Lecture 3

Distance-based classifiers

Machine Learning

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Lecture plan

- Distance-based classifiers (1NN)
- Parameters tuning
- Generalized distance-based classifiers
- Prototype selection
- Anomaly detection

- The presentation is partly prepared with materials of the K.V. Vorontsov’s course “Machine Leaning”.
- Slides are available online: **goo.gl/Wkif2w**

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Problem formulation

X is an object set, Y is an answer set,
$y : X \to Y$ is an unknown dependency, $|Y| \ll \infty$
$X^\ell = \{x_1, \dots, x_n\}$ is a training sample,
$T^\ell = \{(x_1, y_1), \dots, (x_\ell, y_\ell)\}$ is a set of examples.

Task: return an algorithm $a : X \to Y$.

What is this task?

Classification problem formulation

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Task: return an algorithm $a : X \to Y$.

What is this task?

Classification, because $|Y| \ll \infty$.

Duck test

Duck test:

If it looks like a duck, swims like a duck, and quacks like a duck, then it probably is a duck.

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Duck test: *if it looks like a duck, swims like a duck, and quacks like a duck, then it probably is a duck.*

	Looks	Swims	Quacks	A duck?
	like a duck	like a duck	like a duck	**Probably, a duck**
	totally not like a duck	can be a duck	not like a duck	**Probably, not a duck**

How is the classifier formalized?

What is the training sample?

Many ducks, many non-ducks (unducks).

What is classification procedure?

1. Ducks were described with **key features**.
2. **Similarity concept** was used.
3. Logical separator was used for classification.

Main idea

Key hypothesis: similar objects belong to same class.

Main idea: for an object we have to find a class, in which objects are the most similar to the given one.

- Reasoning by analogy (case-based)
- Lazy learning

Formalization of “similarity”

“Similarity” is a distance between objects. We will talk about **metrics**.

Distance: $\rho: X \times X \to [0; +\infty)$.

Metric space is a set with a metric $\rho(x, y)$, defined on it.

Commonly used metrics

Minkowski distance:

$$p(x,y) = \left(\sum_i |x_i - y_i|^p\right)^{\frac{1}{p}},$$

when $p = 2$, it is the Euclidian distance;

when $p = 1$, it is the Manhattan distance.

Mahalanobis distance:

$$p(x,y) = \sqrt{(x-y)^\top S^{-1}(x-y)},$$

where S is covariance matrix for x and y.

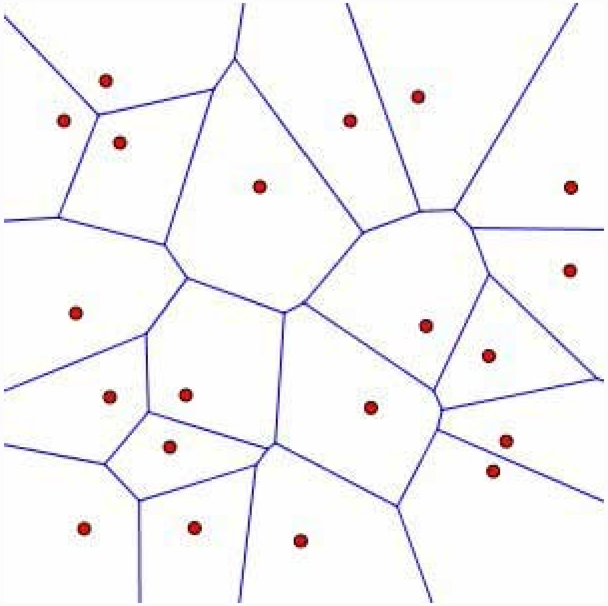
Nearest neighbor method (1NN)

$x_{(u,1)}$ is **nearest neighbor of** u: $x_{(u,1)} = \operatorname{argmin}_{x \in X^\ell} \rho(u, x)$.

Classifier:

$$a(u, T^\ell) = y_{(u,1)}.$$

Voronoi diagram:



1NN discussion

Advantages:
- simplicity;
- lucidity;
- interpretability.

Disadvantage:
- sensibility to noise;
- low efficacy;
- no parameters (explicitly);
- necessity to store all the examples.

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Hold-out validation

Hold-out validation, HO

Split training sample into two parts:

$$T^{\ell} = T^{t} \cup T^{\ell-t}$$

Train, T^{t}	Test, $T^{\ell-t}$

Solve the optimization problem:

$$\mathrm{HO}\left(\mu, T^{t}, T^{\ell-t}\right) = Q\left(\mu(T^{t}), T^{\ell-t}\right) \to \min$$

Complete cross-validation

Choose value of t.

Split the sample with all the possible ways on T^t and $T^{\ell-t}$.

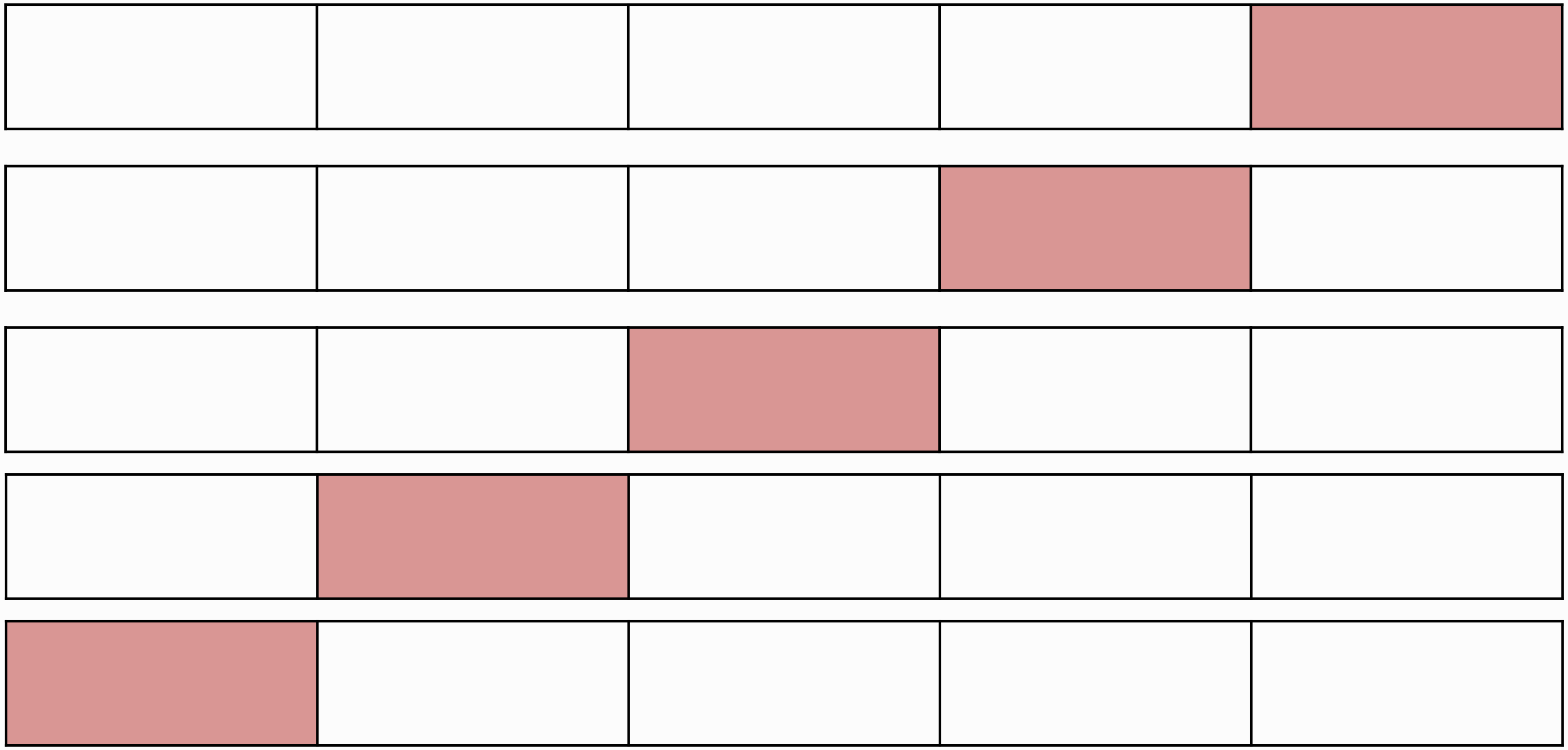
Train, T^t	Test, $T^{\ell-t}$

Solve the optimization problem:

$$\mathrm{CVV}_t = \frac{1}{C_\ell^{\ell-t}} \sum_{T^\ell = T^{\ell-t} \cup T^t} Q\left(\mu(T^t), T^{\ell-t}\right) \to \min$$

Cross-validation

Split sample to k parts k times



k-fold cross-validation

k-fold cross-validation

Each of k blocks is a test sample once.

k is usually 10 (5 is small sample size).

Split $T^\ell = F_1 \cup \ldots \cup F_k$, $|F_i| \approx \frac{\ell}{k}$.

Solve the optimization problem:

$$\mathrm{CV}_k = \frac{1}{k} \sum_{i=1}^{k} Q\big(\mu(T^\ell \setminus F_i), F_i\big) \to \min.$$

$t \times k$-fold cross-validation

Repeat t times: split sample on k blocks, each of k blocks is a test sample once.

k is usually 10, t is usually 10 or less.

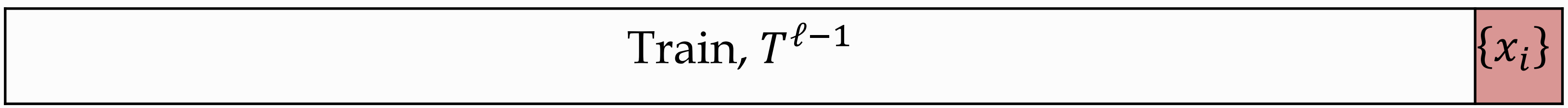
Split T^ℓ t times randomly:
$T^\ell = F_{(1,1)} \cup \dots \cup F_{(k,1)} = \dots = F_{(1,t)} \cup \dots \cup F_{(k,t)}$,
$|F_{(i,j)}| \approx \frac{\ell}{k}$.
Solve the optimization problem:

$$\mathrm{CV}_{t\times k} = \frac{1}{tk} \sum_{j=1}^{t} \sum_{i=1}^{k} Q\left(\mu\left(T^\ell \backslash F_{(i,j)}\right), F_{(i,j)}\right) \to \min.$$

Leave one out

Leave-one-out cross-validation, LOO

Split sample into $\ell - 1$ and 1 objects ℓ times.



Solve the optimization problem:

$$\mathrm{LOO} = \frac{1}{\ell}\sum_{i=1}^{\ell} Q\left(\mu\left(T^{\ell}\backslash p_i\right), p_i\right) \to \min.$$

where $p_i = (x_i, y_i)$.

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How can it be improved?

- More complicated model (more parameters)
- Distance choosing
- Dimension reduction
- Usage of good structures for storing data
- Object set thinning
- Noise filtering
- Prototype selection

kNN

Choose a distance ρ.

Sort objects:

$$\rho\left(u, x_{(u,1)}\right) \leq \rho\left(u, x_{(u,2)}\right) \leq \cdots \leq \rho\left(u, x_{(u,\ell)}\right).$$

Algorithm kNN:

$$a\left(u; T^{\ell}\right) = \operatorname{argmax}_{y \in Y} \sum_{i=1}^{\ell} [y(u,i) = y][i \leq k],$$

$$a\left(u; T^{\ell}\right) = \operatorname{argmax}_{y \in Y} \sum_{i=1}^{k} [y(u,i) = y].$$

Optimization of k

Is equal to the problem of LOO quality functional minimization:

$$\mathrm{LOO}(k, T^{\ell}) = \sum_{i=1}^{\ell} \left[a\left(x_i; T^{\ell} \backslash \{(x_i, y_i)\}, k\right) \neq y_i \right] \to$$

$$\to \min_k$$

Generalized metric classifier

$$a\left(u; T^{\ell}\right) = \operatorname{argmax}_{y \in Y} \sum_{i=1}^{\ell} [y(u,i) = y] w(i,u),$$

where $w(i,u)$ is a function representing importance of ith neighbor of u.

$C_y(u) = \sum_{i=1}^{\ell} [y(u,i) = y] w(i,u)$ is estimation of object u closeness to class y.

$$a\left(u; T^{\ell}\right) = \operatorname{argmax}_{y \in Y} \sum_{i=1}^{\ell} C_y(u).$$

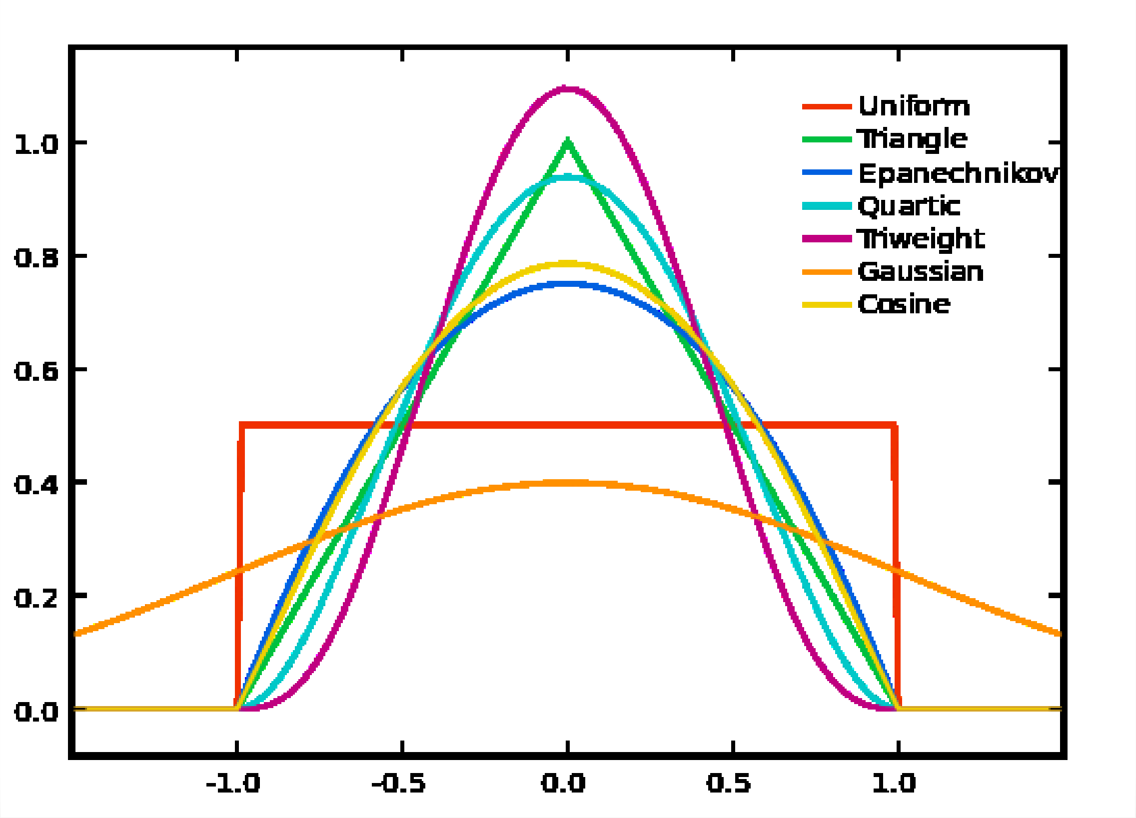
What can be chosen as w?

$w(i, u)$:

- linearly decreasing functions;
- exponentially decreasing functions;
- kernel functions.

Kernel function

Kernel function $K(x)$ is symmetric non-negative function, $\int_{-\infty}^{+\infty} K(x)\,dx = 1$.



Parzen-Rosenblatt window

With fixed window width:

$$a(u; T^\ell; h; K) =$$

$$= \mathrm{argmax}_{y \in Y} \sum_{i=1}^{\ell} [y(u,i) = y] K\left(\frac{\rho(u, x_{(u,i)})}{h}\right),$$

With variable window width:

$$a(u; T^\ell; k; K) =$$

$$= \mathrm{argmax}_{y \in Y} \sum_{i=1}^{\ell} [y(u,i) = y] K\left(\frac{\rho(u, x_{(u,i)})}{\rho(u, x_{(u,k+1)})}\right).$$

Parzen-Rosenblatt window

With fixed window width:

$$a(u; T^\ell; h; K) =$$

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Distance selection (learning)

Distance can be learned.

Example (weighted Minkowski):

$$p(x,y) = \left(\sum_i w_i |x_i - y_i|^p\right)^{\frac{1}{p}}.$$

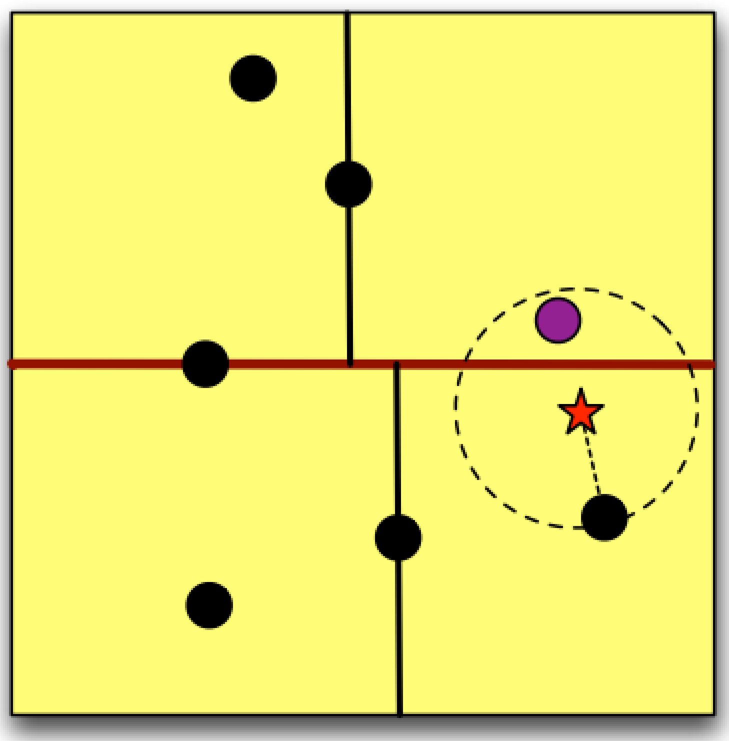
Now the problem is how to choose coefficients w_i.

When $w_i = 0$, the feature is thrown away (feature selection).

A kernelization can be applied.

Structure for storing data

Different greed-like structures can be used. The most effective is ***k-d*-trees**:



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Margin

Margin of object x_i with respect to algorithm $a(u)$:

$$M(x_i) = C_{y_i}(x_i) - \max_{y \in Y \setminus \{y_i\}} C_y(x_i).$$

Margin is the measure of object "typicalness" for its class. The higher margin is, the more typical the object is.

Ranking based on margin

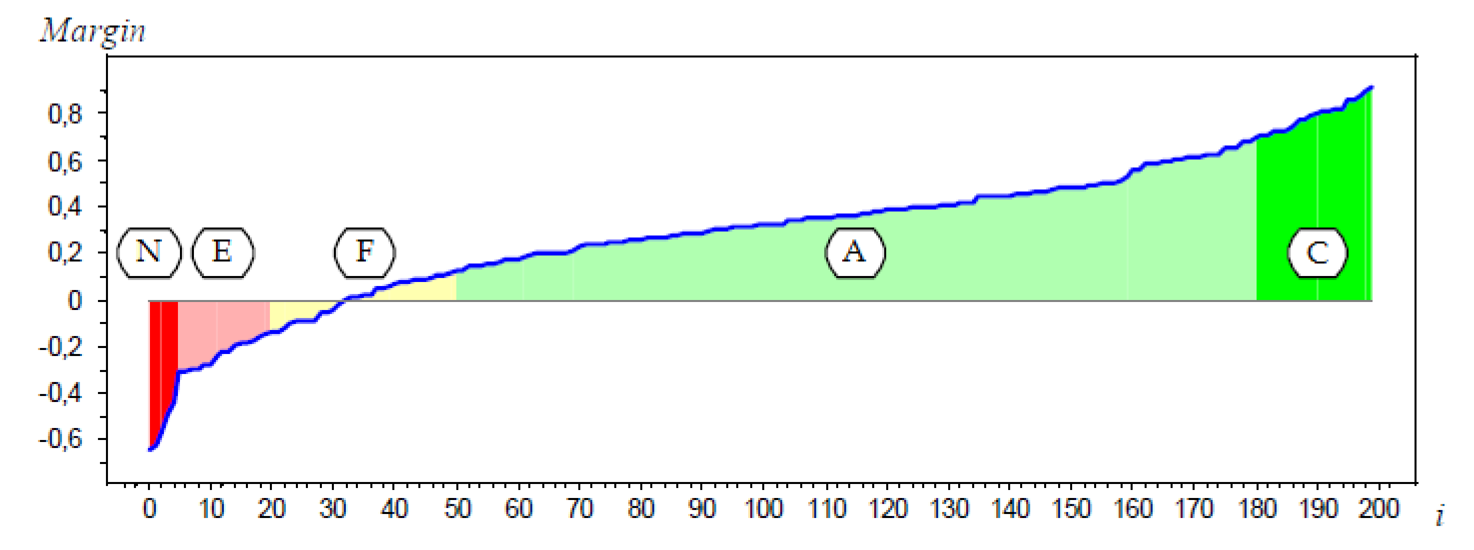
C — **core** (base for classification)

A — **accompaniment** (can be deleted)

F — **frontier** (classification is instable)

E — **erroneous** (misclassification because of bad model)

N — **noisy** (misclassification because of bad data)



Prototype selection problem

Prototype selection problem is how to choose optimal subset of object $\Omega \subseteq X^\ell$.

Distance-based classifier:

$$a(u; \Omega) = \operatorname{argmax}_{y \in Y} \sum_{x_i \in \Omega} [y(u, i) = y] w(i, u).$$

Prototype selection solutions

The problem is NP-hard, so there are lots of approximate solutions.

Two main approaches:

1) linear programming relaxation;
2) greedy algorithms.

Plenty of heuristic approaches.

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What is classification procedure?

1. Ducks were described with **key features**.
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One-class classification problem

The duck test in one-class classifier: we can make suggestions only about belonging to a certain class (ducks). Nothing is said about other classes.

Anomaly (outlier, exception, surprise) **detection** is the problem of one-class classification.

More precise definition

The definition is determined by the class of problems we solve:

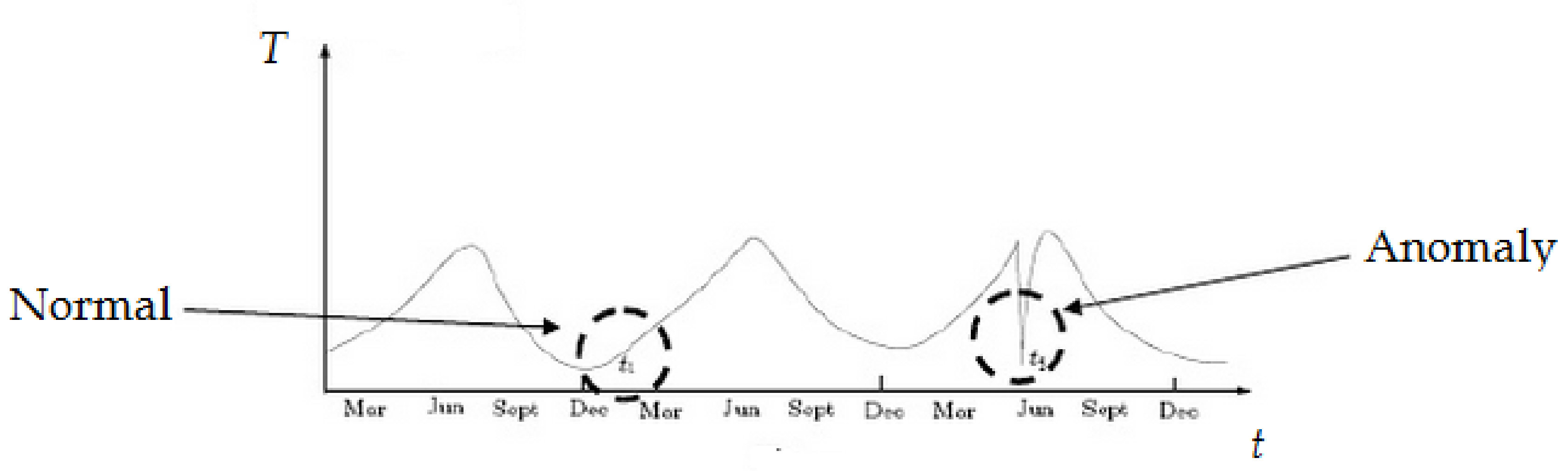
- Labels are known for positive and negative examples: **supervised** rare-class detection.
- Labels are known only for positive examples: **semi-supervised** learning.
- Labels are unknown: **unsupervised** small-cluster detection.

Anomaly detection taxonomy

- Point anomaly detection
- Contextual anomaly detection
- Collective anomaly detection

Contextual anomaly detection

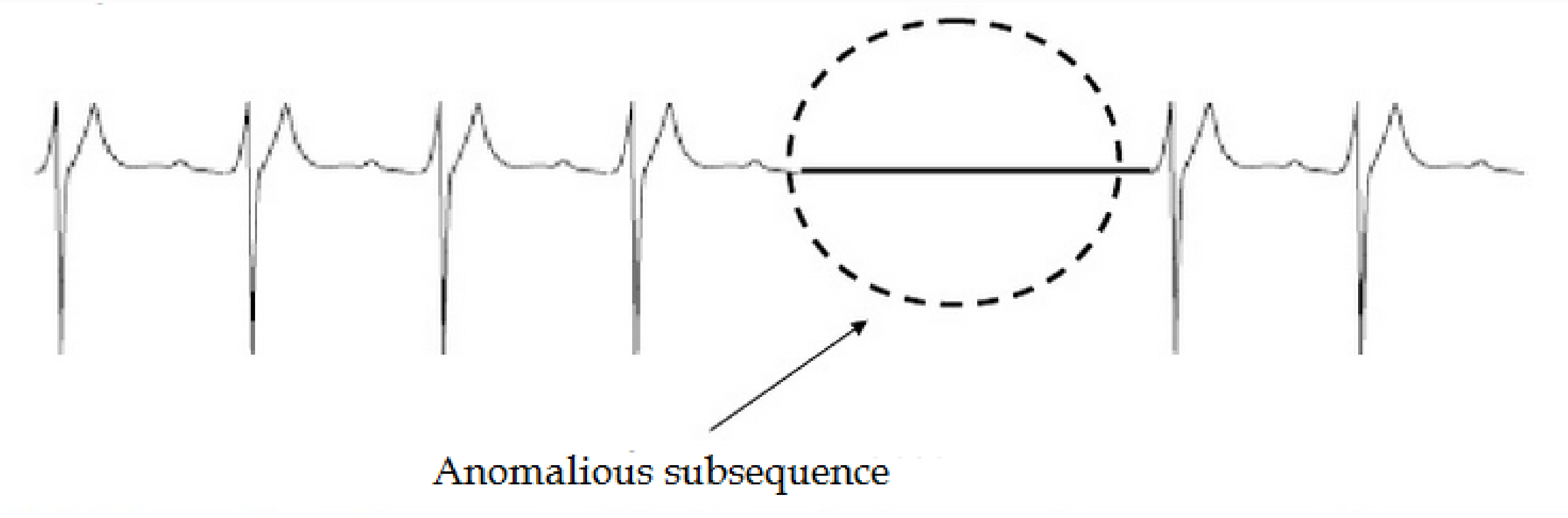
Assumption: all normal instances within a context will be similar (in terms of behavioral attributes), while the anomalies will be different.



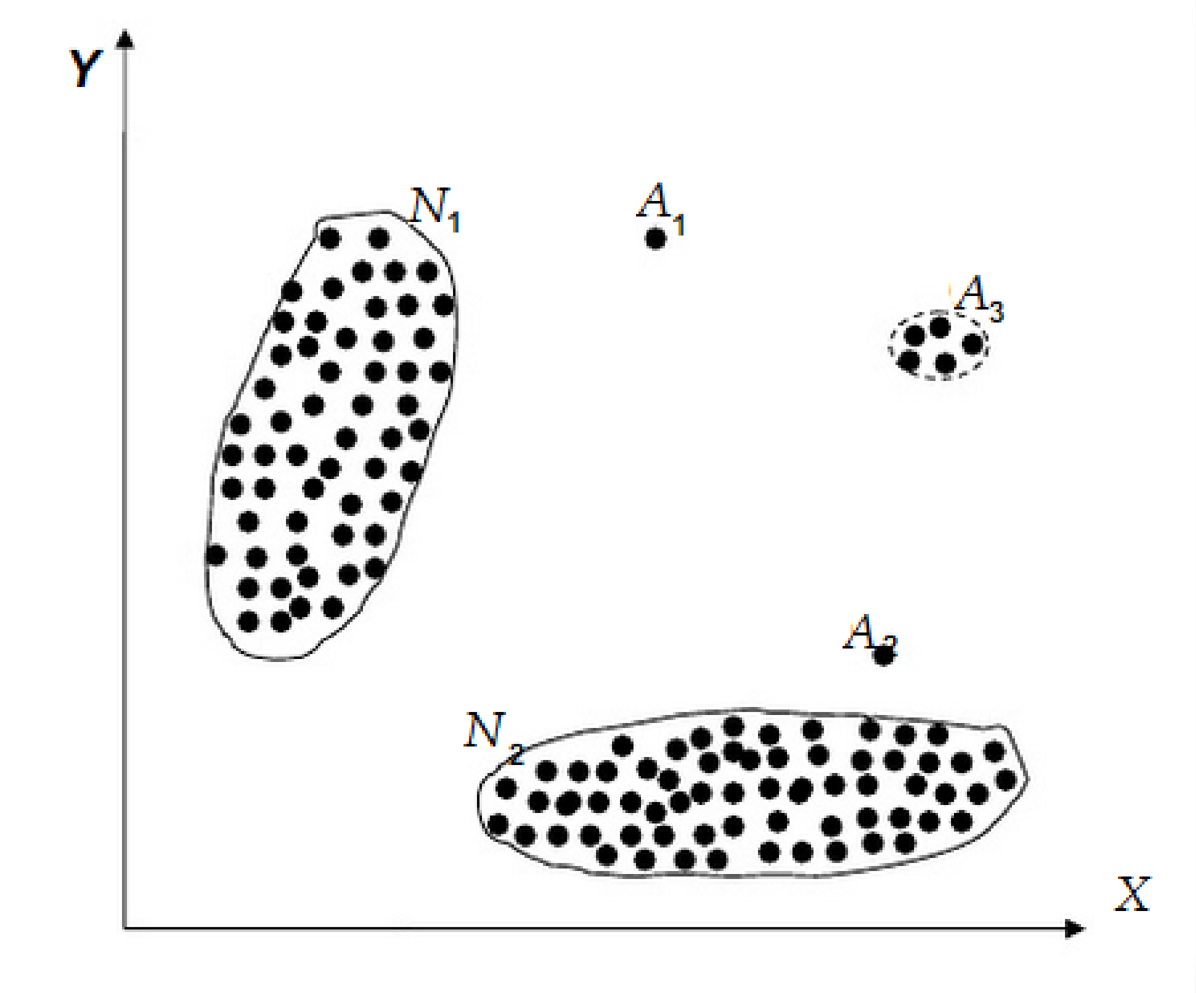
Collective anomaly detection

Data instances are related:

- sequential data
- spatial data
- graph data



Point anomaly detection



NN anomaly detection

Two types of methods:

- **distance based methods**: anomalies are data points most distant from other points
- **density based methods**: anomalies are data points in low density regions