$ - score of class c, given x called *discriminant function*[4].

[4] Are discriminant functions uniquely defined for fixed mapping $X \to Y$?

Examples

linear regression $y \in \mathbb{R}$:

$$f(x|\theta) = \theta_0 + \theta_1 x$$



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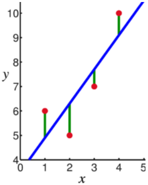
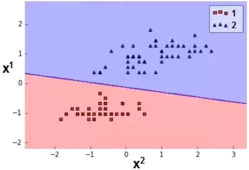


linear classification $y \in \{1, 2\}$:

$$g_c(\mathbf{x}|\theta) = \theta_c^0 + \theta_c^1 x^1 + \theta_c^2 x^2, \; c = 1, 2.$$

$$f(\mathbf{x}|\theta) = \arg\max_c g_c(x|\theta)$$



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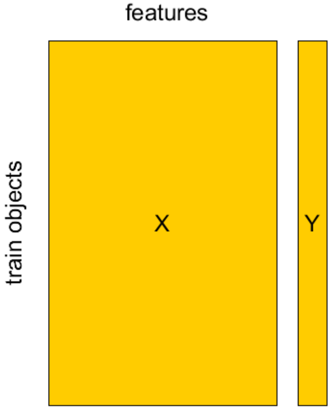
Known set

Known set: $(\mathbf{x}_1, y_1), ...(\mathbf{x}_M, y_M)$,
design matrix $X = [\mathbf{x}_1, ...\mathbf{x}_M]^T$, $Y = [y_1, ...y_M]^T$.



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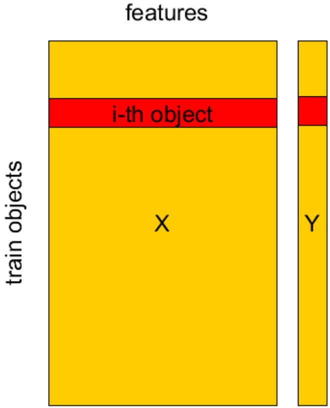

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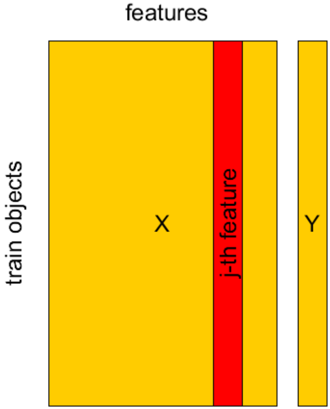
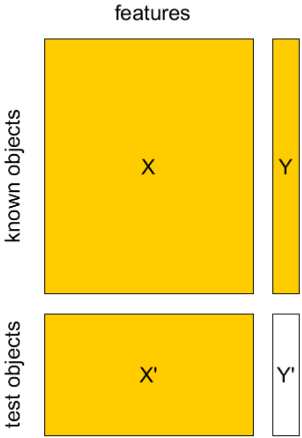


Known set, test set

- Known sample X, Y: $(\mathbf{x}_1, y_1), ...(\mathbf{x}_M, y_M)$
- Test sample X', Y': $(\mathbf{x}_1', y_1'), ...(\mathbf{x}_K', y_K')$



Score versus loss

- In machine learning predictions, functions, objects can be assigned:
  - **score, rating** - this should be maximized
  - **loss, cost** - this should be minimized[5]

[5] how can one convert score$\leftrightarrow$loss?

Loss function $\mathcal{L}(\widehat{y}, y)$[6]

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

[6] Selecting realistic loss is not trivial. Consider e.g. demand forecasting.

Empirical risk

- Want to minimize *expected risk*:

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

[7] We assume that objects are i.i.d.

Empirical risk

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

- Can minimize only *empirical risk*[7]:

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

- Method of empirical risk minimization:

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

[7] We assume that objects are i.i.d.

Estimation of empirical risk

- What is the relationship between $L(\widehat{\theta}|X,Y)$ and $L(\widehat{\theta}|X',Y')$?

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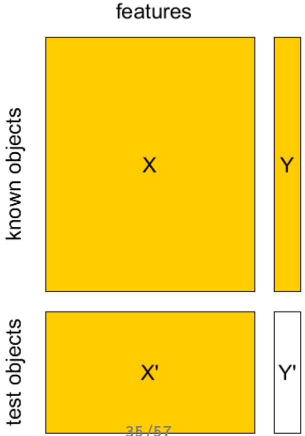
- Typically
$$L(\widehat{\theta}|X,Y) < L(\widehat{\theta}|X',Y')$$
- How to get realistic estimate of $L(\widehat{\theta}|X',Y')$?
    - separate **validation set**
    - **cross-validation**
    - **leave-one-out** method

4. Function estimation
   - Separate validation set
   - Cross-validation
   - A/B testing

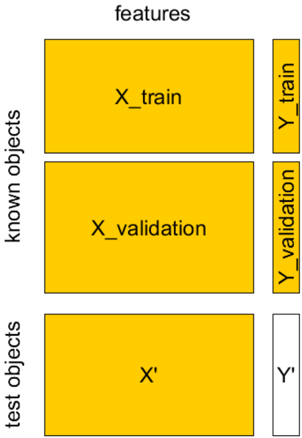
Separate validation set

- Known sample X, Y: $(\mathbf{x}_1, y_1), ...(\mathbf{x}_M, y_M)$
- Test sample X', Y': $(\mathbf{x}_1', y_1'), ...(\mathbf{x}_K', y_K')$



Separate validation set

Divide known set randomly or randomly with stratification:



4 Function estimation

- Separate validation set
- Cross-validation
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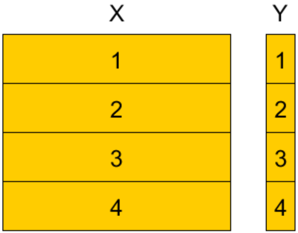
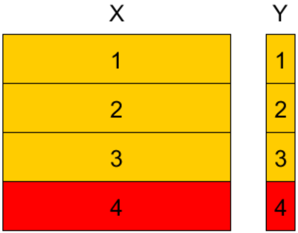
4-fold cross-validation example



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

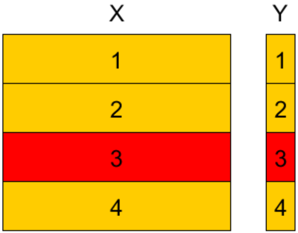
- randomly
- randomly with stratification (w.r.t target value or feature value).

4-fold cross validation example



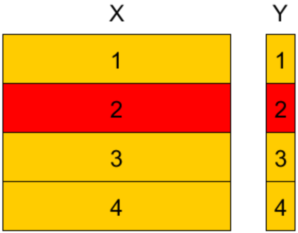
Use folds 1,2,3 for model estimation and fold 4 for model evaluation.

4-fold cross validation example



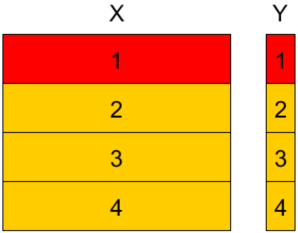
Use folds 1,2,4 for model estimation and fold 3 for model evaluation.

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

[8] 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 $\widehat{\theta}^{-1}, \dots \widehat{\theta}^{-K}$
    - K models $f_{\widehat{\theta}^{-1}}(\mathbf{x}), \dots f_{\widehat{\theta}^{-K}}(\mathbf{x})$.
        - can use ensembles
    - K estimations of empirical risk: $\widehat{L}_k = \frac{1}{|I_k|} \sum_{n \in I_k} \mathcal{L}(f_{\widehat{\theta}^{-k}}(\mathbf{x}_n),\ y_n),\ k = 1, 2, \dots K.$
        - can estimate variance & use statistics![8]

[8] 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.[9] property of observations
- Stratification by target y helps for imbalanced/rare classes.

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

4. Function estimation
   - Separate validation set
   - Cross-validation
   - A/B testing

A/B testing

- Observe test set **after the models were built**.
- A/B testing procedure:
  1. divide test objects randomly into two groups - A and B.
  2. apply base model to A
  3. apply modified model to B
  4. compare final results

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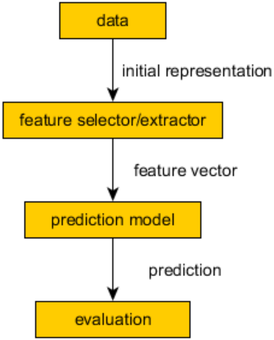
Cross-validation vs. A/B testing

Comparison of cross-validation and A/B test:

	cross-validation	**A/B test**
realism	use retrospective analysis, rely on i.i.d. assumption	full realism
overfitting	possible (when use it multiple times)	almost impossible (possible if A/B split is inadequate)
costs	uses available data, only computational costs	requires time and resources for collecting & evaluating feedback from objects of groups A and B

- When forecast affects true outcome (e.g. in recommender system) A/B test is more adequate.

General modelling pipeline



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

Major niches of ML

- hard to formulate explicit rules
    - complex inter-relationships
        - e.g. image recognition
    - too many attributes
        - e.g. text categorization
- fine-tuning performance on huge datasets
    - e.g. threshold for credibility in credit scoring
- fast adaptation to changing conditions
    - e.g. stock prices/volatility prediction
- further adaptation to usage conditions is required
    - e.g. voice detection

Examples of ML applications by domain

- WEB
  - Web-page ranking
  - Spam filtering
    - e-mails, web pages in search results
- Computer networks
  - Authentication systems
    - by voice, face, fingerprint
    - by behavior
  - Intrusion detection
- Business
  - Fraud detection
  - Churn prediction
- Banking
  - Credit scoring
  - Stock prices forecasting
  - Risks estimation

Examples of ML applications by data type

- 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

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

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Notation used in the course[10]

- **Objects and outputs:**
  - 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
- **General definitions:**
  - D - dimensionality of the feature space: $x \in \mathbb{R}^D$
  - N - the number of objects in the training set
  - C - total number of classes in classification.
  - Possible classes: $\{1, 2, ...C\}$ or $\{\omega_1, \omega_2, ...\omega_C\}$

[10] If this corresponds the context and there are no redefinitions

Notation used in the course

- **Training set:**
  - X - design matrix, $X \in \mathbb{R}^{NxD}$
  - $Y \in \mathbb{R}^N$ - target characteristics of a training set
- **Optimization:**
  - $\mathcal{L}(\widehat{y}, y)$ - loss function for 1 object
    - y is the true value and $\widehat{y}$ is the predicted value.
  - $L(\theta) = \sum_{n=1}^{N} \mathcal{L}(f_\theta(x_n), y_n)$ loss function for the whole the training set.

Notation used in the course

- **Special functions:**
  - $[x]_+ = \max\{x, 0\}$
  - $\mathbb{I}[\text{condition}] = \begin{cases} 1, & \text{if condition is satisfied} \\ 0, & \text{if condition is not satisfied} \end{cases}$
  - $\text{sign}(x) = \begin{cases} 1, & x \geq 0 \\ -1, & x < 0 \end{cases}$
- **Other definitions:**
  - $\widehat{z}$ 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.
  - r.v.=random variable, w.r.t.=with respect to, e.g.=for example.
  - $A \succcurlyeq 0$ means that A is a square positive semi-definite matrix.
- All vectors are vectors-columns, e.g. if $x \in \mathbb{R}^D$ its dimensions are Dx1.

Summary

- Machine learning algorithms reconstruct relationship between features x and outputs y.
- Relationship is reconstructed by optimal function $\widehat{y} = f_{\widehat{\theta}}(x)$ from function class $\{f_\theta(x), \theta \in \Theta\}$.
- θ is particular controls model complexity, models may be too simple and too complex.
- $\widehat{\theta}$ selected to minimize empirical risk $\frac{1}{N}\sum_{n=1}^{N}\mathcal{L}(f_\theta(x_n), y_n)$ for some loss function $\mathcal{L}(\widehat{y}, y)$.
- Overfitting - non-realistic estimate of expected loss on the training set.
- To avoid overfitting - use validation sets, cross-validation, A/B test.