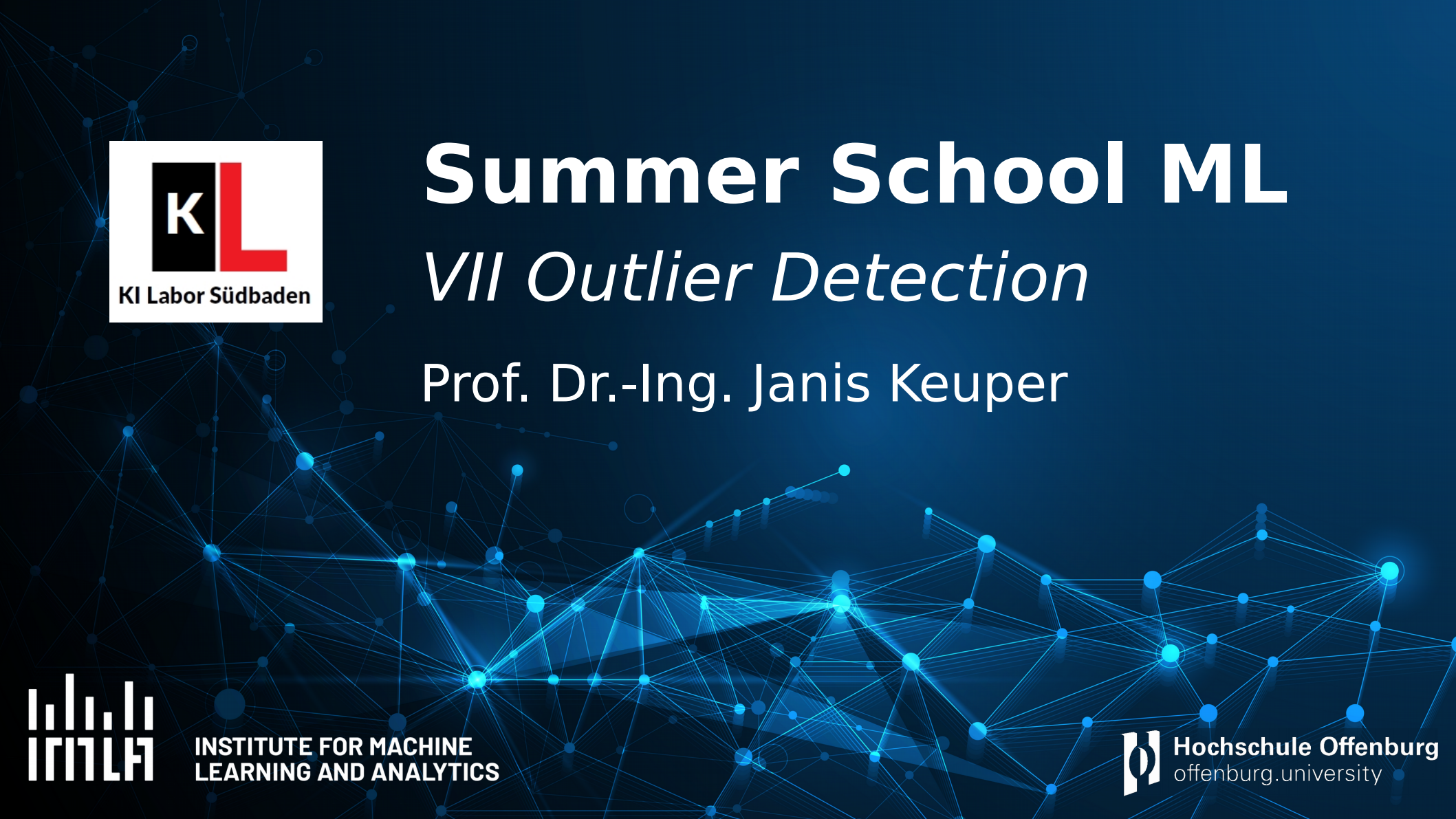

KI Labor Südbaden
Summer School ML
VII Outlier Detection
Prof. Dr.-Ing. Janis Keuper
INSTITUTE FOR MACHINE
LEARNING AND ANALYTICS
Hochschule Offenburg
offenburg.university

Outlier Detection

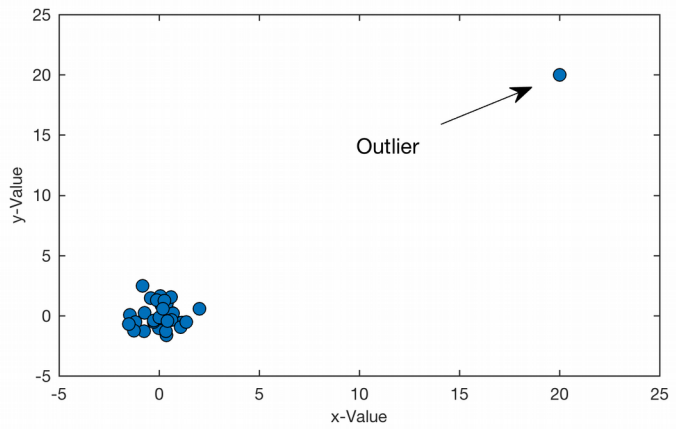
KI Labor Südbaden

Outline

- **Motivation**
- **Traditional ML Methods**
  - DB-Scan Clustering
  - One-Class SVMs
  - Isolation Forests
- **Deep Learning Methods**
  - Auto Encoder

Motivation

Outlier Detection



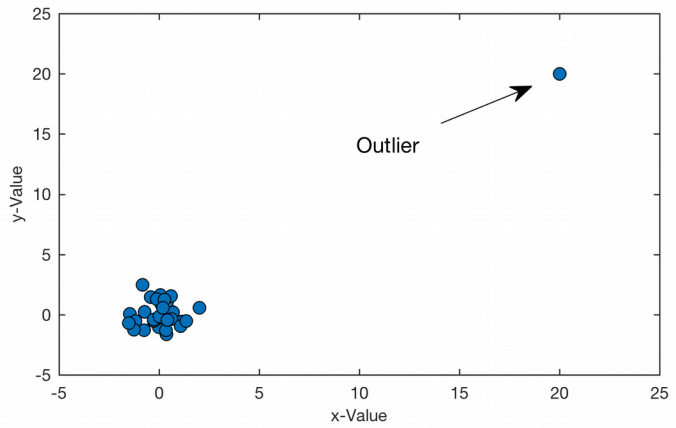
Oversimplification

Machine Learning / Data Mining so far…

- We used supervised and unsupervised methods to learn from data
- Constraint: given training data needs to be a (statistically) good representation of the problem → generalization
- Works well for many applications ...

Motivation

Outlier Detection



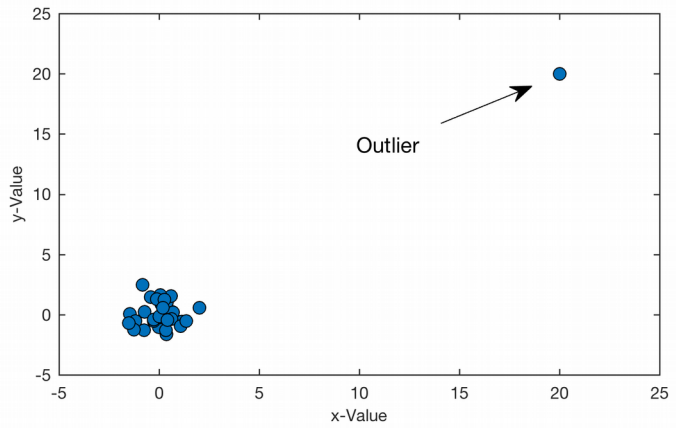
Oversimplification

But, what if we are looking to detect things that we have not seen before ?

- Only “good” examples
- No or only a few “bad” examples
- **Applications:**
  - Find faulty parts (production QC)
  - Find Malware
  - Find Intruders
  - ...

Motivation

Outlier Detection



Oversimplification

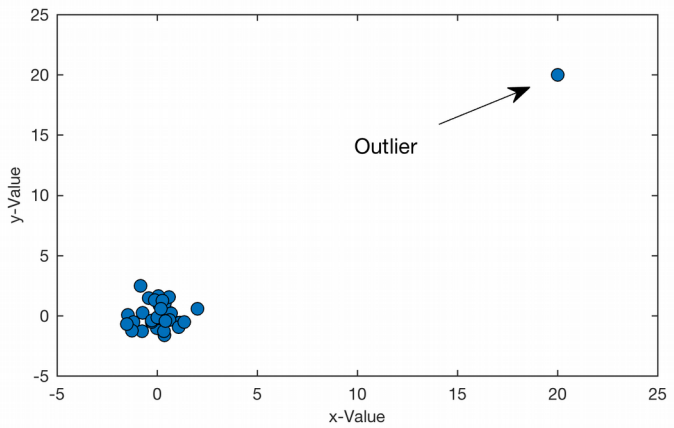
But, what if we are looking to detect things that we have not seen before ?

- Only “good” examples
- No or only a few “bad” examples
- **Applications:**
  - Find faulty parts (production QC)
  - Find Malware
  - Find Intruders
  - ...

→ learn “what is normal” and detect derivations (=outliers)

Motivation

Outlier Detection



Oversimplification

Definition [Wikipedia]

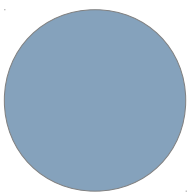
- *"In statistics, an **outlier** is a data point that differs significantly from other observations. An outlier may be due to variability in the measurement or it may indicate experimental error; the latter are sometimes excluded from the data set."*

- *"In data mining, **anomaly detection** (also outlier detection) is the identification of rare items, events or observations which raise suspicions by differing significantly from the majority of the data."*

Outliers with Machine Learning

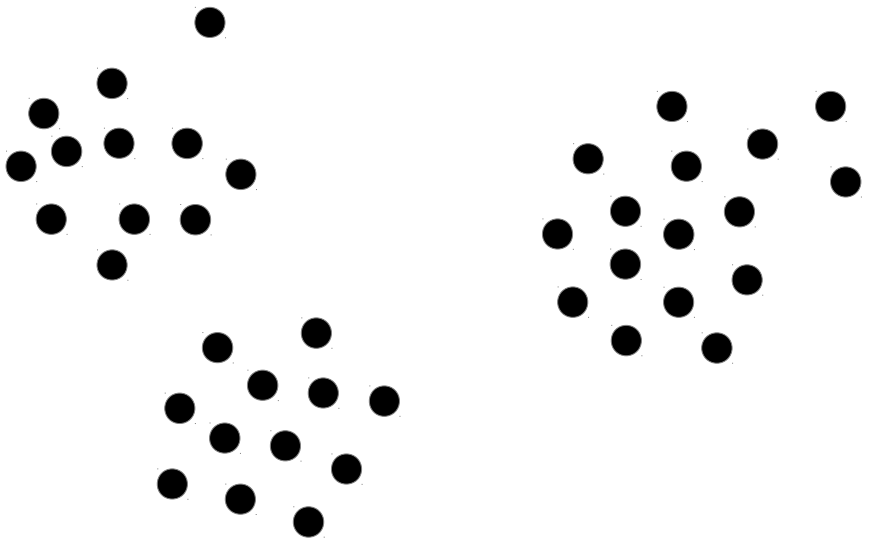
Using DBSCAN clustering [see ML 1 in block 1]

Init:



ε

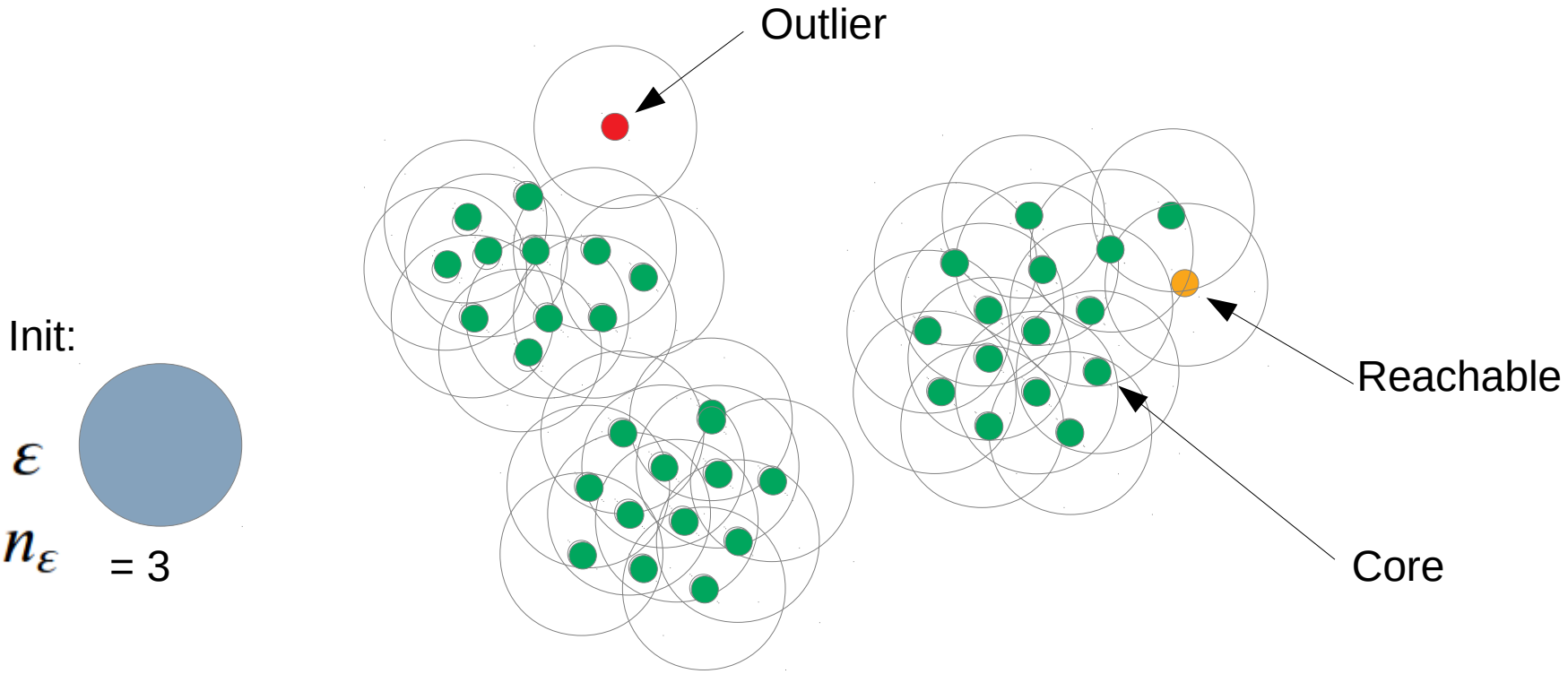
n_ε = 3



Outliers with Machine Learning

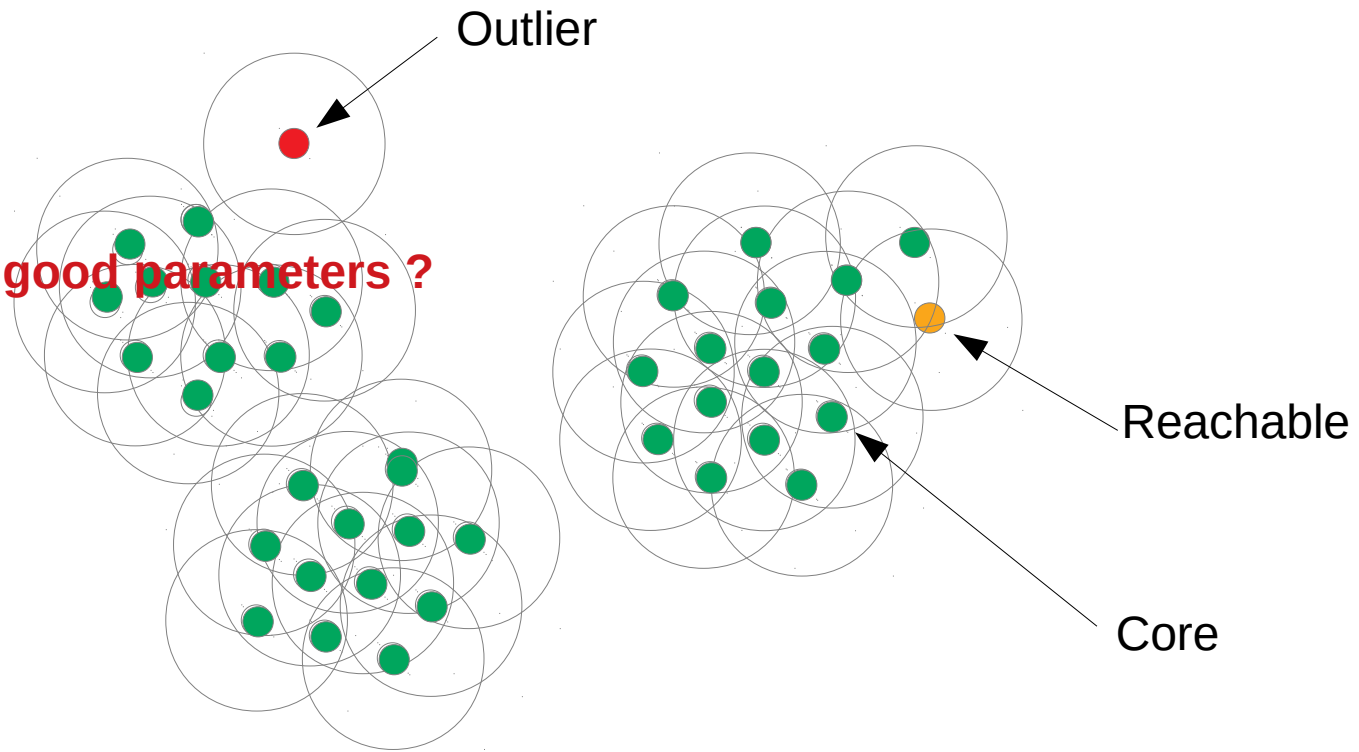
KI Labor Südbaden

Using DBSCAN clustering



Outliers with Machine Learning

Using DBSCAN clustering



Problem: what are good parameters ?

Init:

ε

n_ε = 3

Outliers with Machine Learning

KI Labor Südbaden

Using One-Class SVMs [recall SVMs from ML IV block 2]

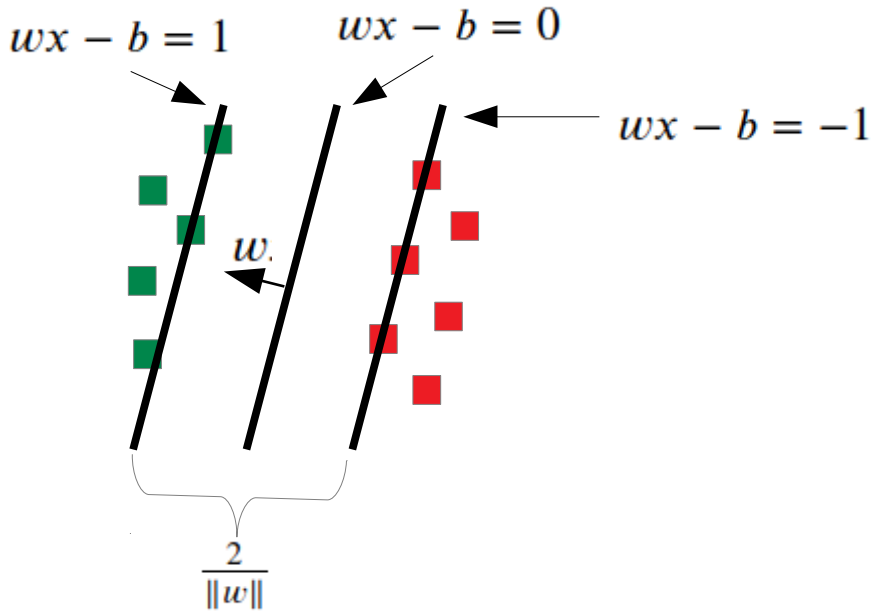
SVM: binary supervised classification

→ New optimization problem
→ maximize “Margin”:
→ equals minimizing the uncertainty

$$\arg\min_{w} \sum_{i=0}^{N} \xi_i + \lambda \|w_i\|^2$$

$$\text{subject to } y_i(w \cdot x_i - b) \geq 1 - \zeta_i \text{ and } \zeta_i \geq 0, \text{ for all } i.$$

$$\zeta_i = \max(0, 1 - y_i(w \cdot x_i - b))$$



Outliers with Machine Learning

KI Labor Südbaden

Using One-Class SVMs (following Schöllkopf)

Support Vector Method for Novelty Detection

Bernhard Schölkopf*, Robert Williamson§,
Alex Smola§, John Shawe-Taylor†, John Platt*

* Microsoft Research Ltd., 1 Guildhall Street, Cambridge, UK
§ Department of Engineering, Australian National University, Canberra 0200
† Royal Holloway, University of London, Egham, UK
* Microsoft, 1 Microsoft Way, Redmond, WA, USA
bsc@jplatt@microsoft.com, Bob.Williamson@Alex.Smola@anu.edu.au, jst@dcs.rhbnc.ac.uk

Abstract

Suppose you are given some dataset drawn from an underlying probability distribution P and you want to estimate a "simple" subset S of input space such that the probability that a test point drawn from P lies outside of S equals some a priori specified ν between 0 and 1.

We propose a method to approach this problem by trying to estimate a function f which is positive on S and negative on the complement. The functional form of f is given by a kernel expansion in terms of a potentially small subset of the training data; it is regularized by controlling the length of the weight vector in an associated feature space. We provide a theoretical analysis of the statistical performance of our algorithm.

The algorithm is a natural extension of the support vector algorithm to the case of unlabelled data.

1 INTRODUCTION

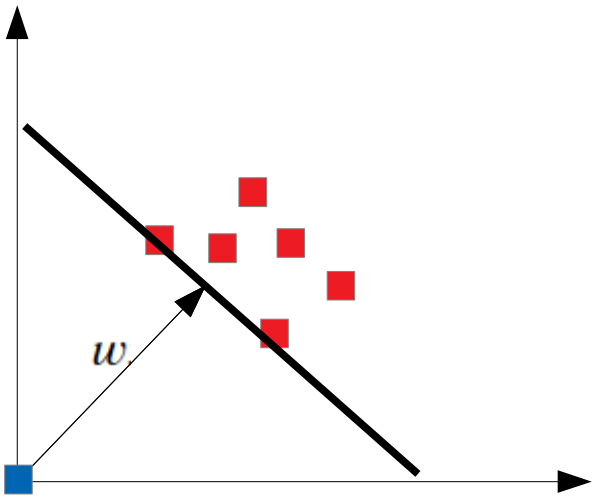
During recent years, a new set of kernel techniques for supervised learning has been developed [8]. Specifically, support vector (SV) algorithms for pattern recognition, regression estimation and solution of inverse problems have received considerable attention. There have been a few attempts to transfer the idea of using kernels to compute inner products in feature spaces to the domain of *unsupervised* learning. The problems in that domain are, however, less precisely specified. Generally, they can be characterized as estimating

Now: unitary supervised classification

→ New optimization problem

→ maximize “Margin” between origin and data

→ equals minimizing the uncertainty



Outliers with Machine Learning

KI Labor Südbaden

Using One-Class SVMs (following Schöllkopf)

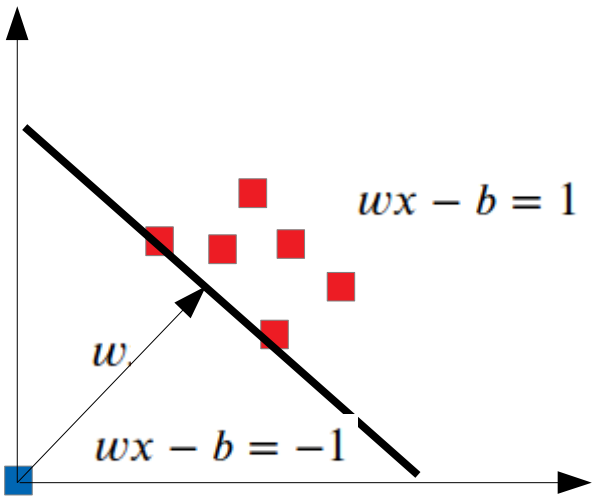
Now: unitary supervised classification

→ New optimization problem
→ maximize “Margin” between origin and data
→ equals minimizing the uncertainty

$$\min_{w,\,\xi_i,\,\rho} \frac{1}{2}\|w\|^2 + \frac{1}{\nu n}\sum_{i=1}^{n}\xi_i - \rho$$

subject to:

$$(w \cdot \phi(x_i)) \geq \rho - \xi_i \qquad \text{for all } i = 1, \ldots, n$$
$$\xi_i \geq 0 \qquad \text{for all } i = 1, \ldots, n$$



Outliers with Machine Learning

KI Labor Südbaden

Using One-Class SVMs (following Schöllkopf)

Now: unitary supervised classification

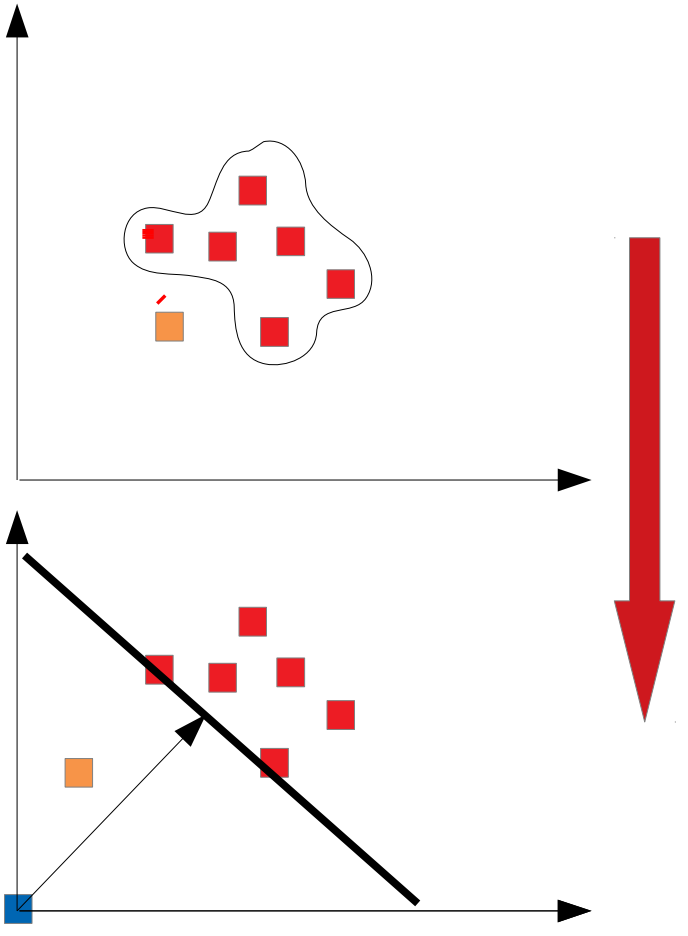
→ New optimization problem
→ maximize “Margin” between origin and data
→ equals minimizing the uncertainty

$$\min_{w,\,\xi_i,\,\rho} \frac{1}{2}\|w\|^2 + \frac{1}{\nu n}\sum_{i=1}^{n}\xi_i - \rho$$

subject to:

$$(w \cdot \phi(x_i)) \geq \rho - \xi_i \qquad \text{for all } i = 1, \ldots, n$$

$$\xi_i \geq 0 \qquad \text{for all } i = 1, \ldots, n$$



Non-linear transformation (a.k.a “kernel trick”)

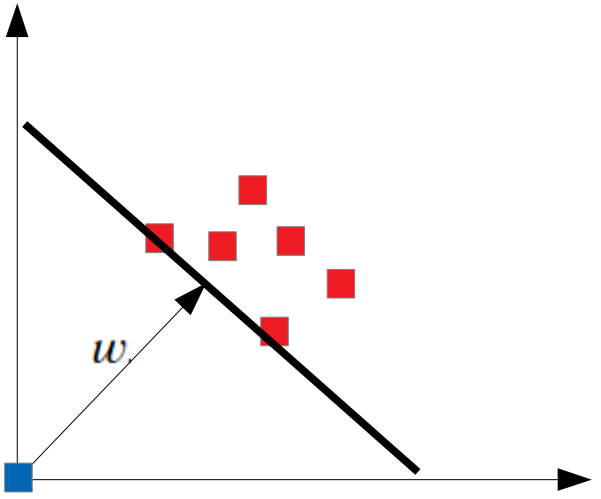
Outliers with Machine Learning

Using One-Class SVMs (following Schöllkopf)

In Scikit-Learn:

```
>>> from sklearn.svm import OneClassSVM
>>> X = [[0], [0.44], [0.45], [0.46], [1]]
>>> clf = OneClassSVM(gamma='auto').fit(X)
>>> clf.predict(X)
array([-1,  1,  1,  1, -1])
>>> clf.score_samples(X)  # doctest: +ELLIPSIS
array([1.7798..., 2.0547..., 2.0556..., 2.0561..., 1.7332...])
```

https://scikit-learn.org/stable/modules/generated/sklearn.svm.OneClassSVM.html



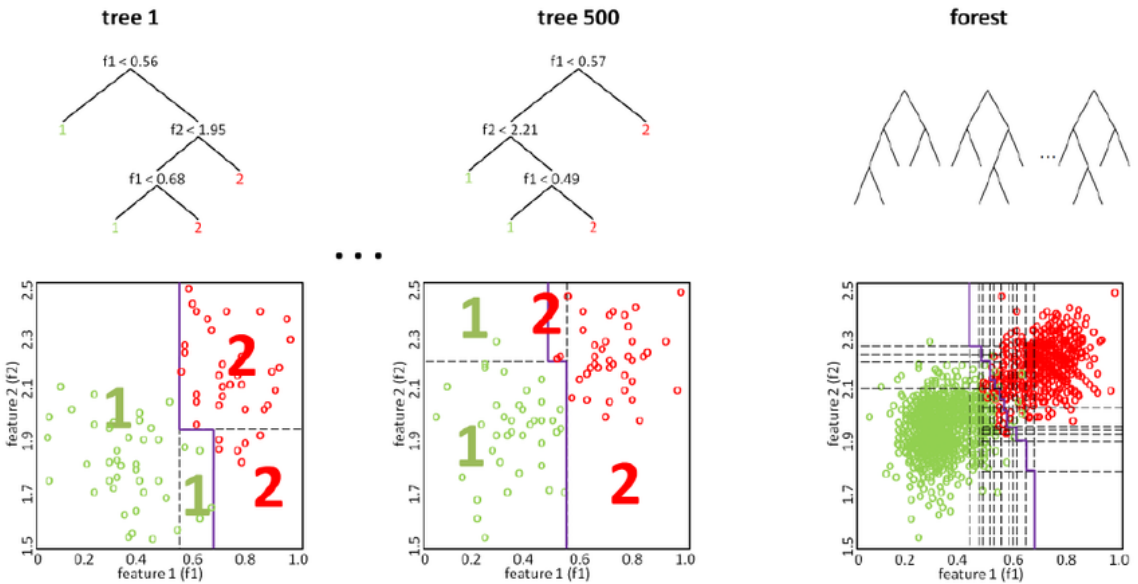
Outliers with Machine Learning

KI Labor Südbaden

Using Isolation Forests [Recall Random Forests from ML II in Block 1]

Random Forests:

- Ensemble of simple decision trees
- Classification as voting
- Combination of piecewise linear models

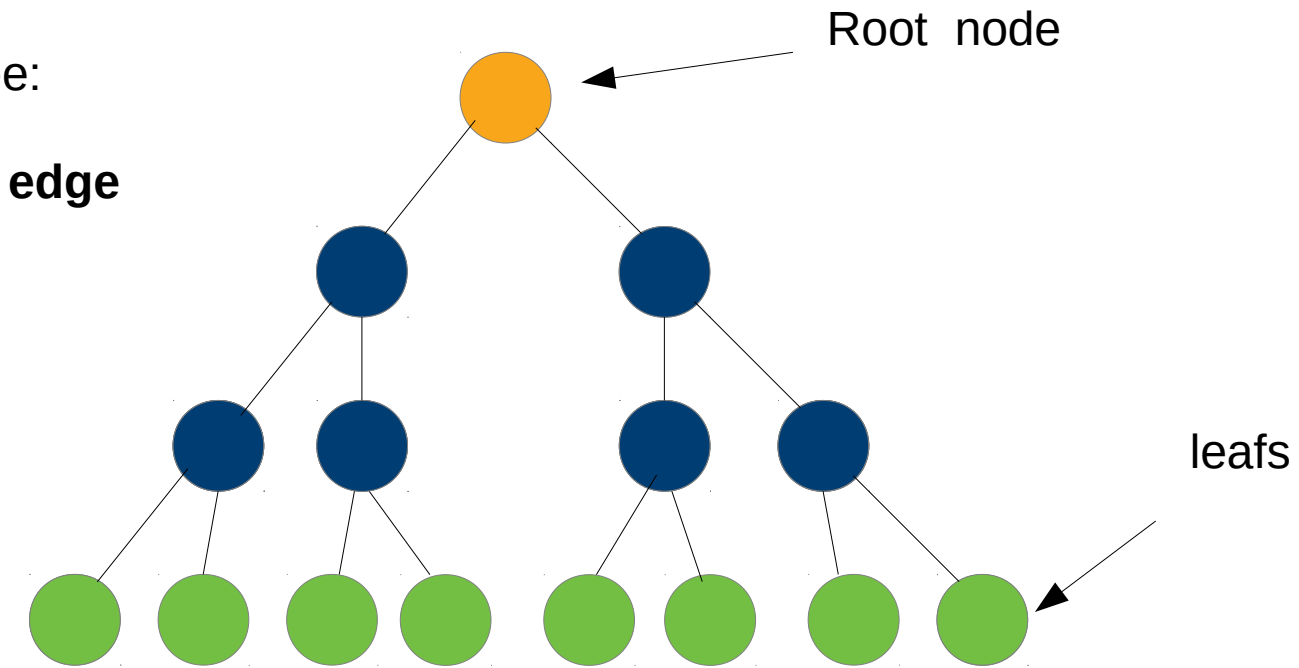


Random Forests

Recall Decision Trees: the base classifier for Random/Isolation Forests

Typically Binary Tree:

Vertex (Node) and edge

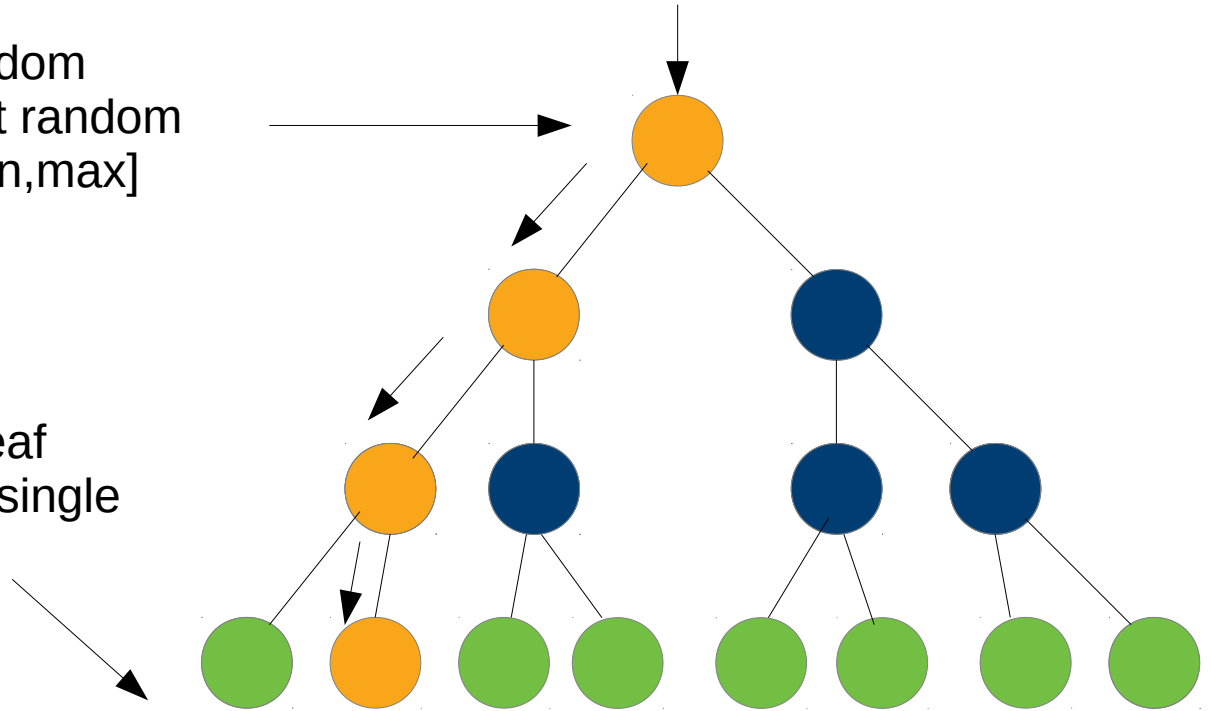


Random Forests

Isolation Forest, just like RF, BUT

Split: random feature at random value [min,max]

Split till leaf contains single sample



Random Forests

Isolation Forest

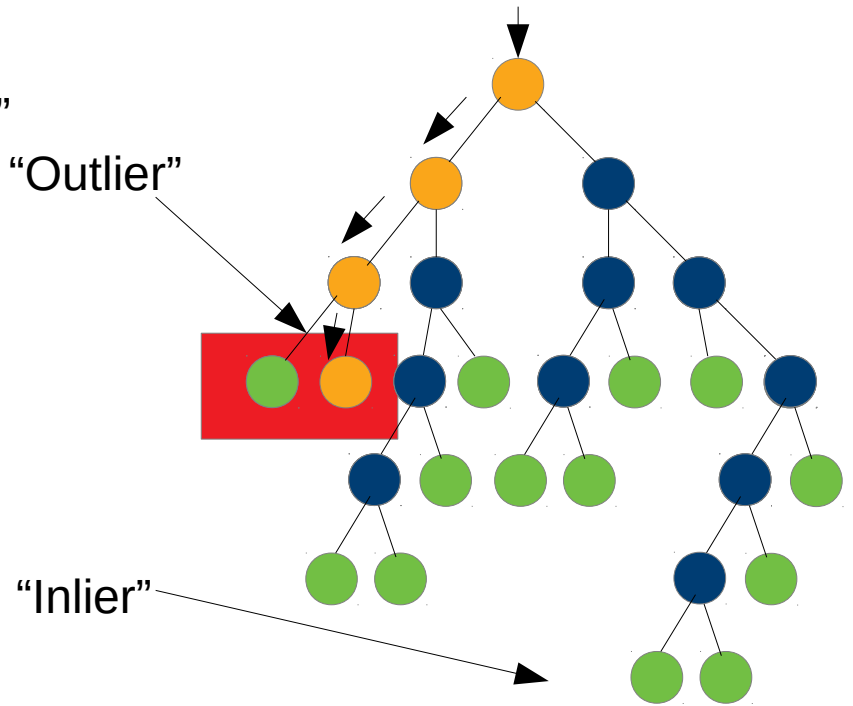
Effect: trees become much deeper

Depth of as sample as “of out of distribution”
Measure:

$$s(x,n) = 2^{-\frac{E(h(x))}{c(n)}}$$

where h(x) is the path length of observation x, c(n) is the average path length of unsuccessful search in a Binary Search Tree and n is the number of external nodes.

→ 1 outlier, 0 inlier

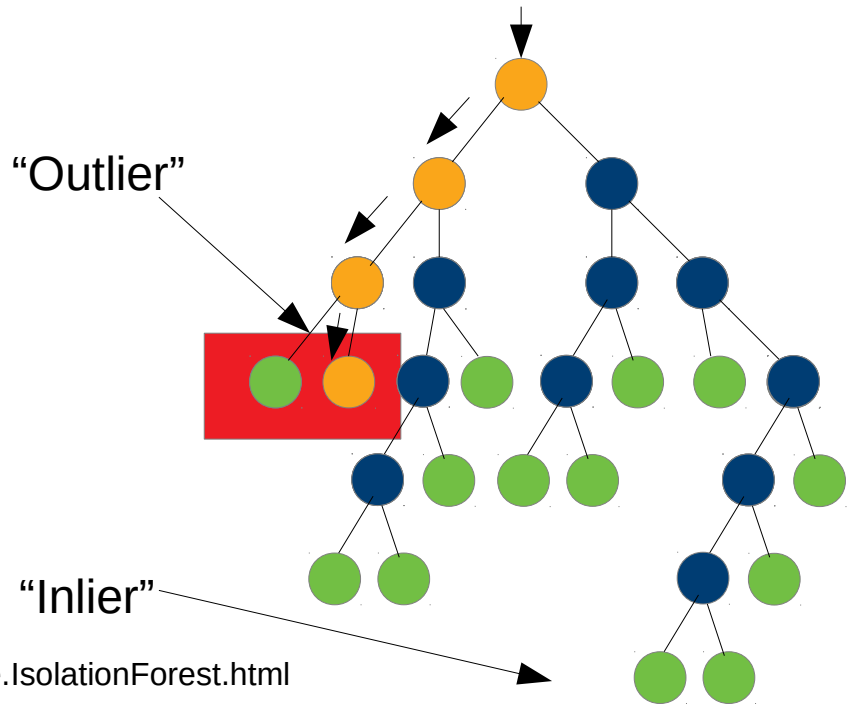


Random Forests

Isolation Forest

In Scikit-Learn:

```
>>> from sklearn.ensemble import IsolationForest
>>> X = [[-1.1], [0.3], [0.5], [100]]
>>> clf = IsolationForest(random_state=0).fit(X)
>>> clf.predict([[0.1], [0], [90]])
array([ 1,  1, -1])
```



https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.IsolationForest.html

Discussion