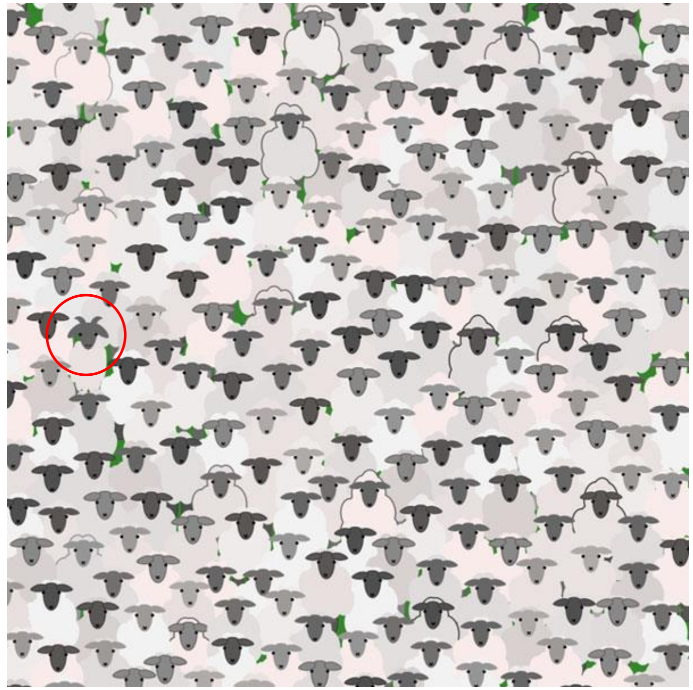

Lecture 3: Novelty Detection

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School of Industrial Management Engineering
Korea University

AGENDA

Machine Learning

- Definition
  - ✓ 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 at task in T, as measured by P, improves with experience E," – Mitchell (1997)

Supervised Learning

- Goal: predict a single "target" or "outcome" variable
- Finds relations between X and Y
- Train (learn) data where target value is known
- Score data where target value is not known

Unsupervised Learning

- Explores intrinsic characteristics
- Estimates underlying distribution
- Segment data into meaningful groups or detect patterns
- There is no target (outcome) variable to predict or classify

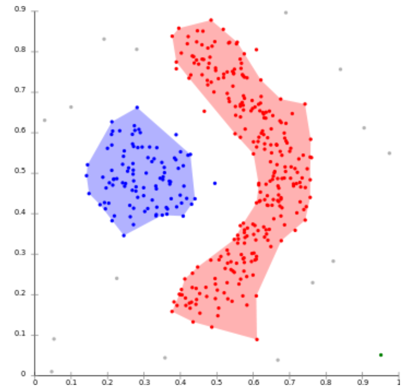
Unsupervised Learning

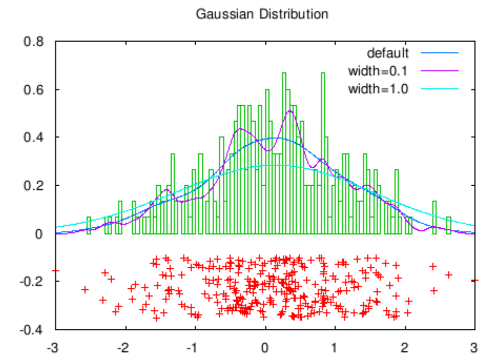
A given dataset $\mathbf{X}$

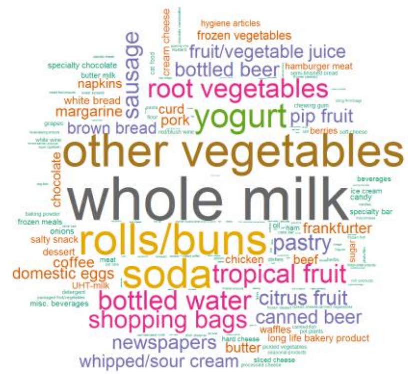
	Var. 1	Var. 2	…	Var. d
Ins. 1	..	..	…	..
Ins. 2	..	..	…	..
…	…	…	…	…
Ins. N	..	..	..	..

[Unsupervised learning](#)

- Explores intrinsic characteristics
- Estimates underlying distribution
- Density estimation, clustering, association rule mining, network (graph) analysis, etc.





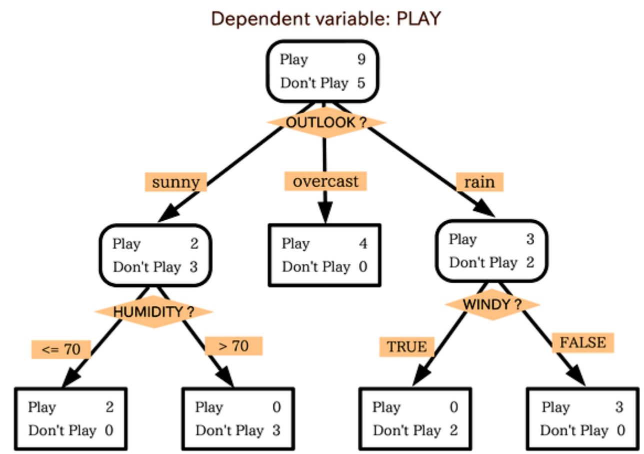


Supervised Learning

A given dataset **X** & **Y**

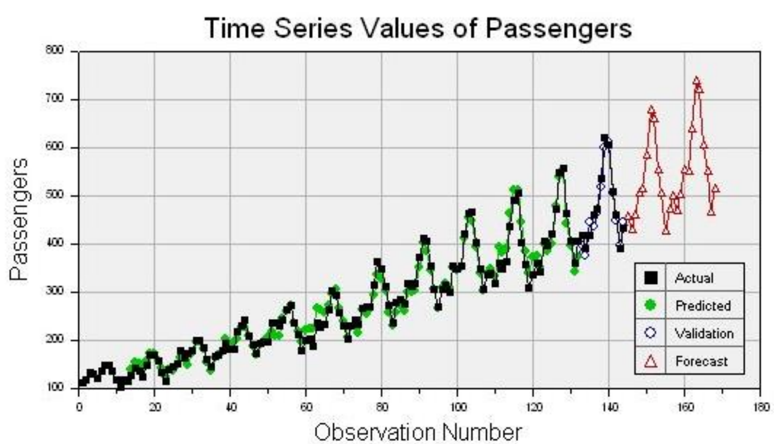
	Var. 1	Var. 2	...	Var. d	Y
Ins. 1	..	..	...	..	..
Ins. 2	..	..	...	..	..
...	...	...	...	...	...
Ins. N	..	..	..	..	..

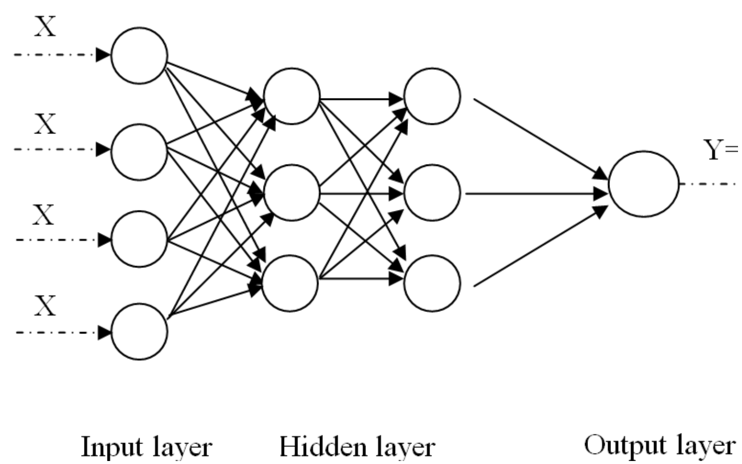
$y = f(x)$



Supervised learning

- Finds relations between X and Y: estimate the underlying function $y = f(x)$
- Classification, regression, novelty detection





Supervised Learning: Novelty Detection

- What is novel data (outliers)?

> *"Observations that deviate so much from other observations as to arouse suspicions that they were generated by a different mechanism (Hawkins, 1980)"*
>
> *"Instances that their true probability density is very low (Harmeling et al., 2006)"*

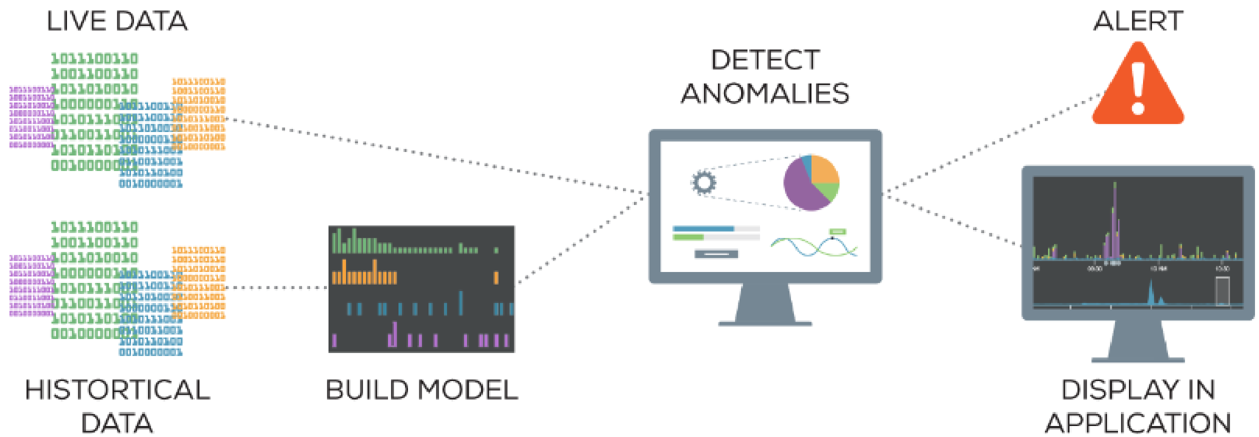
- Outliers are different from noise data
  - ✓ Noise is random error or variance in a measured variable
  - ✓ Noise should be removed before outlier detection
- Outliers are interesting
  - ✓ It violates the mechanism that generates the normal data

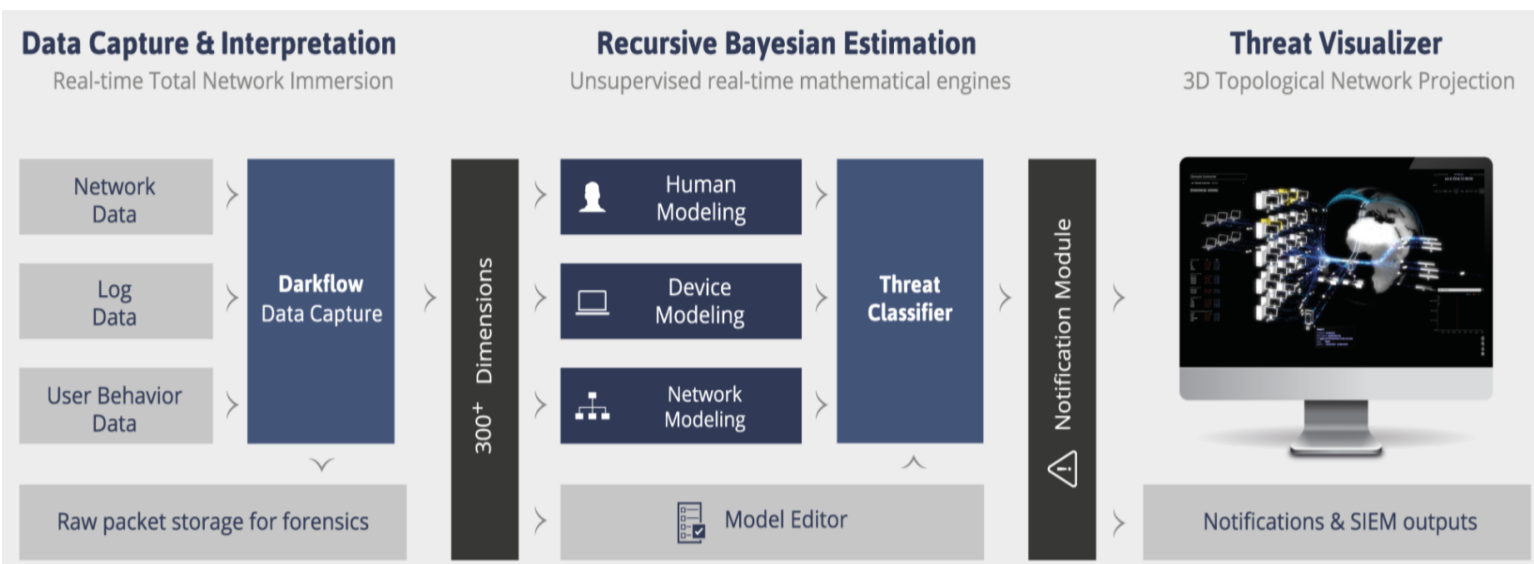
Supervised Learning: Novelty Detection

- Applications
  - ✓ Industrial monitoring
  - ✓ IT security
  - ✓ Healthcare informatics
  - ✓ Sensor network
  - ✓ Computer vision
  - ✓ Credit card fraud detection
  - ✓ Telecom fraud detection
  - ✓ Customer segmentation/Medical analysis

Supervised Learning: Novelty Detection

- Applications: System Security





Supervised Learning: Novelty Detection

Data Preparation

Vectorization

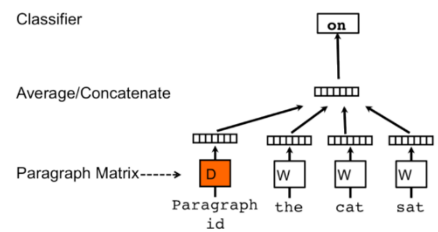
Host-based

ADFA-LD Dataset

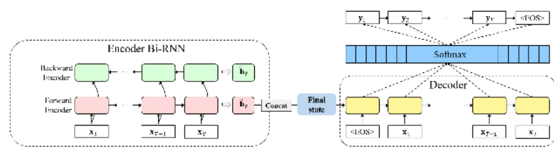
Syscall Trace

```
265 104 265 104 3 175
104 142 3 3 3 104 146
265 104 142 142 175
146 142 146 142 265 3
175 175 142 142 175
119 265 142 146 265
146 119 142 146 142
142 142 142 146 104
265 3 119 3 265 119
146 146 146 265 146
142 142 146 142 119
```

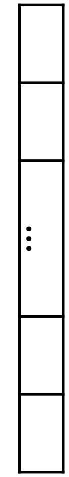
Doc2vec

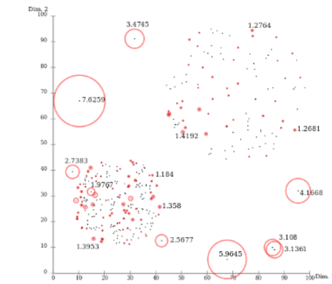


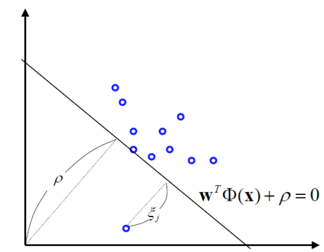
RNN-AutoEncoder

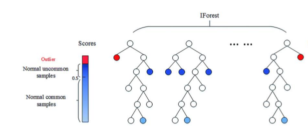


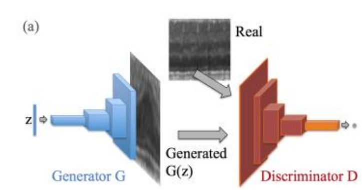
D-dimensional vector







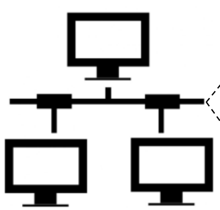


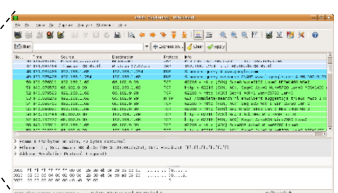


Network-based

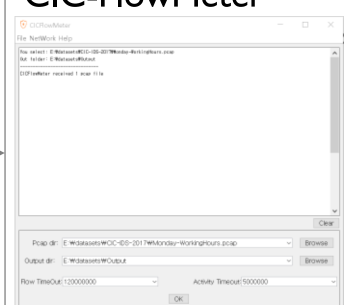
CICIDS2017 Dataset

Packet Capture

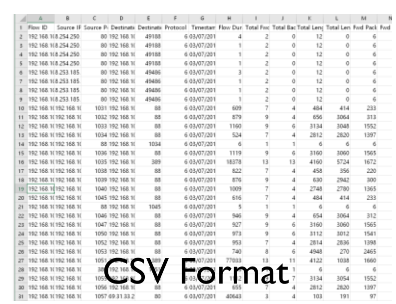




CIC-FlowMeter



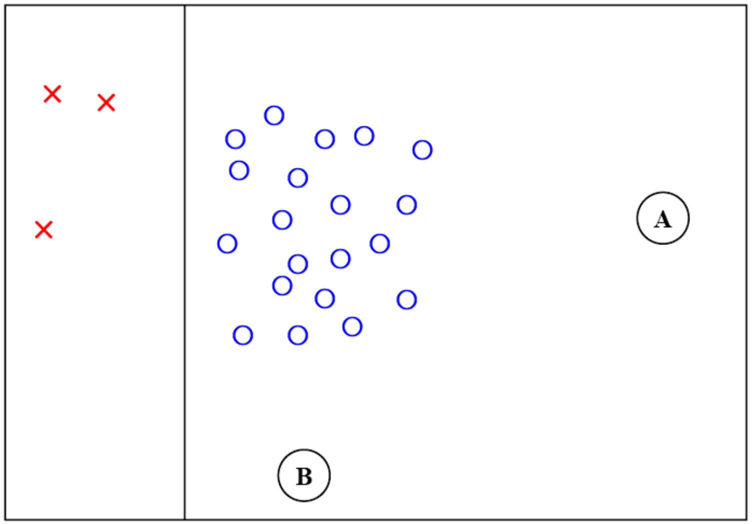
Features



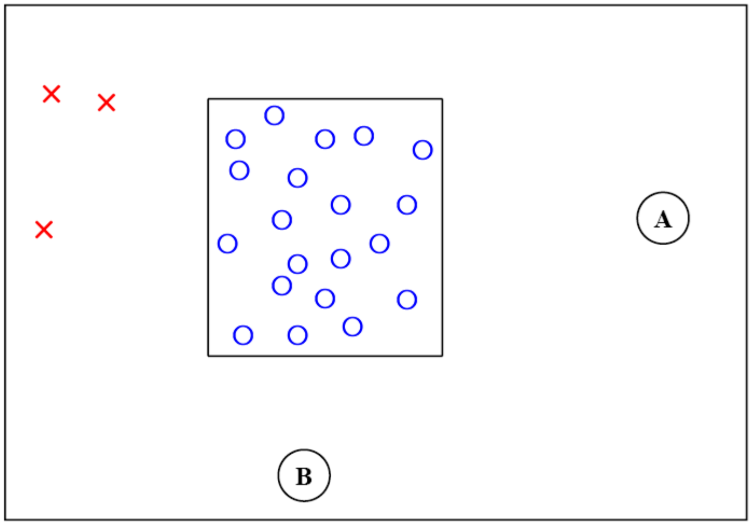
CSV Format

Supervised Learning: Novelty Detection

- Classification vs. Novelty Detection



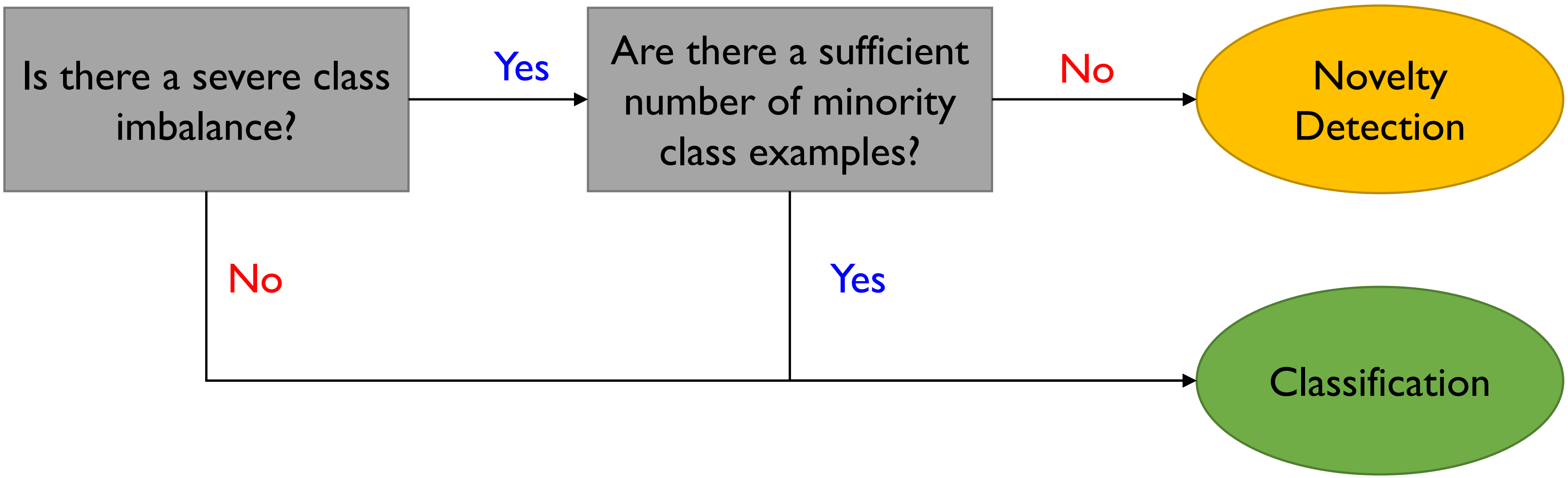
Binary classification



Novelty detection

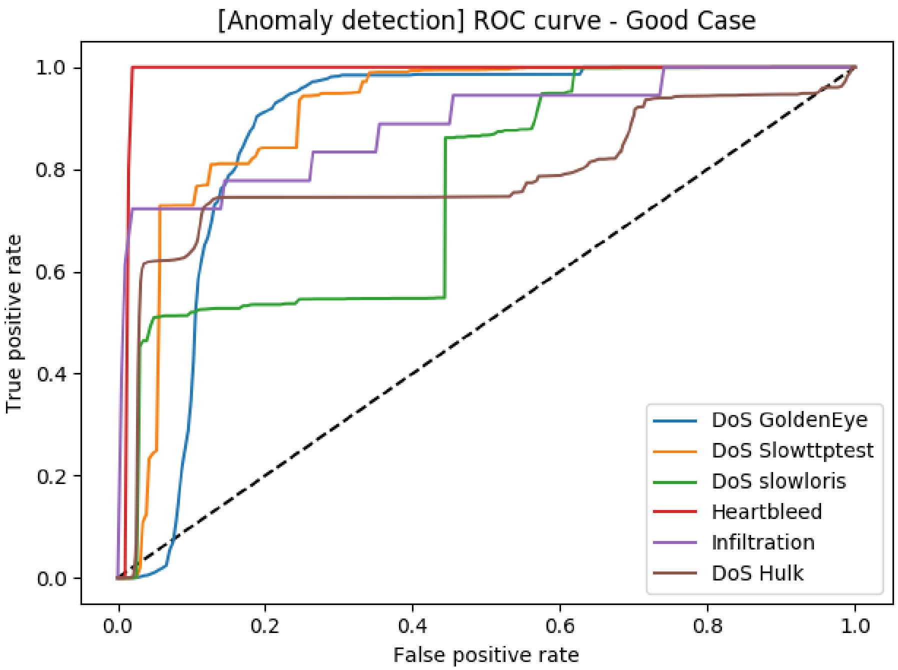
Supervised Learning: Novelty Detection

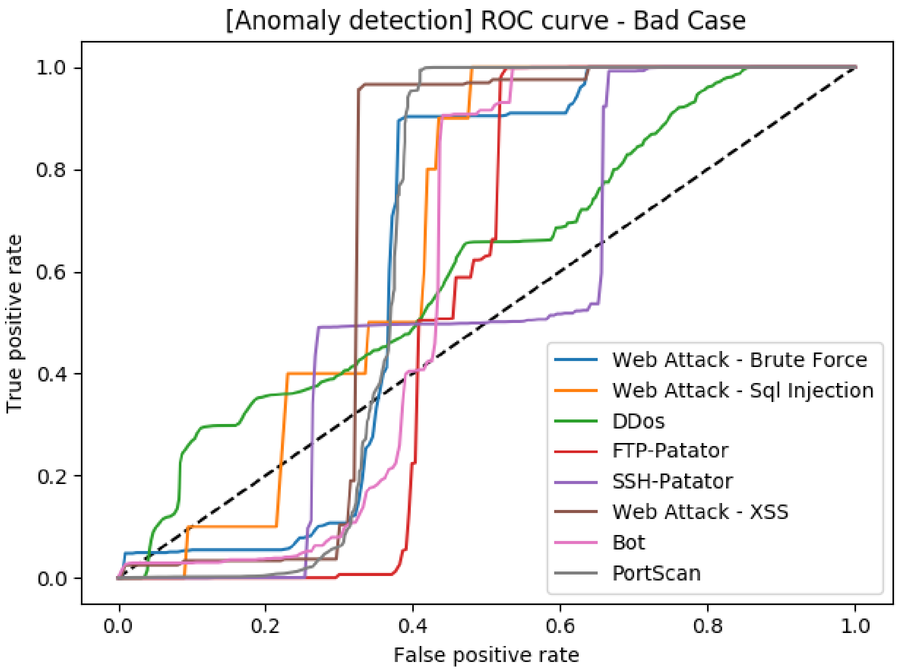
- Classification vs. Novelty Detection
  - ✓ Which one to use?



Supervised Learning: Novelty Detection

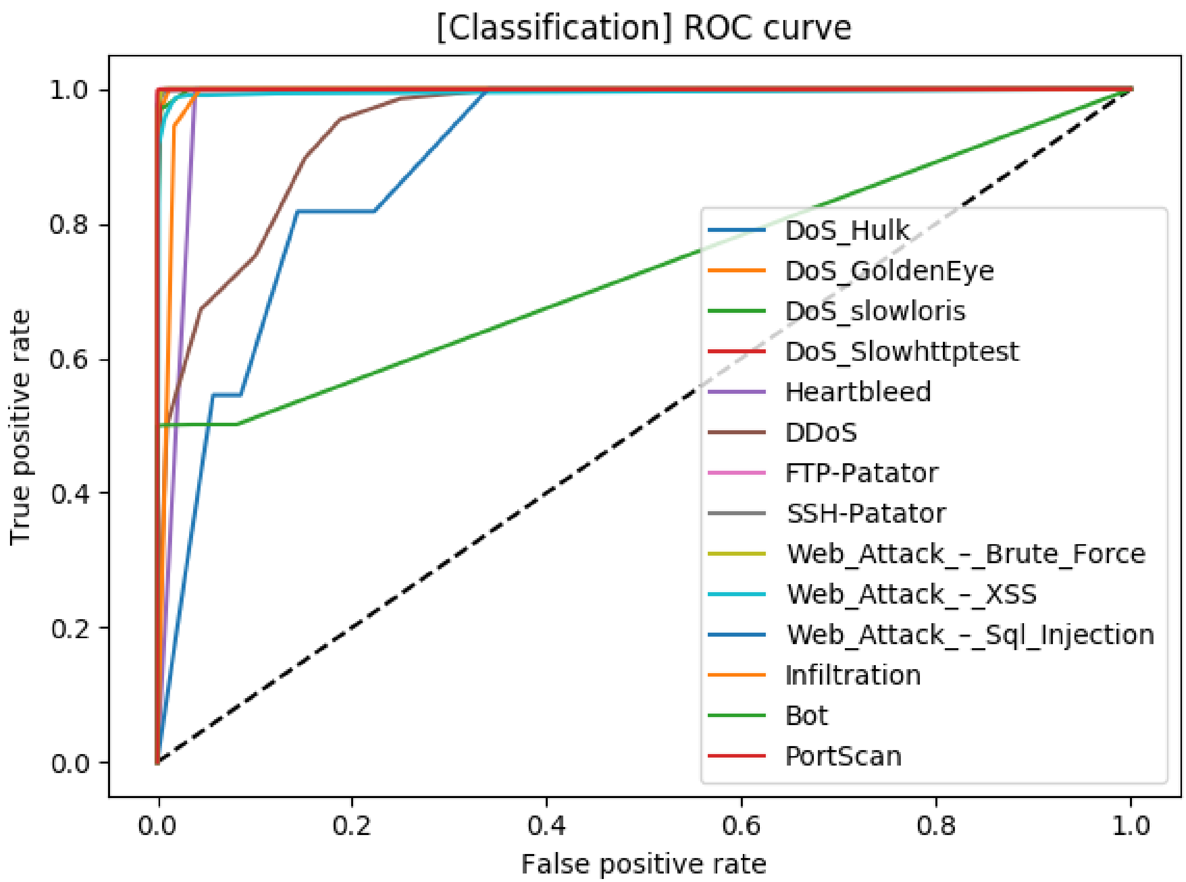
- Classification vs. Novelty Detection
  - ✓ Performance comparison for network traffic anomaly detection





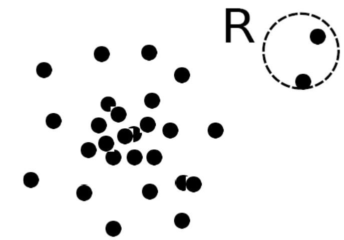
Supervised Learning: Novelty Detection

- Classification vs. Novelty Detection
  - ✓ Performance comparison for network traffic anomaly detection

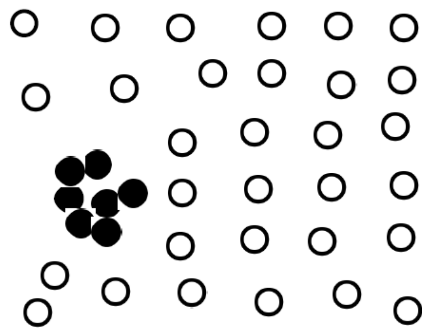


Type of Novel Data (Outliers)

- Global outlier
  - ✓ Object that significantly deviates from the rest of the data set
  - ✓ Ex) Credit card fraud detection
  - ✓ Issue: find an appropriate measurement of deviation



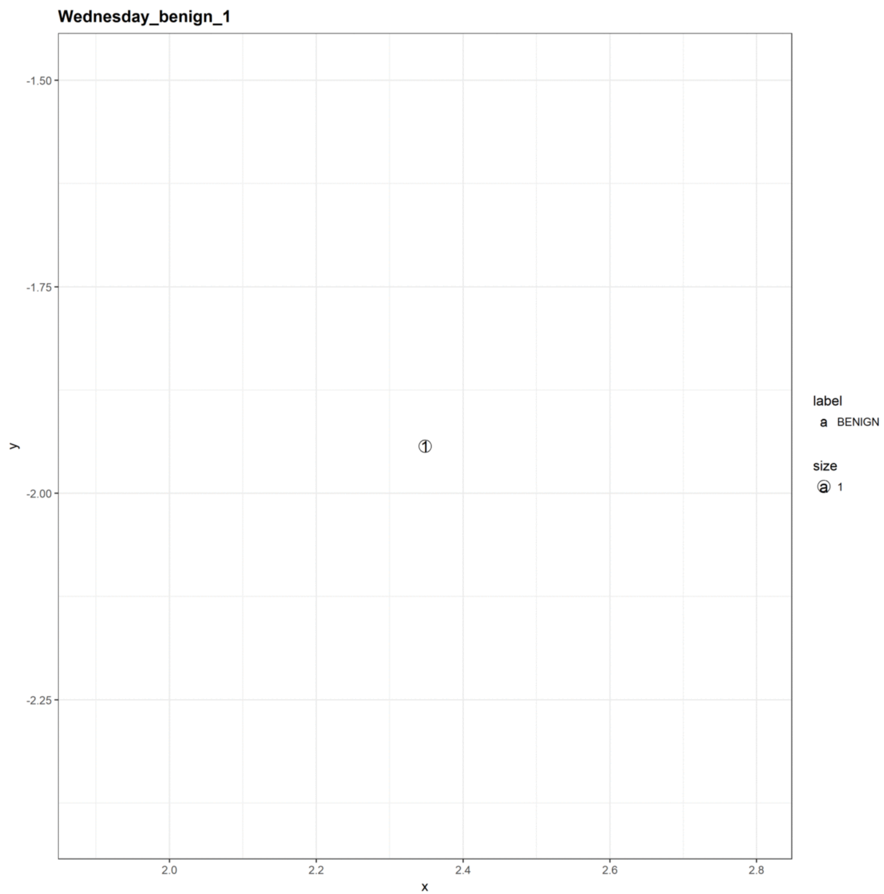
- Contextual outlier (local outlier)
  - ✓ Object that deviates significantly based on a selected context
  - ✓ Ex) 30℃ in Alaska vs. 30℃ in Sahara
  - ✓ Issue: How to define or formulate meaningful context?



- Collective outlier
  - ✓ A subset of data objects collectively deviate significantly from the whole data set, even if the individual data objects may not be outliers
  - ✓ Ex) Denial-of-Service (DoS) attack

Type of Novel Data (Outliers)

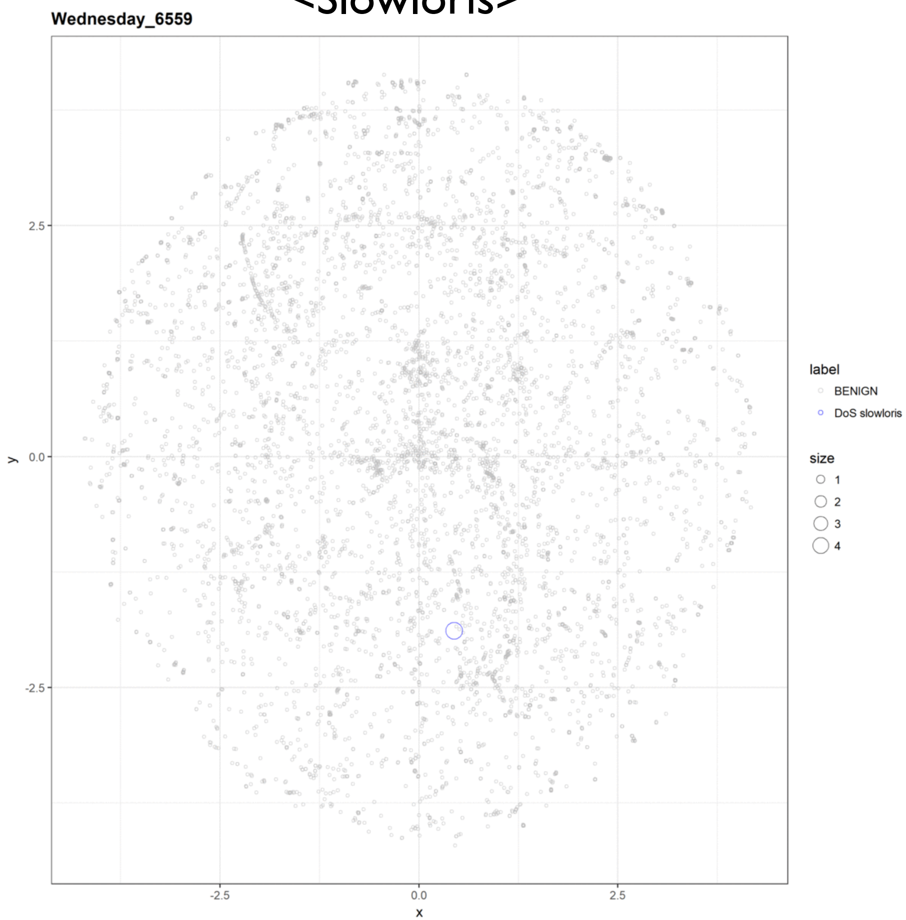
- Collective outlier: An example
  - ✓ Normal traffic (animation by Minsik Park)



Type of Novel Data (Outliers)

- Collective outlier: An example
  - ✓ DoS traffic (animation by Minsik Park)

<Slowloris>



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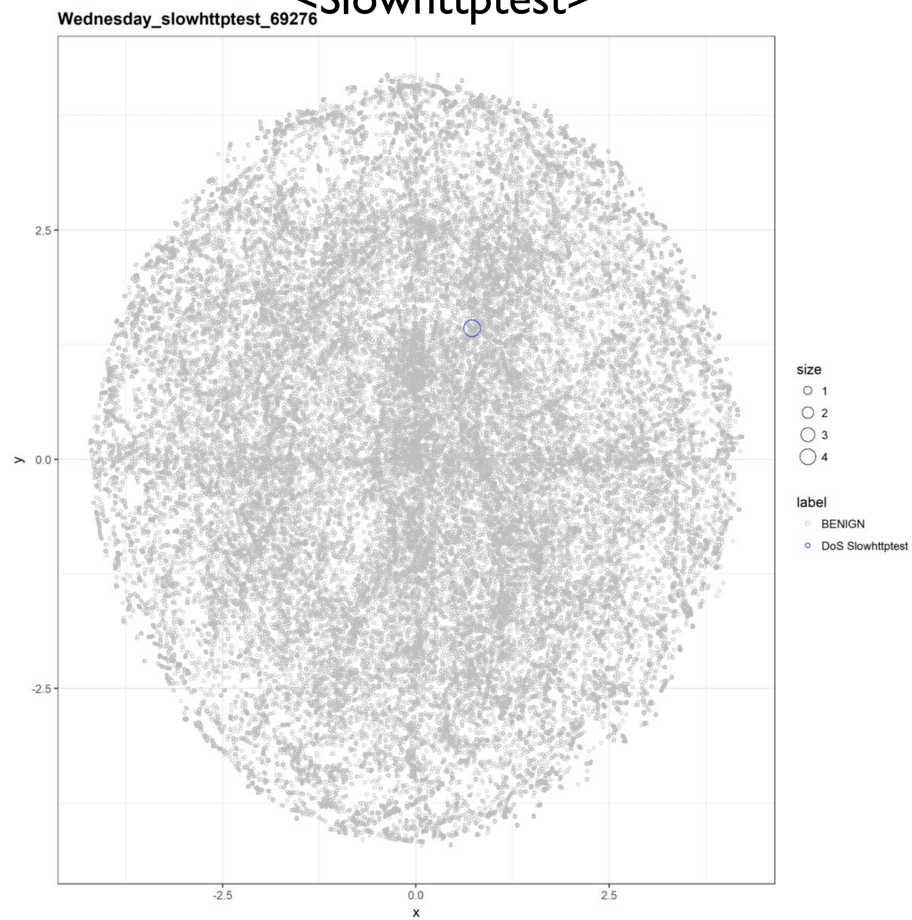


Challenges

- Modeling normal objects and outliers properly
  - ✓ The border between normal and outlier objects is often a gray area
- Application-specific outlier detection
  - ✓ Choice of distance measure among objects and the model of relationship among objects are often application-dependent
  - ✓ E.g., clinic data: a small deviation could be an outlier; while in marketing analysis, larger fluctuations
- Understandability
  - ✓ Understand why these are outliers: Justification of the detection
  - ✓ Specify the degree of an outlier: the unlikelihood of the object being generated by a normal mechanism

Challenges

- Novelty detection actually matters

○ 분석목표 : 제품 원료품질 검사 데이터(X)로 제품불량(Y)을 예측

○ 데이터 분포

- X 변수 : 재료 품질검사 데이터 560 개 항목
- Y 범주 : 불량, 정상
- 비중 : 정상 93%, 불량 7%

○ 분석기법

- 지도학습 : KNN, Random Forest
- 비지도학습 : Gausian Mixture 모델

○ 분석과정 및 결과

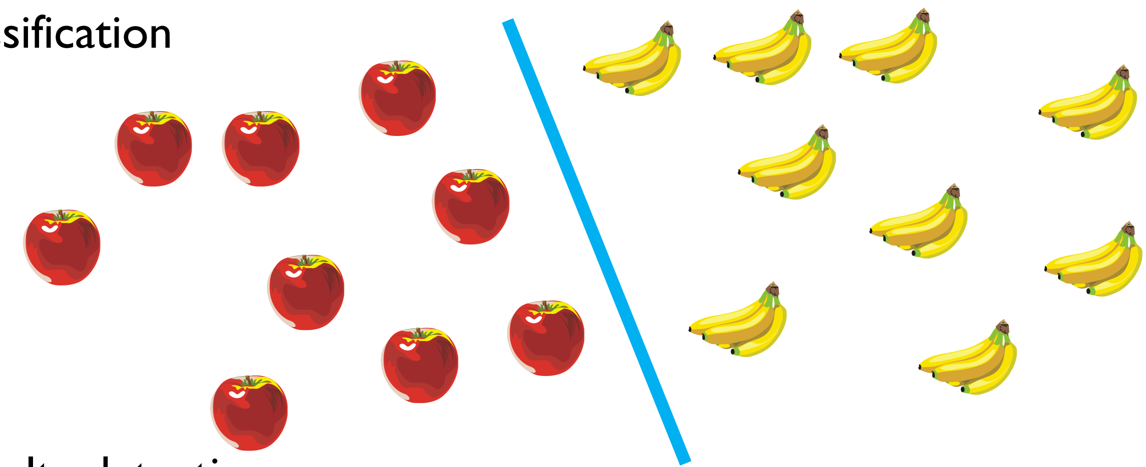
1) 전체 데이터로 학습
   - Accuracy 93%
   - 문제점 : 불량데이터에 대한 예측성능이 매우 낮음 (Precision 0.38, Recall 0.01, f1-score 0.02)
2) 정상, 불량 학습데이터 비중을 맞춤 (1 : 1)
   - Accuracy 66%
   - 문제점 : 불량데이터 예측성능은 향상되었으나 (Precision 0.38, Recall 0.71), 전체 Accuracy 낮아 짐 (66%)
3) 이상치 탐지 분석 (가우시안 혼합모델)
   - 비정상 데이터에 대한 예측성능이 지도학습과 유사한 수준으로 낮음
4) PolyNomial 방법
   - X 변수를 증가시키는 방법 : 분류분석이고, 이미 X변수가 많아서 시도하지 않음

○ 문의사항

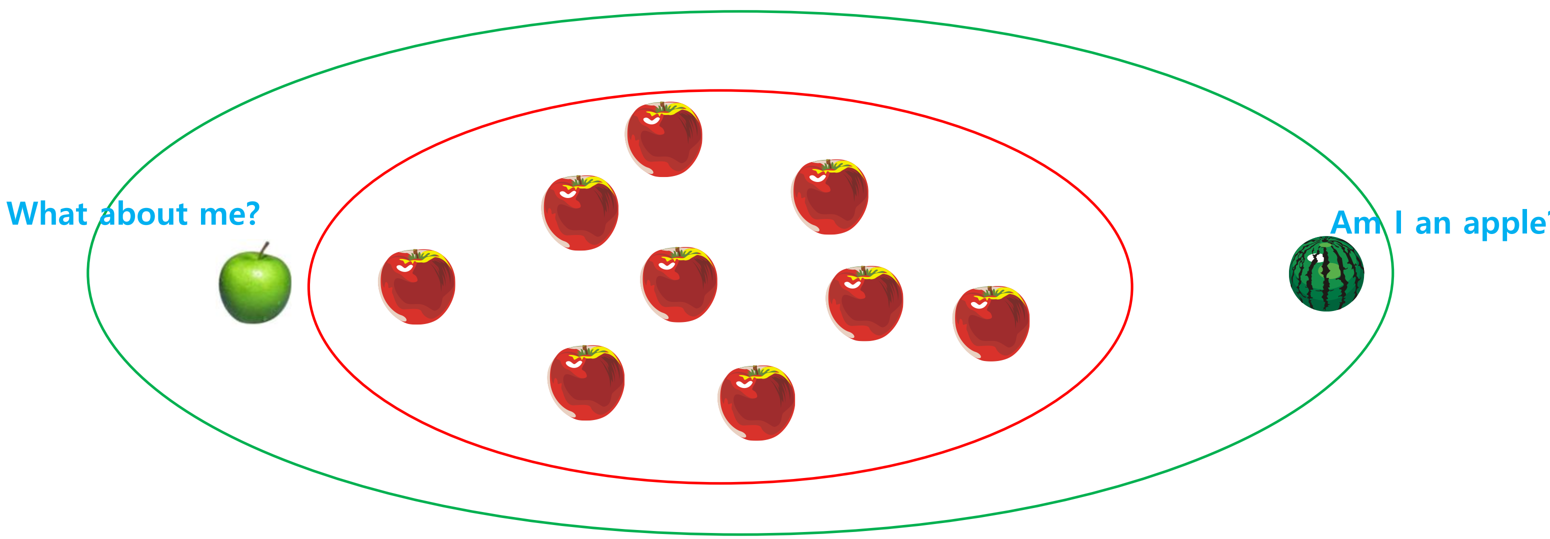
- 판단기준 : 편중된 데이터에 대해서 어느 정도의 수치가 나왔을 때 연관성이 있다고 판단해야 할지 판단기준은?
- 분석방향 : 편중된 데이터에 대해서 불량(이상치)을 예측할 수 있도록 모델학습 시, 시도해 볼만한 방법은?

Supervised Learning: Novelty Detection

- The way by which the classification and novelty detection learns from data
  - ✓ Classification

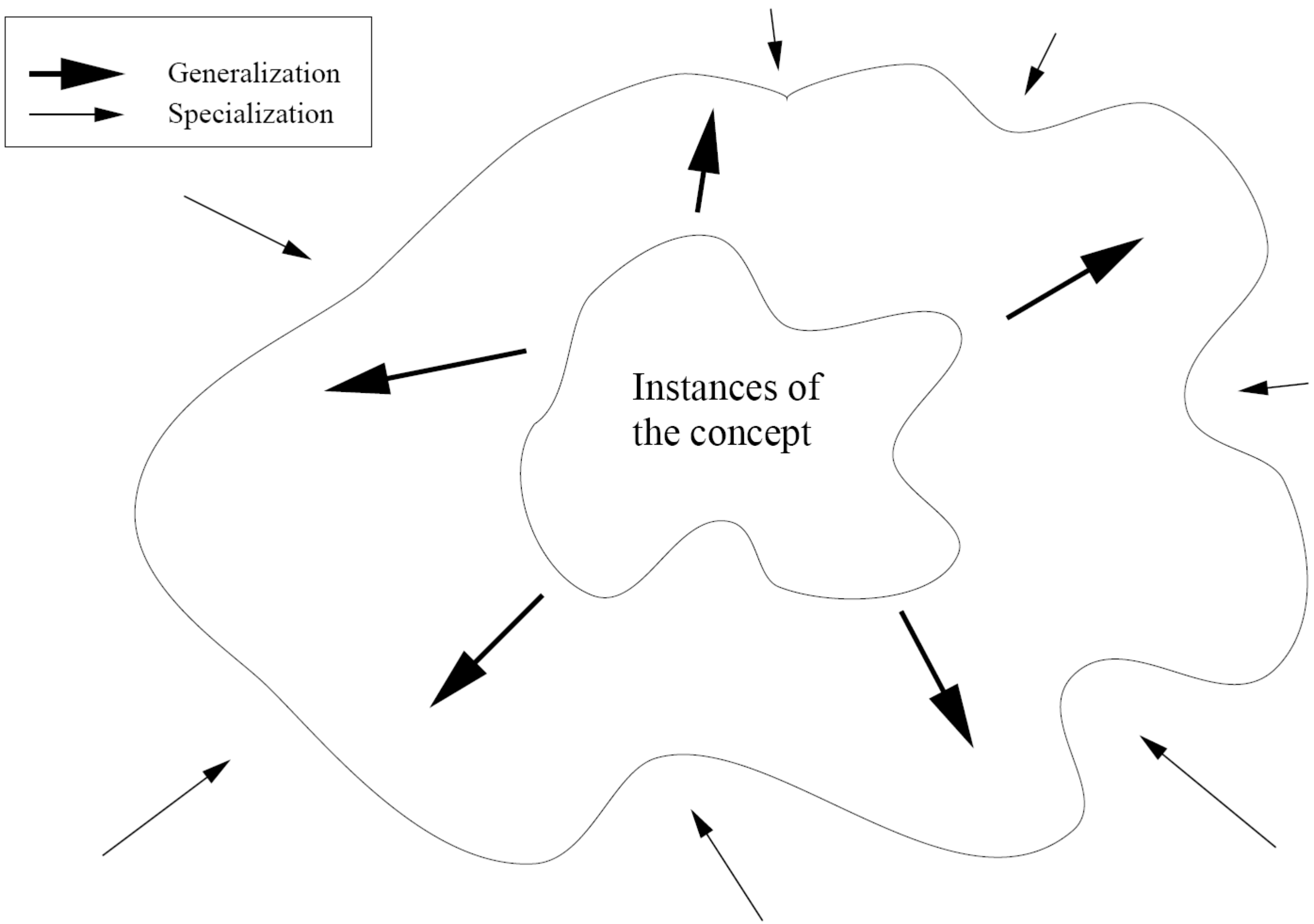


  - ✓ Novelty detection



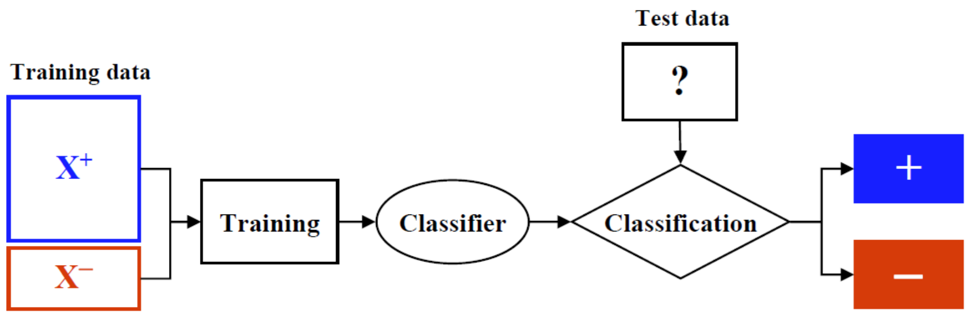
Supervised Learning: Novelty Detection

- Generalization vs. Specialization

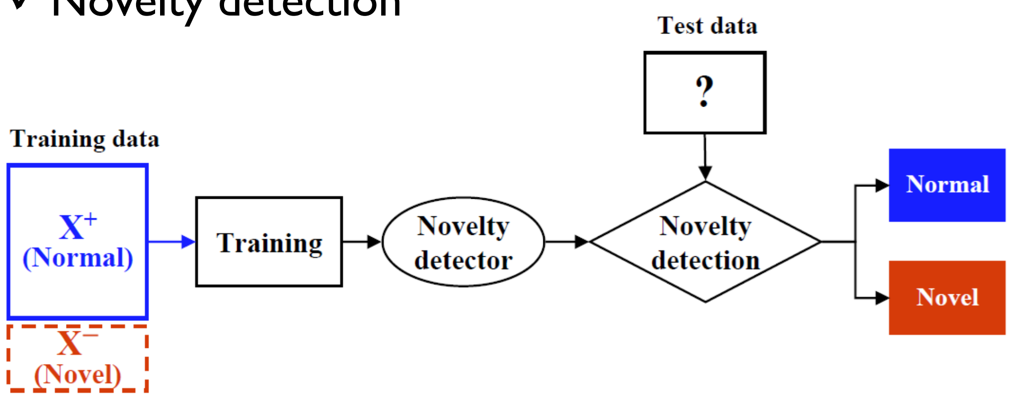


ND Approach

- Assumption
  - ✓ There are considerably more "normal" observations than "abnormal" observations in the data
  - ✓ Classification



  - ✓ Novelty detection



Performance Measures

- Performance Measures
  - ✓ Confusion matrix for novelty detection

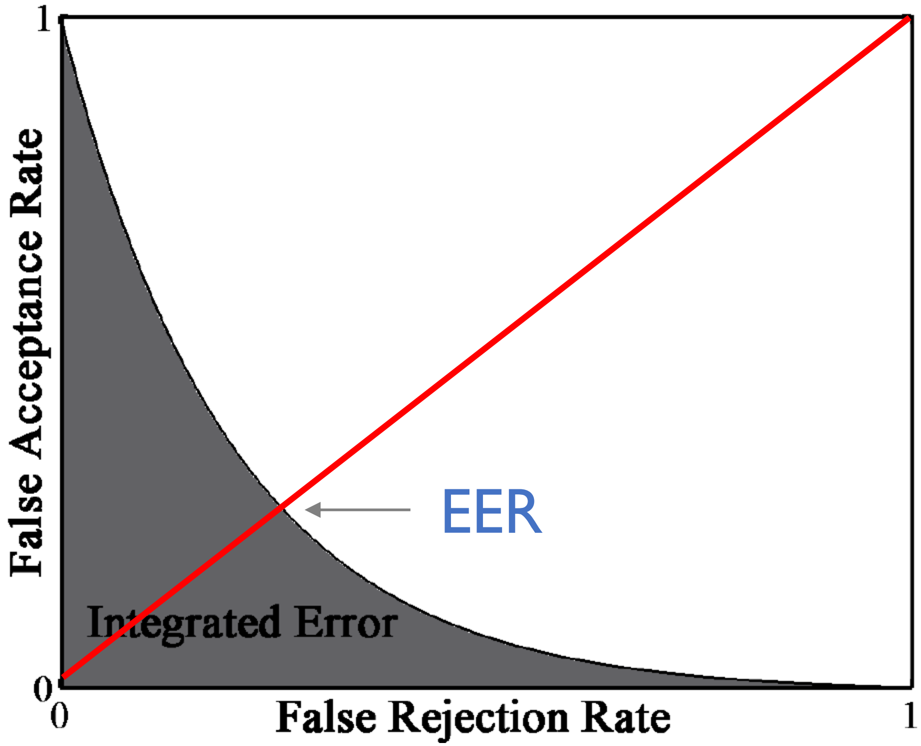
		Predicted class	
		Novel	Normal
Actual class	Novel	A	B
	Normal	C	D

  - ✓ Performance measures when the cut-off (threshold) is set

Metric	Description
Detection Rate	(Identified as novel)/(Actually novel) = A/(A+B)
False Rejection Rate (FRR)	(Rejected as novel)/(Actually normal) = C/(C+D)
False Acceptance Rate (FAR)	(Accepted as normal)/(Actually novel) = B/(A+B)

Performance Measures

- To evaluate an intrinsic performance of novelty detection algorithms
  - ✓ Equal error rate (EER): Error rate where the FAR and FRR are the same
  - ✓ Integrated Error (IE): the area under the FRR-FAR curve
    - AUROC for classification: the higher the better
    - IE for novelty detection: the lower the better

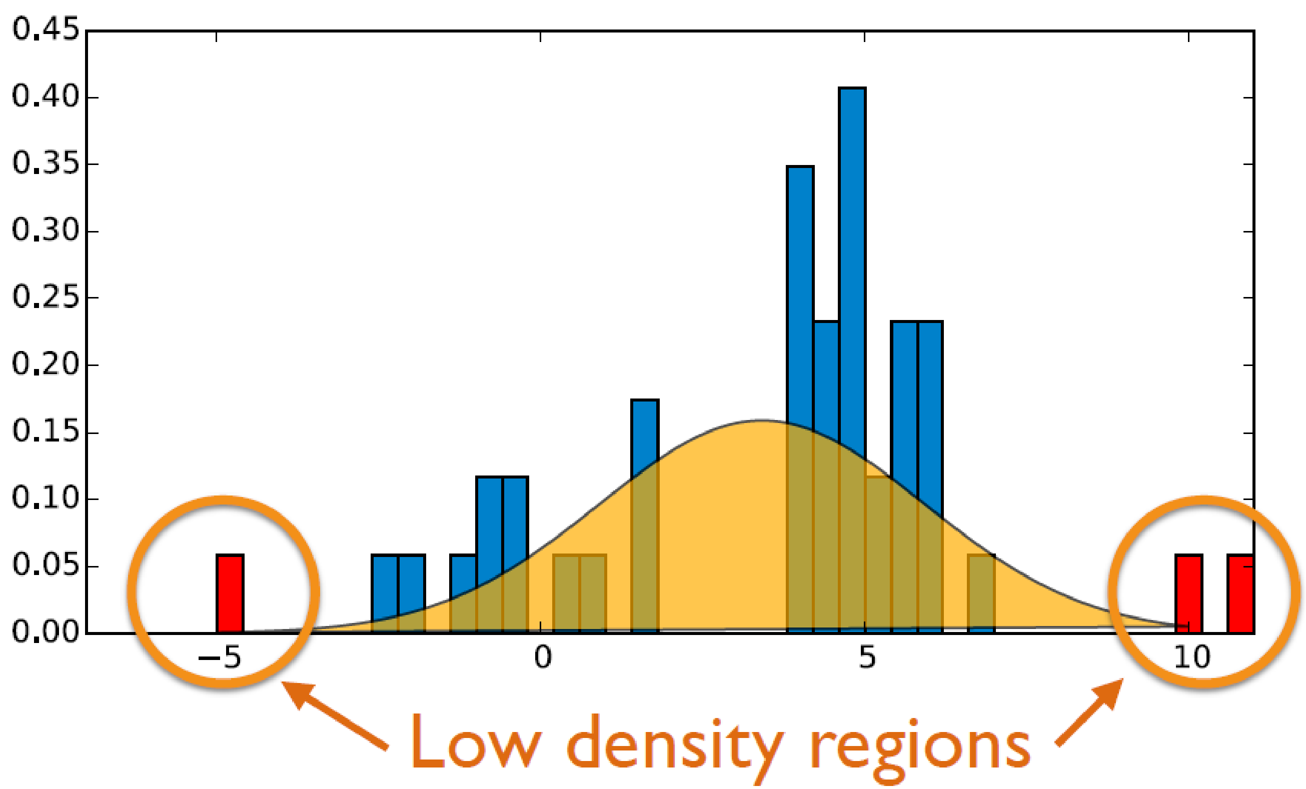


AGENDA

Density-based Novelty Detection

Gramfort (2006)

- Purpose
  - ✓ Estimate the data-driven density function
  - ✓ If a new instance has a low probability according the trained density function, it will be identified as novel



Density-based Novelty Detection

- Purpose
  - ✓ Estimate the data-driven density function
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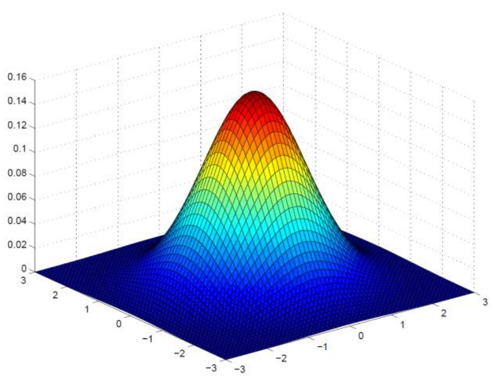
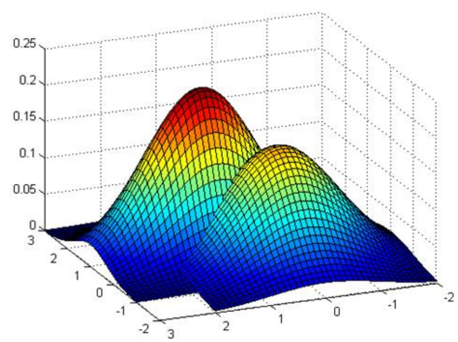
Gaussian Density Estimation



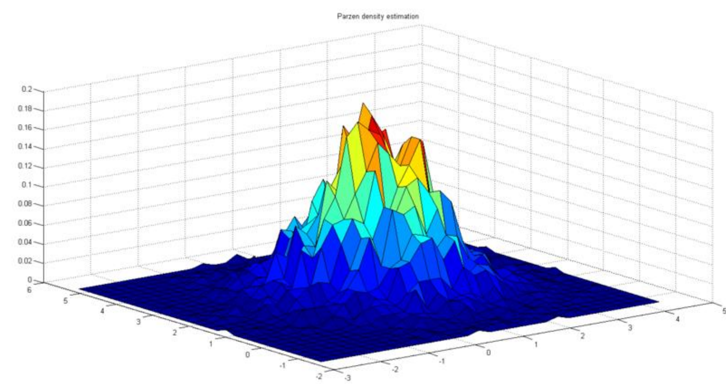
Number of modals = 1

Mixture of Gaussian Density Estimation



1 < Number of modals < Number of instances

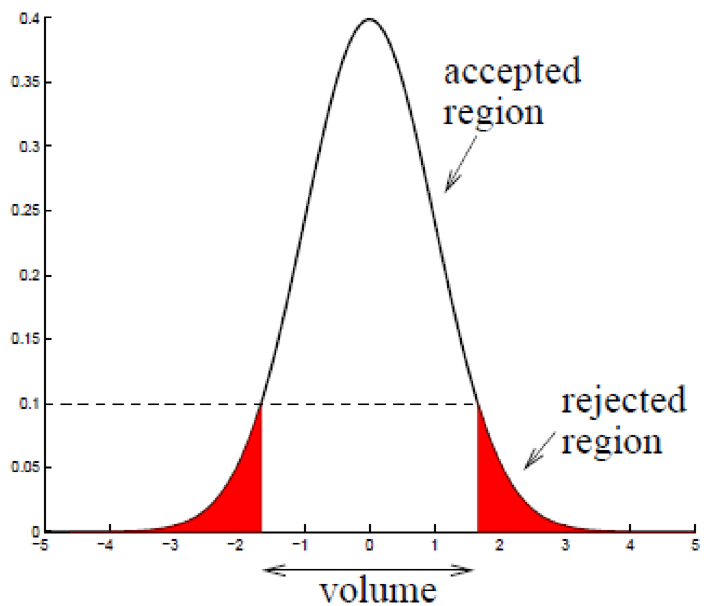
Kernel Density Estimation

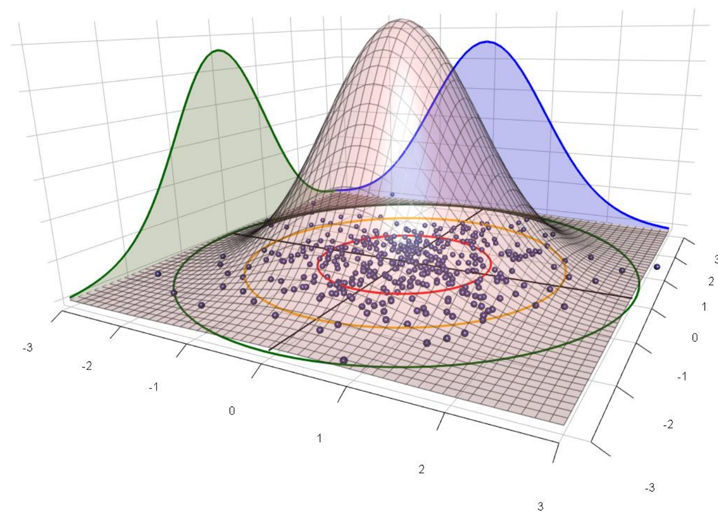


Number of modals = Number of instances

Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ Assume that the observed data are drawn from a Gaussian distribution





$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} exp\left[\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

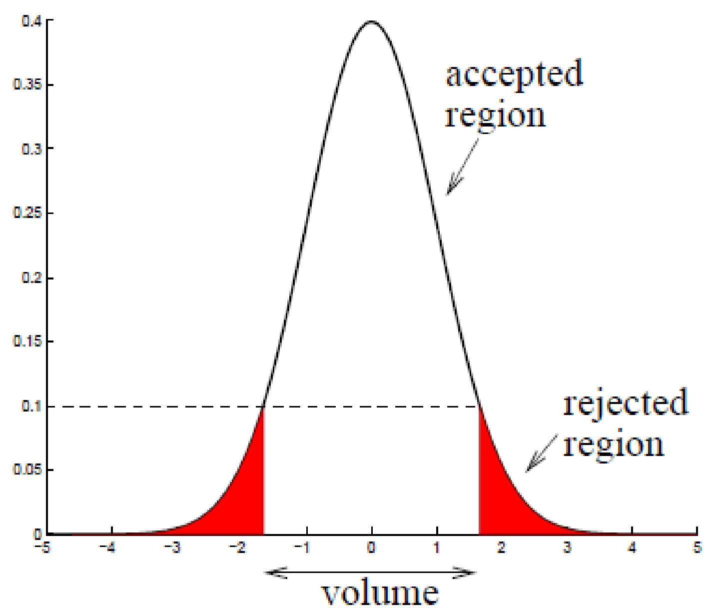
$$\boldsymbol{\mu} = \frac{1}{n}\sum_{\mathbf{x}_i\in\mathbf{X}^+}\mathbf{x}_i \text{ (mean vector)}, \quad \boldsymbol{\Sigma} = \frac{1}{n}\sum_{\mathbf{x}_i\in\mathbf{X}^+}(\mathbf{x}_i-\boldsymbol{\mu})(\mathbf{x}_i-\boldsymbol{\mu})^T \text{ (covariance matrix)}$$

Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ Advantages
    - Insensitive to scaling of the data

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}|^{1/2}} exp\left[\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

    - Possible to compute analytically the optimal threshold



Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ Parameter estimation: μ and σ^2
  - ✓ For one-dimensional data,

$$L = \prod_{i=1}^{N} P(x_i|\mu,\sigma^2) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x_i-\mu)^2}{2\sigma^2}\right)$$

$$Log\ L = -\frac{1}{2}\sum_{i=1}^{N}\frac{(x_i-\mu)^2}{\sigma^2} - \frac{N}{2}\log(2\pi\sigma^2)$$

Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ Maximum likelihood estimation, let's set $\gamma = 1/\sigma^2$

$$Log\ L = -\frac{1}{2}\sum_{i=1}^{N}\gamma(x_i - \mu)^2 - \frac{N}{2}\log(2\pi) + \frac{N}{2}\log(\gamma)$$

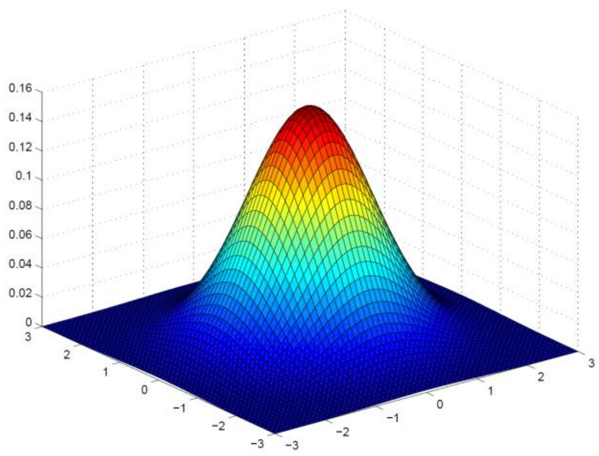
$$\frac{\partial Log\ L}{\partial \mu} = \gamma\sum_{i=1}^{N}(x_i - \mu) = 0\ \rightarrow \mu = \frac{1}{N}\sum_{i=1}^{N}x_i$$

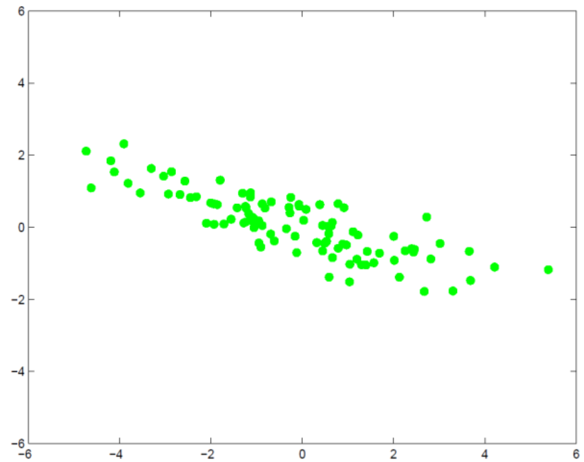
$$\frac{\partial Log\ L}{\partial \gamma} = -\frac{1}{2}\sum_{i=1}^{N}(x_i - \mu)^2 + \frac{N}{2\gamma} = 0 \rightarrow \sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$$

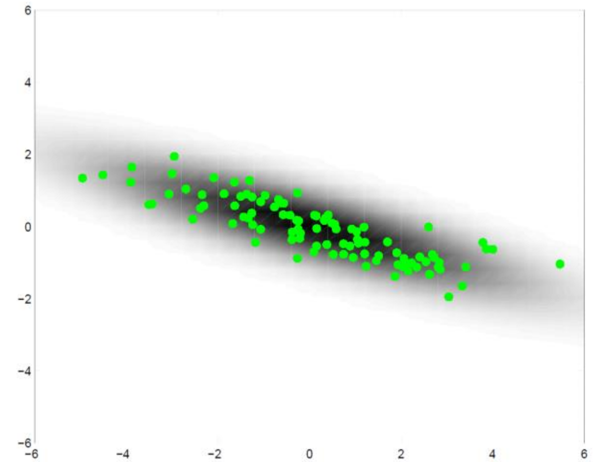
Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ In general,

$$\boldsymbol{\mu} = \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}_i, \quad \boldsymbol{\Sigma} = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \boldsymbol{\mu})(\mathbf{x}_i - \boldsymbol{\mu})^T$$



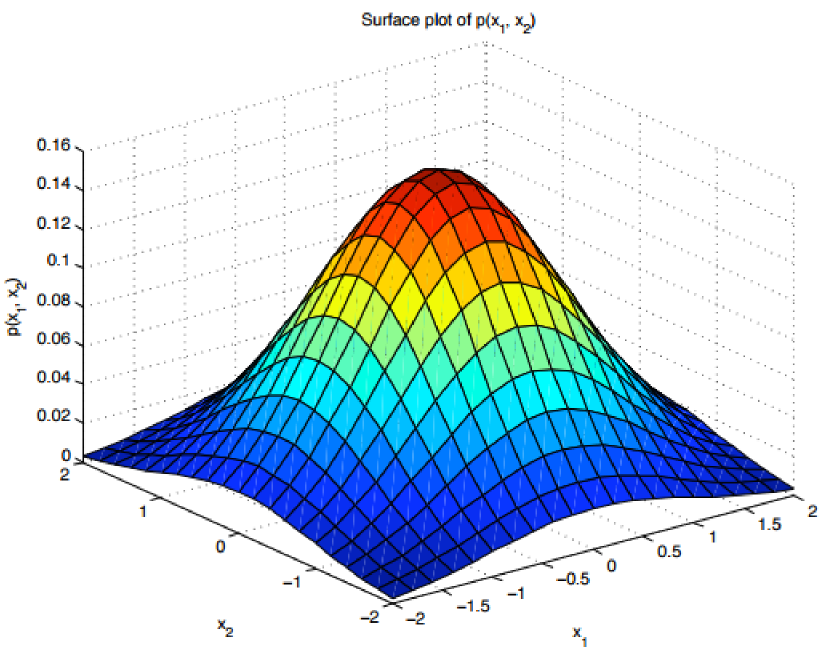


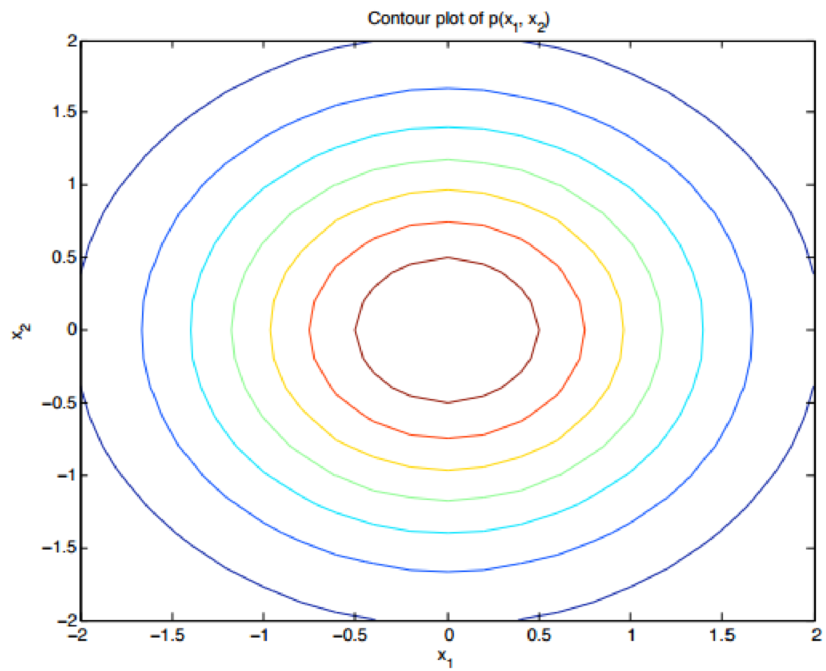


Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ The shape of Gaussian distribution according to the Covariance matrix type

Spherical $$\Sigma = \sigma^2 \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}$$



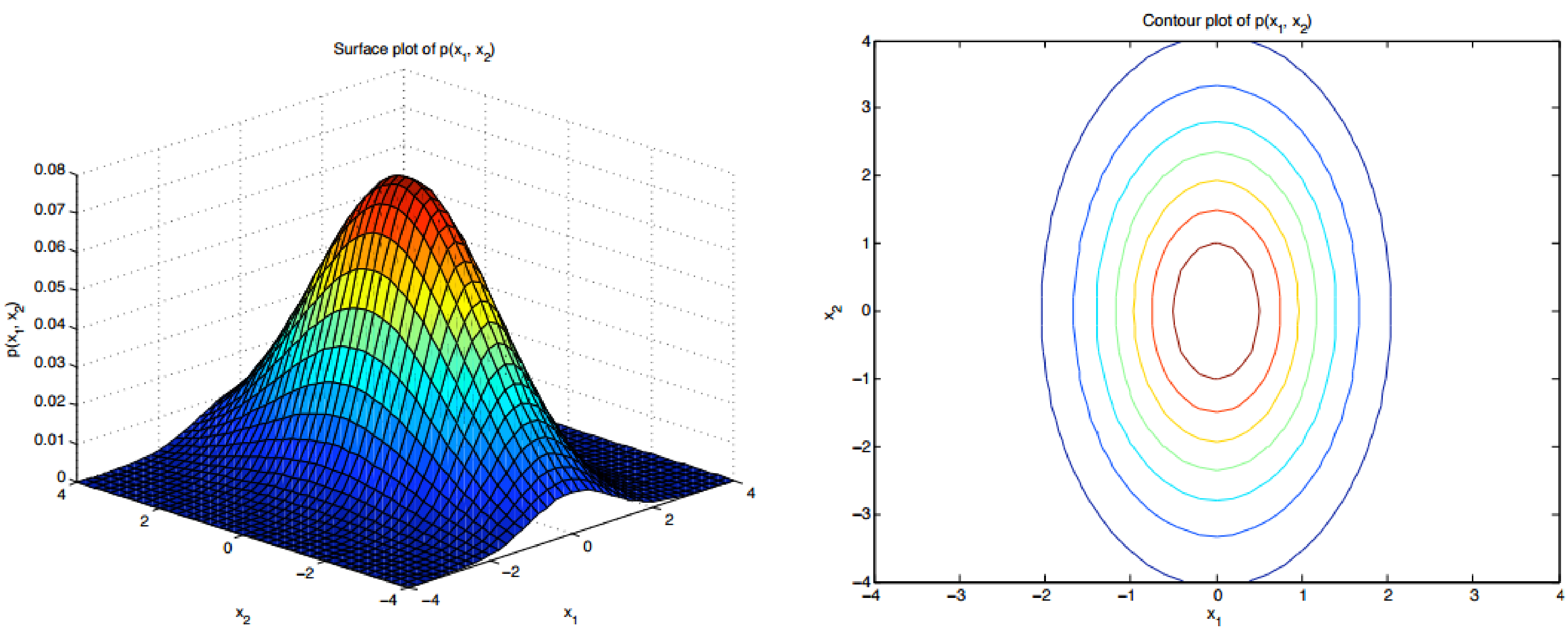


(a) Spherical Gaussian (diagonal covariance, equal variances)

Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ The shape of Gaussian distribution according to the Covariance matrix type

Diagonal $$\Sigma = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_d^2 \end{bmatrix}$$



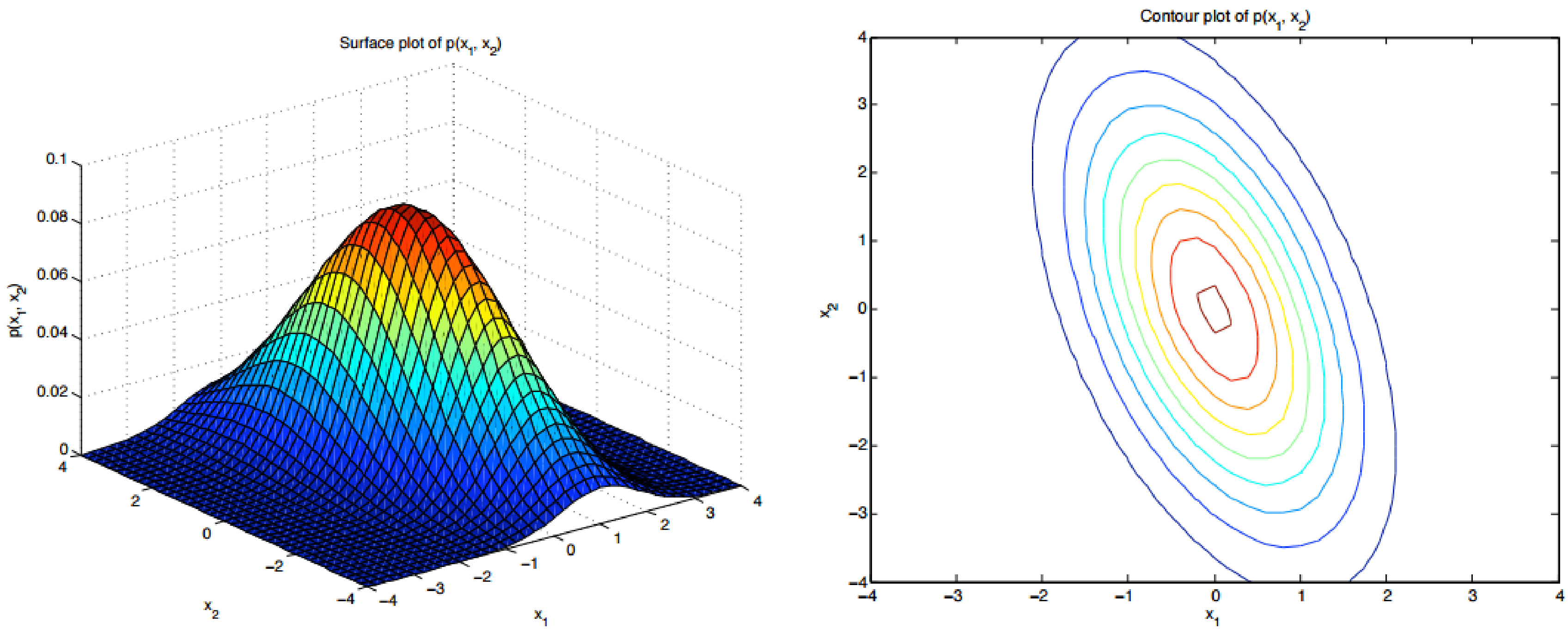
(b) Gaussian with diagonal covariance matrix

Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ The shape of Gaussian distribution according to the Covariance matrix type

Full

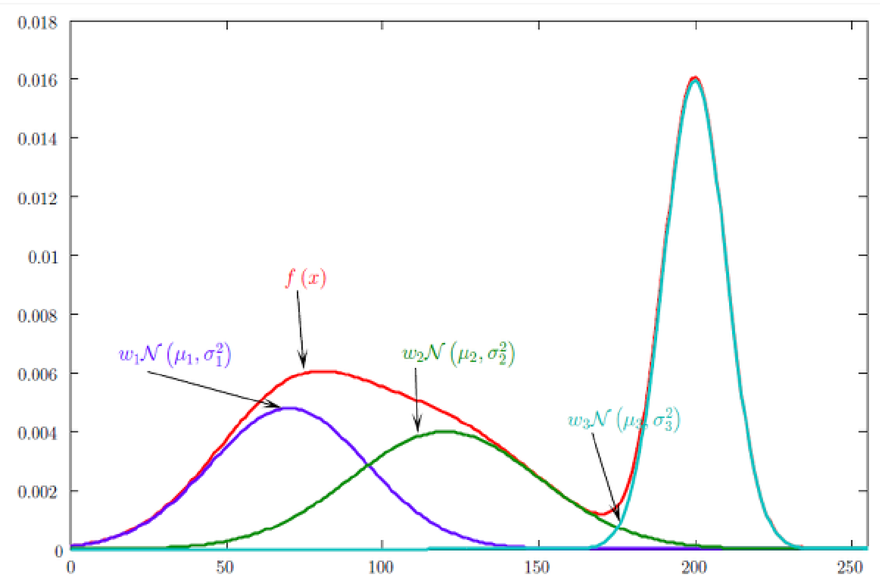
$$\Sigma = \begin{bmatrix} \sigma_{11} & \cdots & \sigma_{1d} \\ \vdots & \ddots & \vdots \\ \sigma_{d1} & \cdots & \sigma_{dd} \end{bmatrix}$$



(c) Gaussian with full covariance matrix

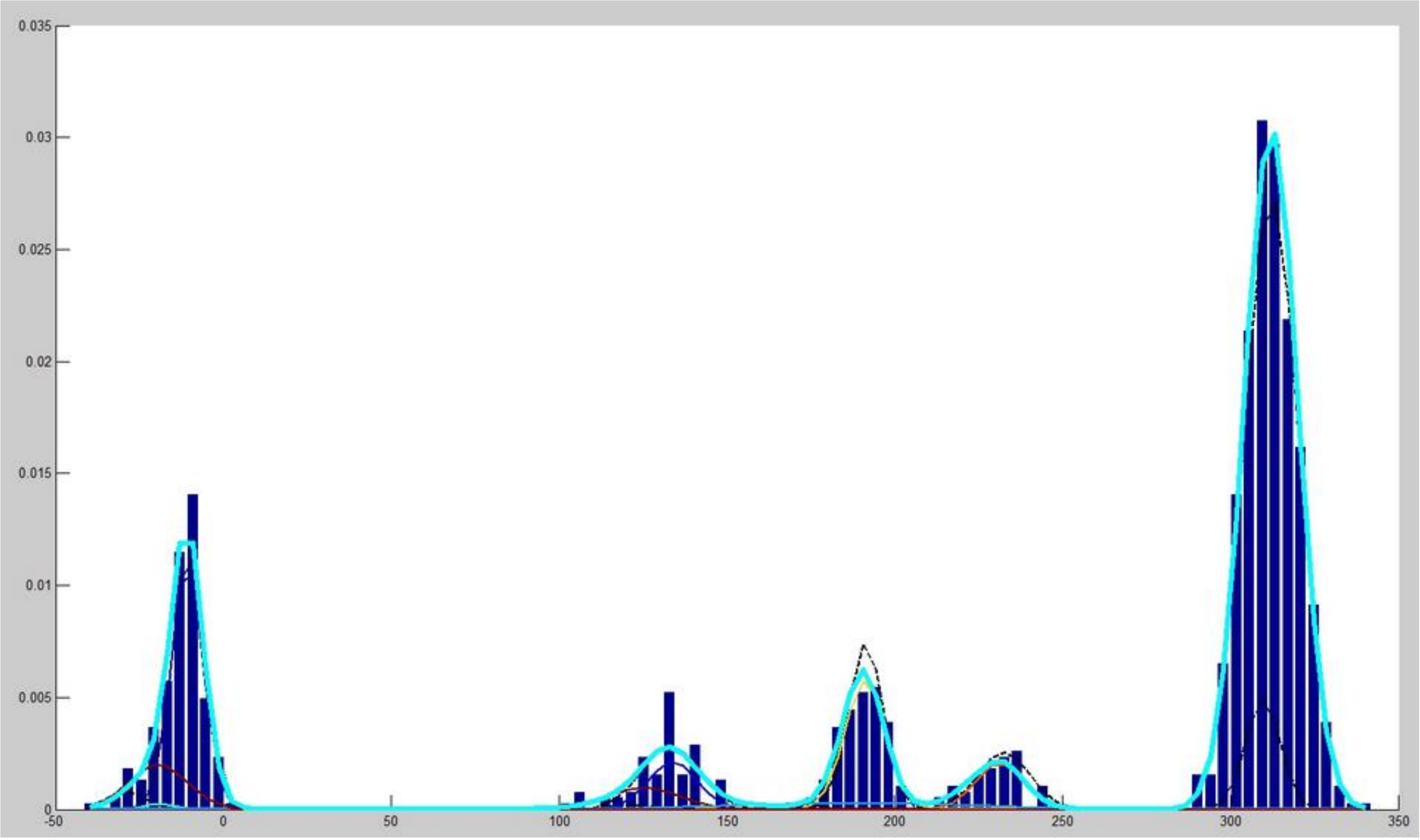
Mixture of Gaussian Density Estimation

- Mixture of Gaussian (MoG) Density Estimation
  - ✓ Gaussian Density Estimation
    - assumes a very strong model of the data: unimodal and convex
  - ✓ MoG
    - an extension of Gaussian that allows multi-modal distribution
    - a linear combination of normal distributions
    - Has a smaller bias than the single Gaussian distribution, but requires far more data for training



Mixture of Gaussian Density Estimation

- MoG example



Mixture of Gaussian Density Estimation

- Components of MoG
  - ✓ Probability of an instance belonging to the normal class

$$p(\mathbf{x}|\lambda) = \sum_{m=1}^{M} w_m g(\mathbf{x}|\boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m)$$

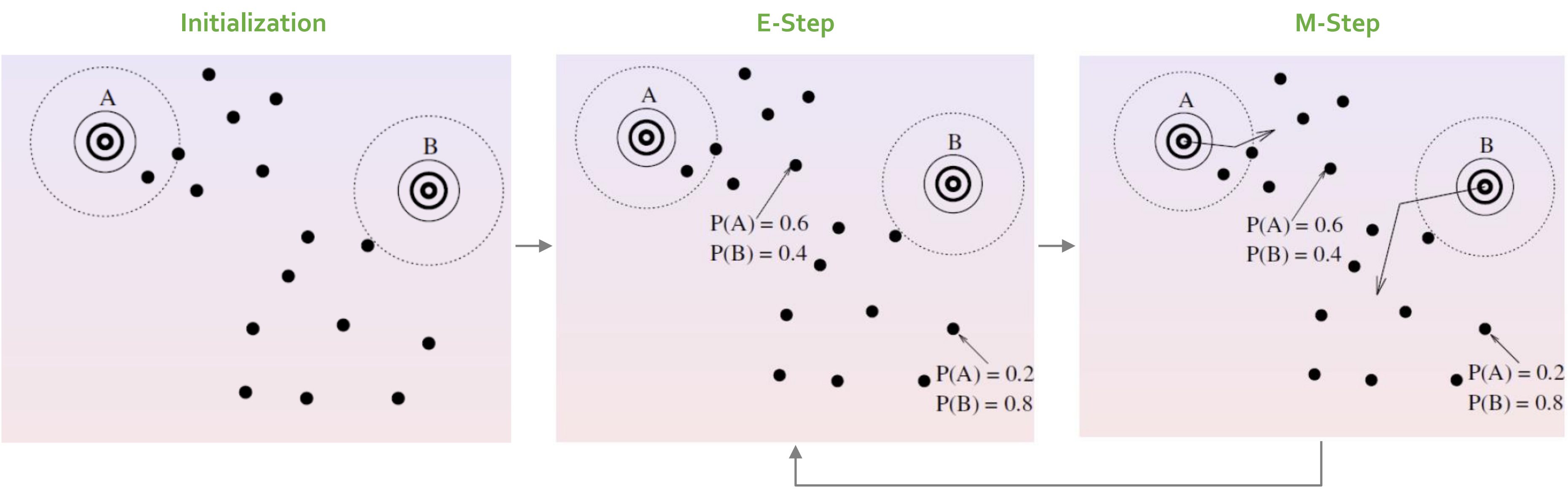
  - ✓ Distribution of each Gaussian model

$$g(\mathbf{x}|\boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}_m|^{1/2}} exp\left[\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_m)^T \boldsymbol{\Sigma}_m^{-1}(\mathbf{x}-\boldsymbol{\mu}_m)\right]$$

$$\lambda = \{w_m, \boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m\}, \quad m = 1, \cdots, M$$

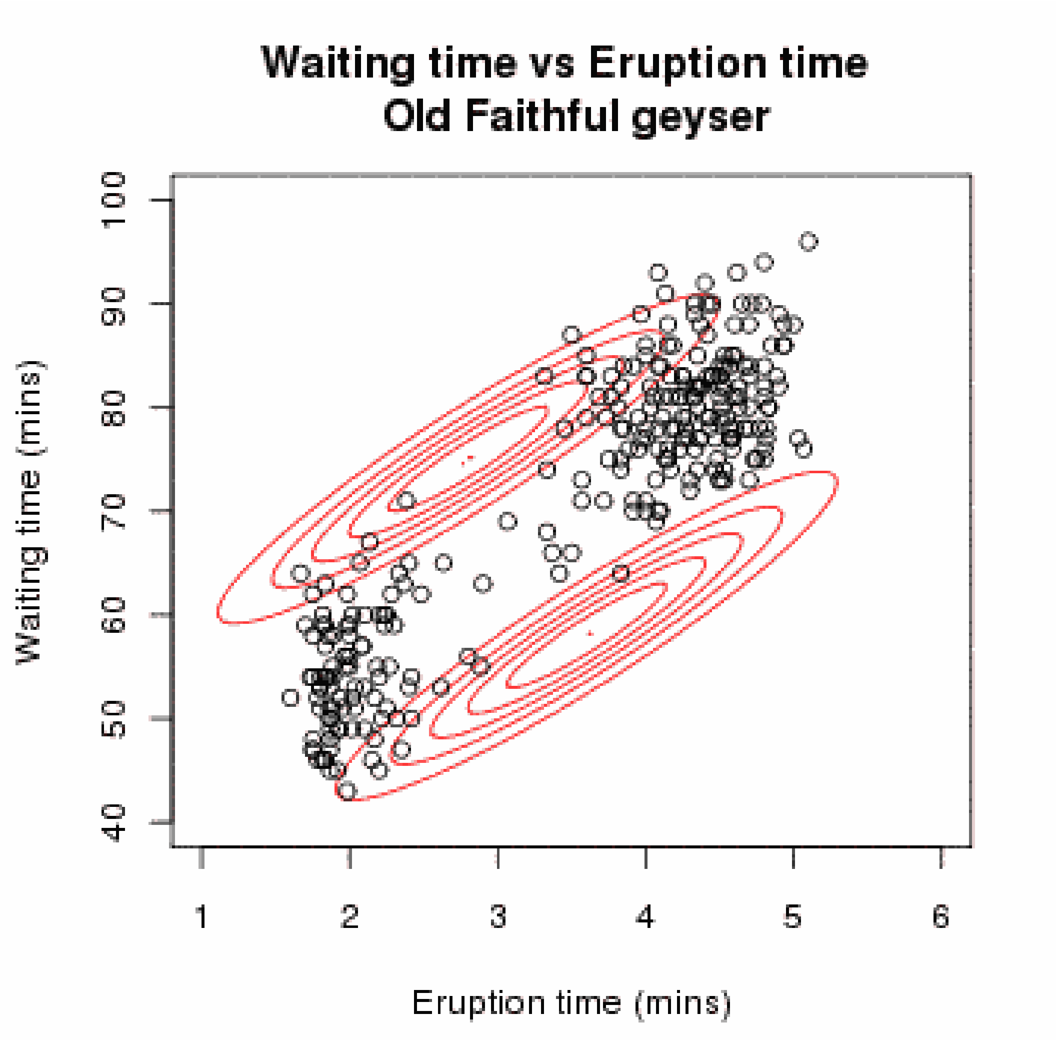
Mixture of Gaussian Density Estimation

- Expectation-Maximization Algorithm
  - ✓ E-Step: Given the current estimate of the parameters, compute the conditional probabilities
  - ✓ M-Step: Update the parameters to maximize the expected likelihood found in the E-Step



Mixture of Gaussian Density Estimation

- Expectation-Maximization Algorithm: Illustrative example



Mixture of Gaussian Density Estimation

- EM algorithm for MoG
  - ✓ Expectation

$$p(m|\mathbf{x}_i,\lambda) = \frac{w_m g(\mathbf{x}_i|\boldsymbol{\mu}_m,\boldsymbol{\Sigma}_m)}{\sum_{k=1}^{M} w_k g(\mathbf{x}_t|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}$$

  - ✓ Maximization
    - Mixture weight

$$w_m^{(new)} = \frac{1}{N}\sum_{i=1}^{N} p(m|\mathbf{x}_i,\lambda)$$

    - Means and variances

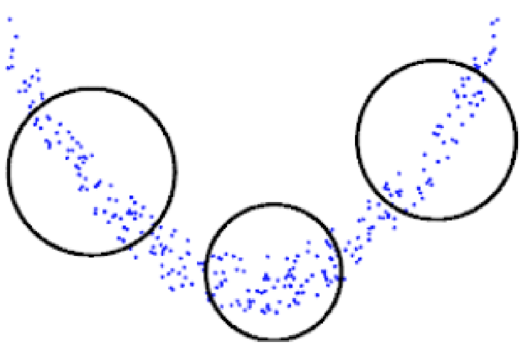
$$\boldsymbol{\mu}_m^{(new)} = \frac{\sum_{i=1}^{N} p(m|\mathbf{x}_i,\lambda)\mathbf{x}_i}{\sum_{i=1}^{N} p(m|\mathbf{x}_i,\lambda)}, \quad \sigma_m^{2(new)} = \frac{\sum_{i=1}^{N} p(m|\mathbf{x}_i,\lambda)\mathbf{x}_i^2}{\sum_{i=1}^{N} p(m|\mathbf{x}_i,\lambda)} - \boldsymbol{\mu}_m^{2(new)}$$

Mixture of Gaussian Density Estimation

- The shape of MoG according to the covariance matrix

Spherical

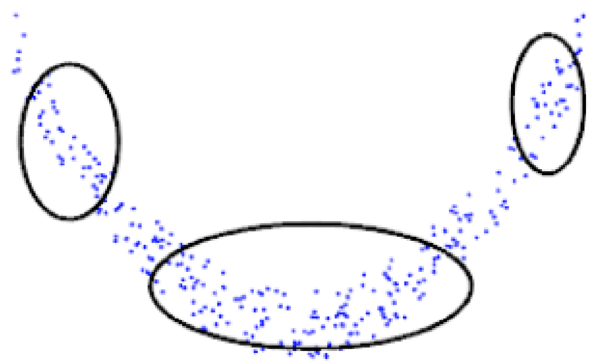
$$\Sigma = \sigma^2 \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}$$



- Less precise
- Very efficient to compute

Diagonal

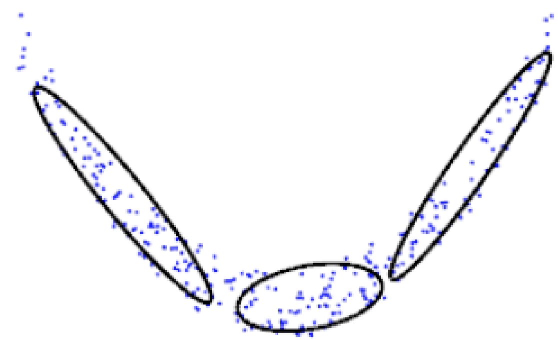
$$\Sigma = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_d^2 \end{bmatrix}$$



- More precise
- Efficient to compute

Full

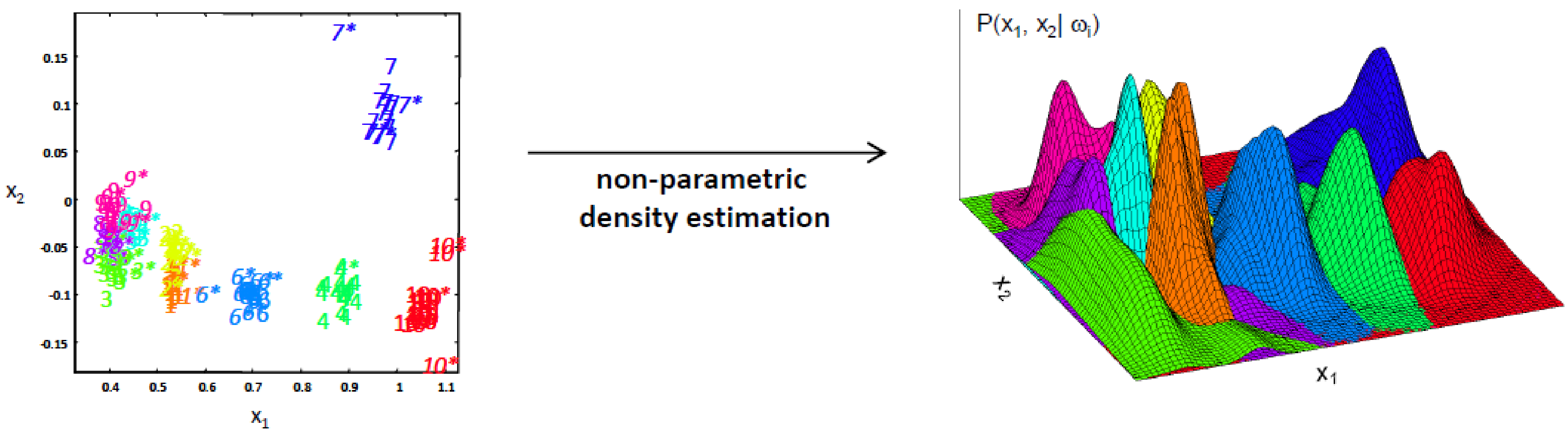
$$\Sigma = \begin{bmatrix} \sigma_{11} & \cdots & \sigma_{1d} \\ \vdots & \ddots & \vdots \\ \sigma_{d1} & \cdots & \sigma_{dd} \end{bmatrix}$$



- Very precise
- Less efficient to compute

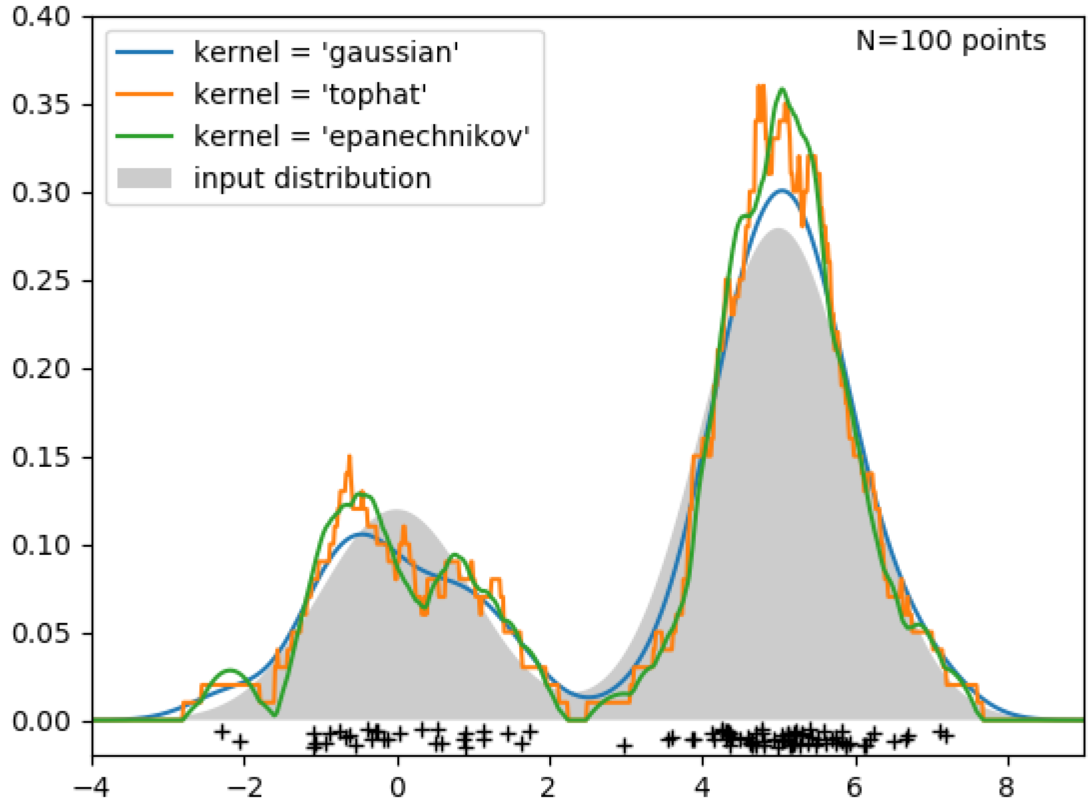
Kernel-density Estimation

- Kernel-density Estimation
  - ✓ Attempts to estimate the density directly from the data without assuming a particular form for the underlying distribution



Kernel-density Estimation

- Kernel-density Estimation: 1-D example



Kernel-density Estimation

- Kernel-density Estimation
  - ✓ The probability that a vector x, drawn from a distribution p(x), will fall in a given region R of the sample space

$$P = \int_R p(x')dx'$$

  - ✓ Suppose that N vectors $\{\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n\}$ are drawn from the distribution; the probability that k of these N vectors fall in R is given by

$$P(k) = \binom{N}{k} P^k (1-P)^{N-k}$$

  - ✓ It can be shown that (from the binomial distribution) the mean and variance of the ratio k/N are

$$E\left[\frac{k}{N}\right] = P, \qquad Var\left[\frac{k}{N}\right] = \frac{P(1-P)}{N}$$

Kernel-density Estimation

- Kernel-density Estimation
  - ✓ As $N \rightarrow \infty$, the distribution becomes sharper (the variance gets smaller), so we can expect that a good estimate of the probability P can be obtained from the mean fraction of the points that fall within R

$$P \cong \frac{k}{N}$$

  - ✓ If we assume that R is so small that p(x) does not vary appreciably within it, then

$$P = \int_R p(x')dx' \cong p(x)V$$

  - ✓ where V is the volume enclosed by region R
  - ✓ Merging the two previous results

$$P = \int_R p(x')dx' \cong p(x)V = \frac{k}{N}, \qquad p(x) = \frac{k}{NV}$$

Kernel-density Estimation

- Kernel-density Estimation

$$p(x) = \frac{k}{NV}, \qquad where \begin{Bmatrix} V\text{: volume surrounding } x \\ N\text{: the total number of examples} \\ k\text{: the number of examples inside } V \end{Bmatrix}$$

✓ Estimation becomes more accurate as we increase the number of sample points N and shrink the volume V

✓ In practice, the total number of examples is fixed so that we have to find a compromise for V

- Large enough to include enough examples within R
- Small enough to support the assumption that p(x) is constant within R

✓ Fix V and determine k from the data: Kernel-density estimation

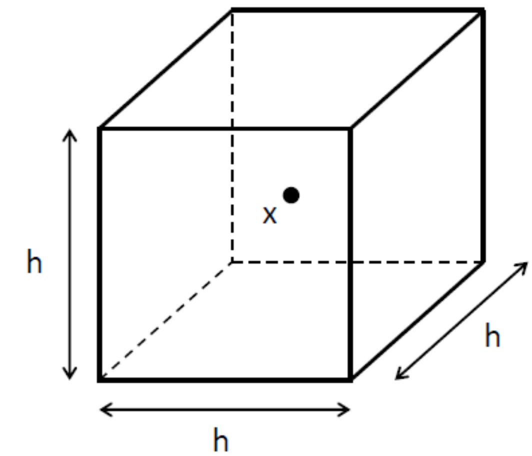
✓ Fix k and determine V from the data: k-nearest neighbor density estimation

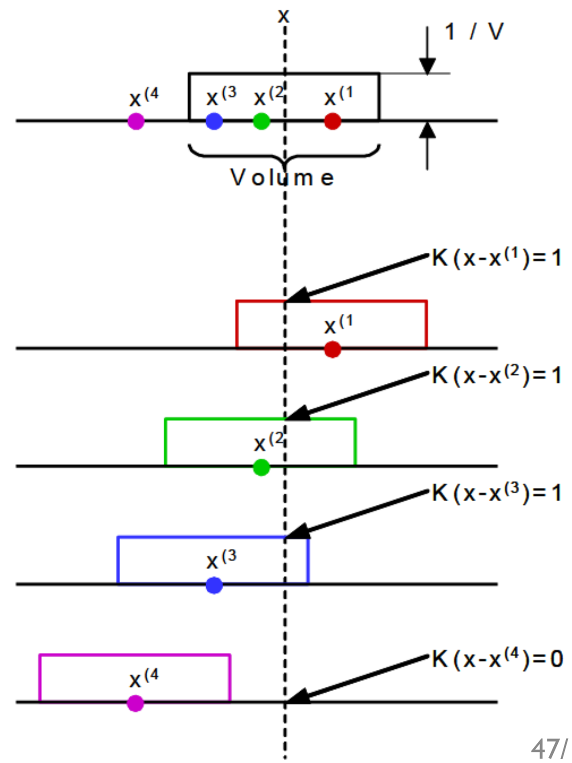
Parzen Window Density Estimation

- Parzen Window Density Estimation
  - ✓ Assume that the region R that encloses the k examples is a hypercube with sides of length h centered at x
    - Its volume is given by V = h^d, d: N. dimensions
  - ✓ Define a kernel function K(u)

$$K(u) = \begin{cases} 1 & |u_j| < \frac{1}{2} \ \forall j = 1, \ldots d \\ 0 & otherwise \end{cases}$$

$$k = \sum_{i=1}^{N} K\left(\frac{\mathbf{x}^i - \mathbf{x}}{h}\right) \qquad p(x) = \frac{1}{Nh^d} \sum_{i=1}^{N} K\left(\frac{\mathbf{x}^i - \mathbf{x}}{h}\right)$$



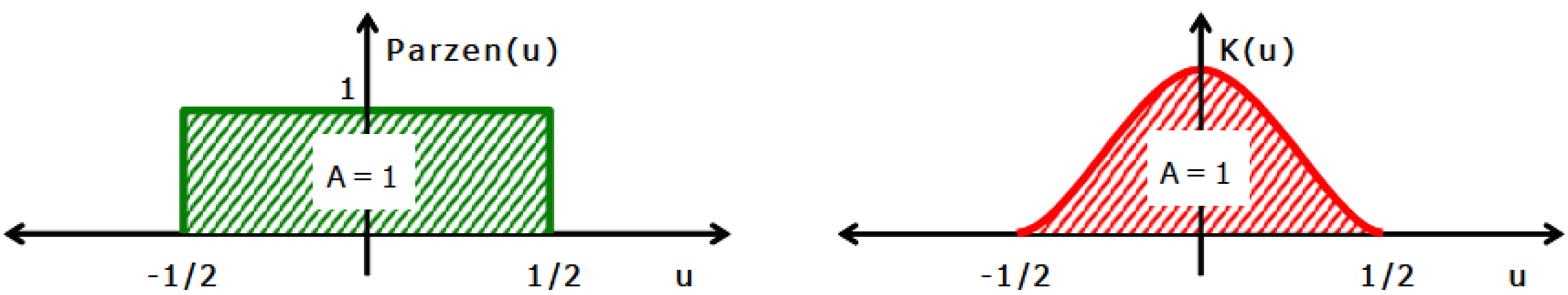


Parzen Window Density Estimation

- Drawbacks of K(u)
  - ✓ Yields density estimate that have discontinuities
  - ✓ Weights equally all points $\mathbf{x}^i$, regardless of their distance to the estimation point $\mathbf{x}$
- Smooth kernel function

$$P = \int_R K(x)\,dx = 1$$

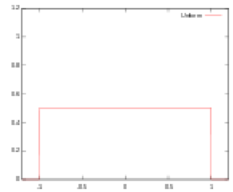
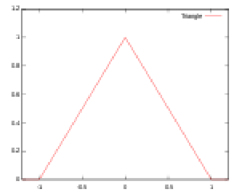
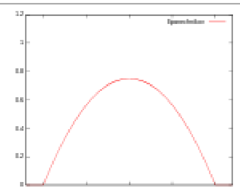
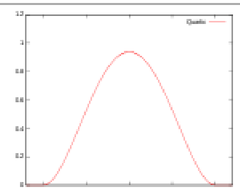
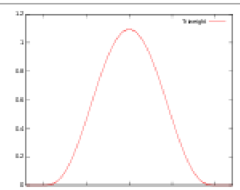
  - ✓ Commonly use a radially symmetric and unimodal pdf, such as Gaussian

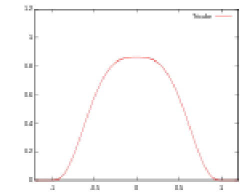
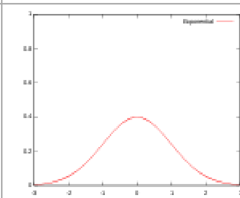
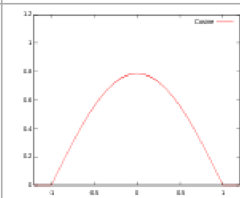


$$p(x) = \frac{1}{N}\sum_{i=1}^{N} K\left(\frac{\mathbf{x}^i - \mathbf{x}}{h}\right)$$

Parzen Window Density Estimation

- Example of smooth kernels

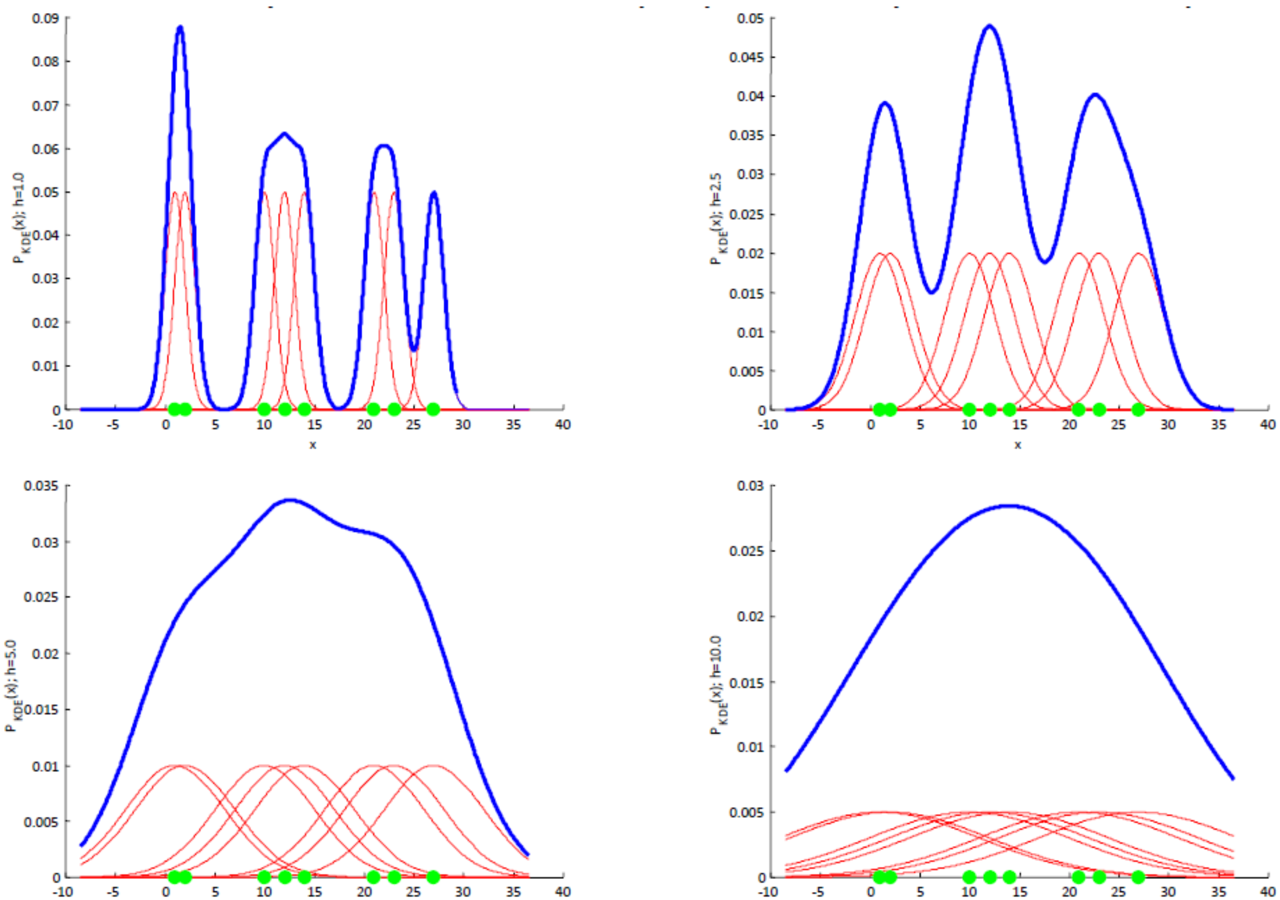
Uniform	$K(u) = \frac{1}{2}\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Triangular	$K(u) = (1 - \lvert u\rvert)\,\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Epanechnikov	$K(u) = \frac{3}{4}(1 - u^2)\,\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Quartic (biweight)	$K(u) = \frac{15}{16}(1 - u^2)^2\,\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Triweight	$K(u) = \frac{35}{32}(1 - u^2)^3\,\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	

Tricube	$K(u) = \frac{70}{81}(1 - \lvert u\rvert^3)^3\,\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Gaussian	$K(u) = \frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}u^2}$	
Cosine	$K(u) = \frac{\pi}{4}\cos\left(\frac{\pi}{2}u\right)\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Logistic	$K(u) = \frac{1}{e^u + 2 + e^{-u}}$	
Silverman kernel[4]	$K(u) = \frac{1}{2}e^{-\frac{\lvert u\rvert}{\sqrt{2}}} \cdot \sin\left(\frac{\lvert u\rvert}{\sqrt{2}} + \frac{\pi}{4}\right)$	

https://en.wikipedia.org/wiki/Kernel_(statistics)

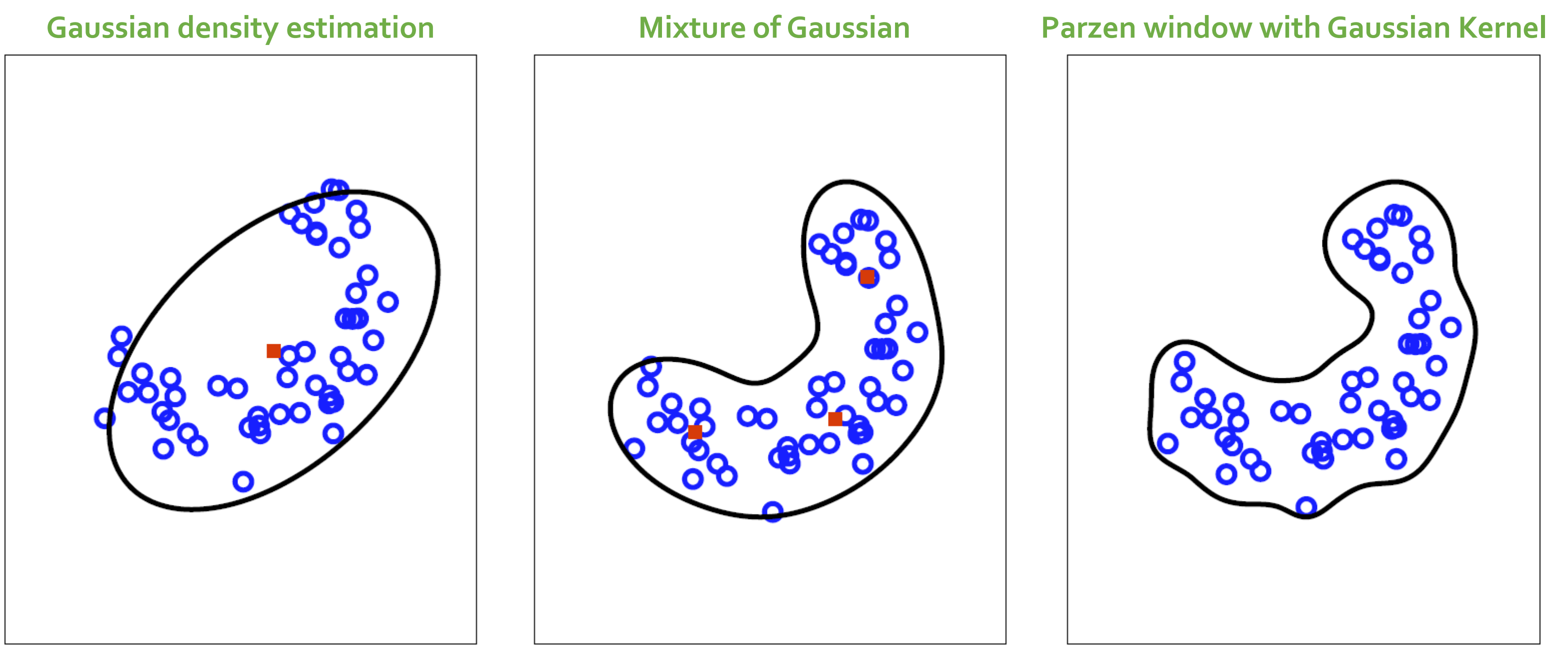
Parzen Window Density Estimation

- Smoothing parameter (bandwidth) h
  - ✓ A large h will over-smooth the density distribution
  - ✓ A small h will result in a spiky density distribution



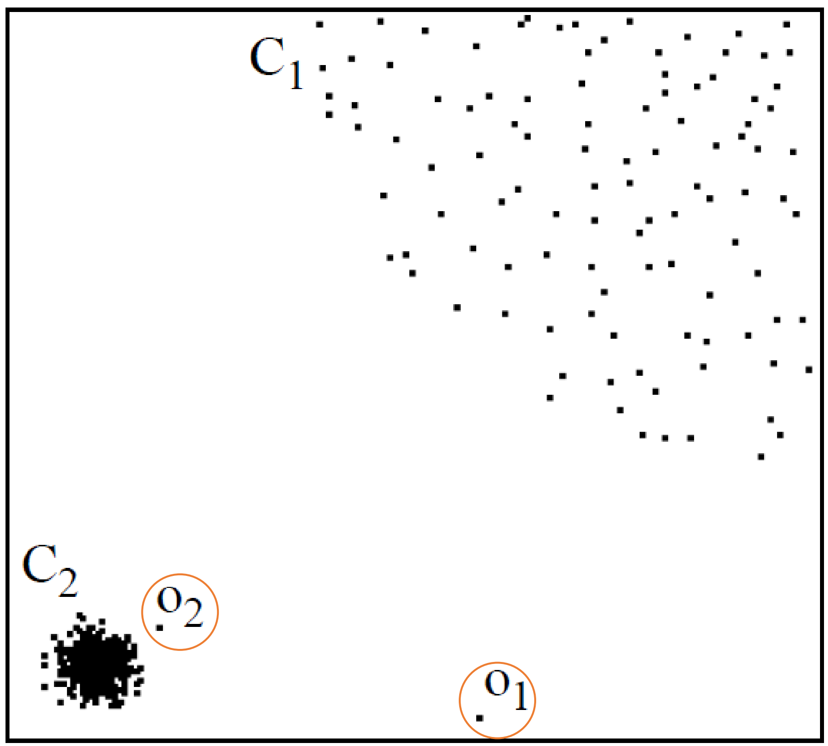
Parzen Window Density Estimation

- Kernel Density Estimation
  - ✓ The smoothing parameter h can be optimized through EM algorithm



Local Outlier Factors (LOF)

- Motivation
  - ✓ Compute the novelty score of an instance by considering local density around it



Local Outlier Factors (LOF)

- Local Outlier Factors (LOF)
  - ✓ Definition 1: k-distance of an object p
    - For any positive integer k, the k-distance of object p, denoted as k-distance(p), is defined as the distance d(p,o) between p and an object o in D such that
    - for at least k objects o' in D\{p} it holds that $d(p, o') \leq d(p, o)$
    - for at most k-1 objects o' in D\{p} it holds that $d(p, o') < d(p, o)$
    - Simply it is the distance to the k-th nearest neighbor considering ties.

1st	2nd	3rd	4th	5th	6th	7th	3-distance
1	2	3	3	3	4	5	3
1	2	2	2	3	4	5	2
1	1	1	1	2	3	4	1

Local Outlier Factors (LOF)

- Local Outlier Factors (LOF)
  - ✓ Definition 2: k-distance neighborhood of an object p
    - Given the k-distance of p, the k-distance neighborhood of p contains every object whose distance from p is not grater than the k-distance

$$N_k(p) = \{q \in D \backslash \{p\} |\, d(p,q) \leq k - distance(p)\}$$

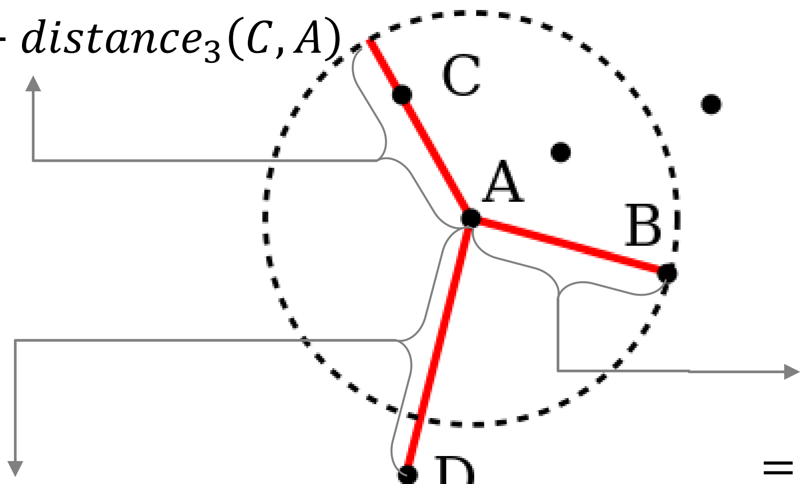
    - Example

1st	2nd	3rd	4th	5th	6th	7th	$k - distance(3)$	$N_3(p)$
1	2	3	3	3	4	5	3	5
1	2	2	2	3	4	5	2	4
1	1	1	1	2	3	4	1	4

Local Outlier Factors (LOF)

- Local Outlier Factors (LOF)
  - ✓ Definition 3: reachability distance
    - $rechability - distance_k(p, o) = \max\{k - distance(o), d(p, o)\}$
    - Examples

$rechability - distance_3(C, A)$



$3 - distance(A)$

$= rechability - distance_3(B, A)$

$rechability - distance_3(D, A)$

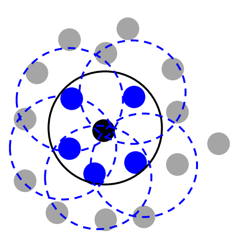
Local Outlier Factors (LOF)

- Local Outlier Factors (LOF)
  - ✓ Definition 4: local reachability density of an object p

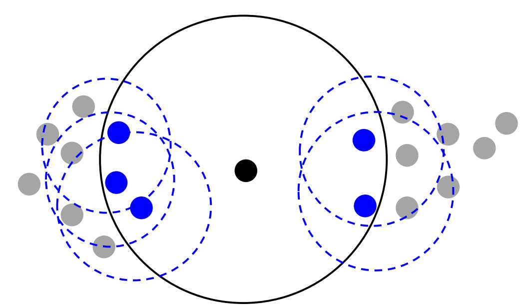
$$lrd_k(p) = \frac{|N_k(p)|}{\sum_{o \in N_k(p)} reachability - distance_k(p,o)}$$

- Case 1: p is located in the middle of a denser area: the denominator of $lrd_k(p)$ becomes small, which results in a large $lrd_k(p)$
- Case 2: p is located in a spare are between two dense data clusters: the denominator of $lrd_k(p)$ becomes large, which results in a small $lrd_k(p)$

Case 1



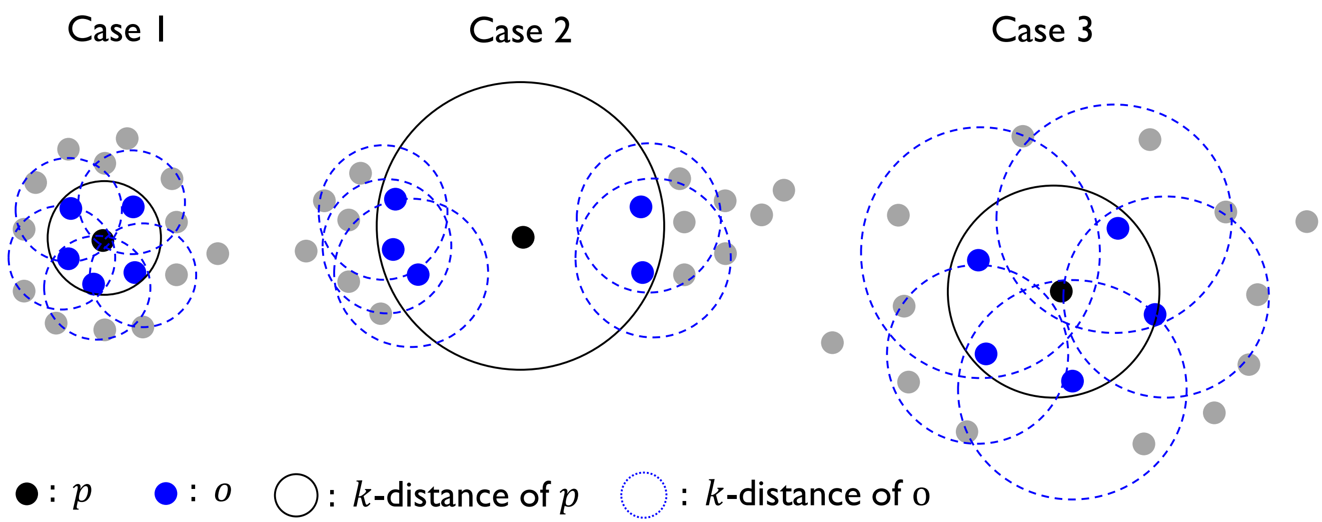
Case 2



Local Outlier Factors (LOF)

- Local Outlier Factors (LOF)
  - ✓ Definition 5: local outlier factor of an object p

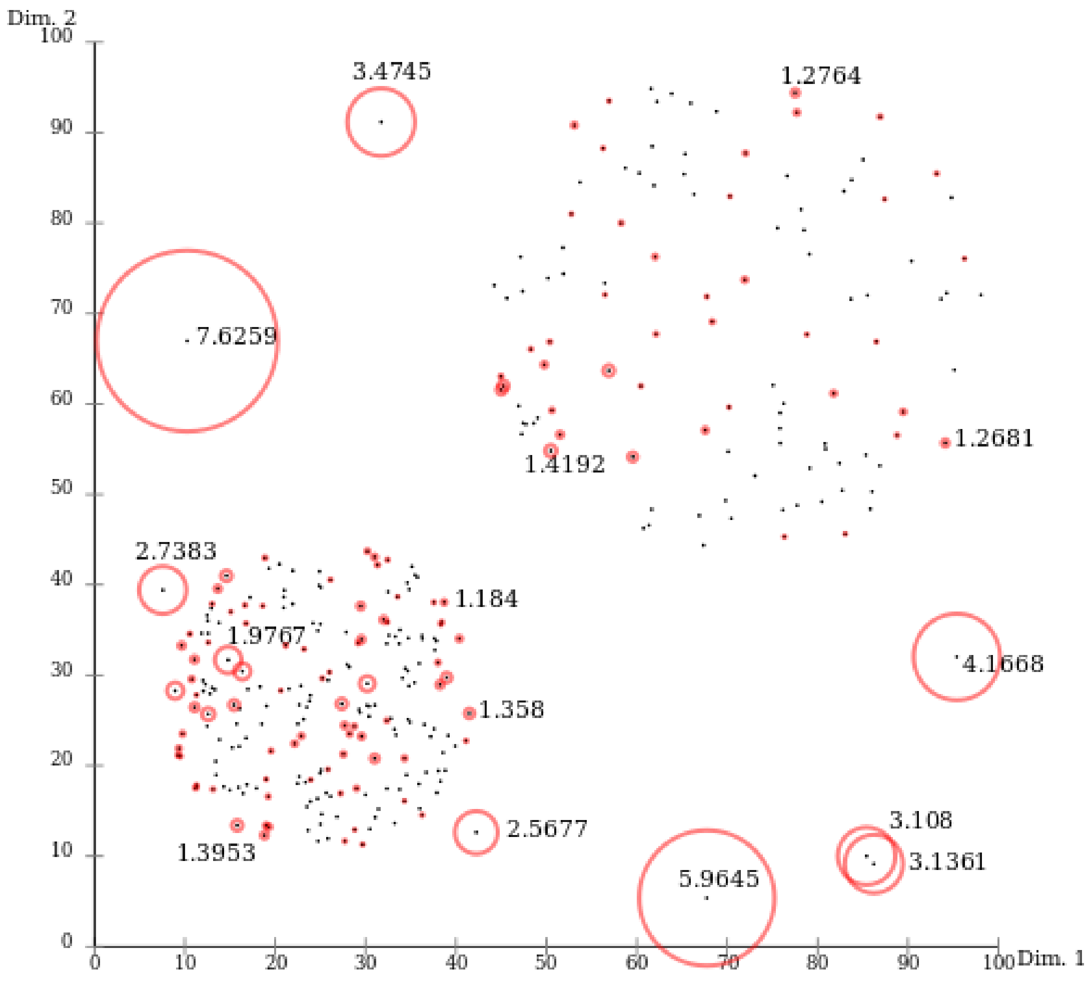
$$LOF_k(p) = \frac{\sum_{o \in N_k(p)} \frac{lrd_k(o)}{lrd_k(p)}}{|N_k(p)|} = \frac{\frac{1}{lrd_k(p)} \sum_{o \in N_k(p)} lrd_k(o)}{|N_k(p)|}$$



Case	$lrd_k(p)$	$lrd_k(o)$	$LOF_k(p)$
Case 1	Large	Large	Small
Case 2	Small	Large	Large
Case 3	Small	Small	Small

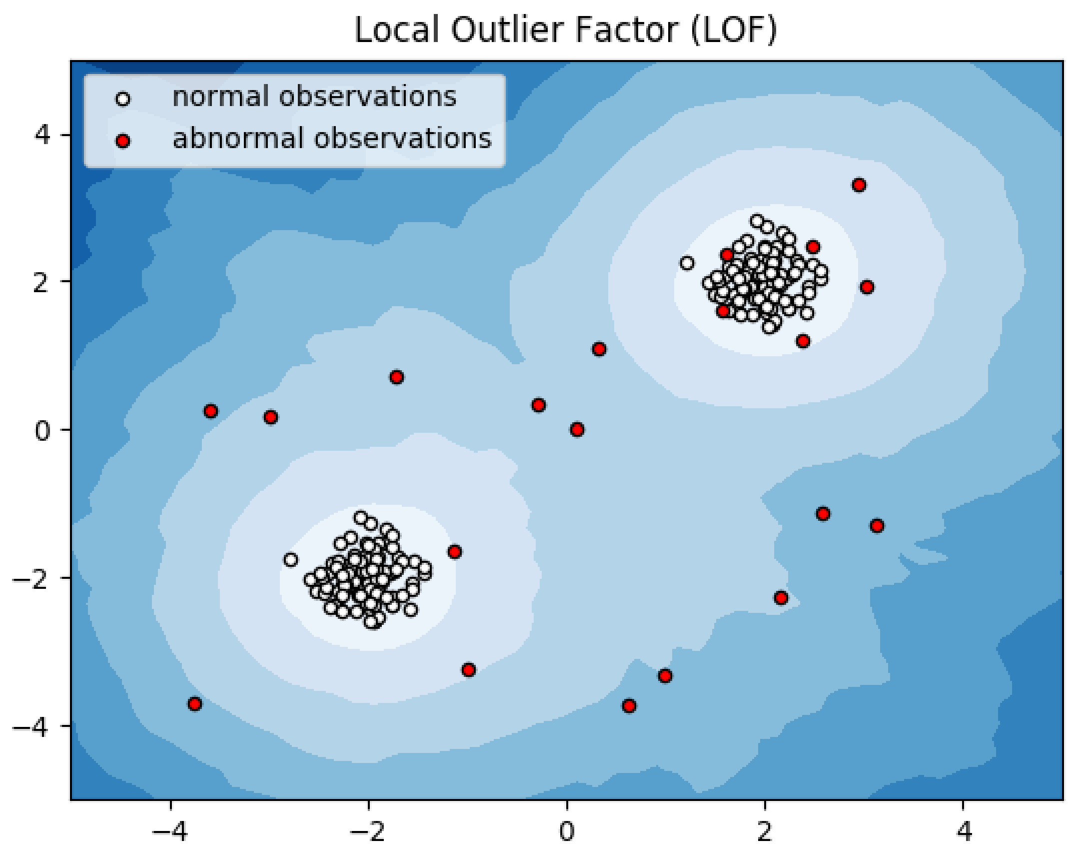
Local Outlier Factors (LOF)

- Local Outlier Factors (LOF)
  - ✓ For each point, compute the density of its local neighborhood



Local Outlier Factors (LOF)

- Local Outlier Factors (LOF)
  - ✓ LOF contour plot



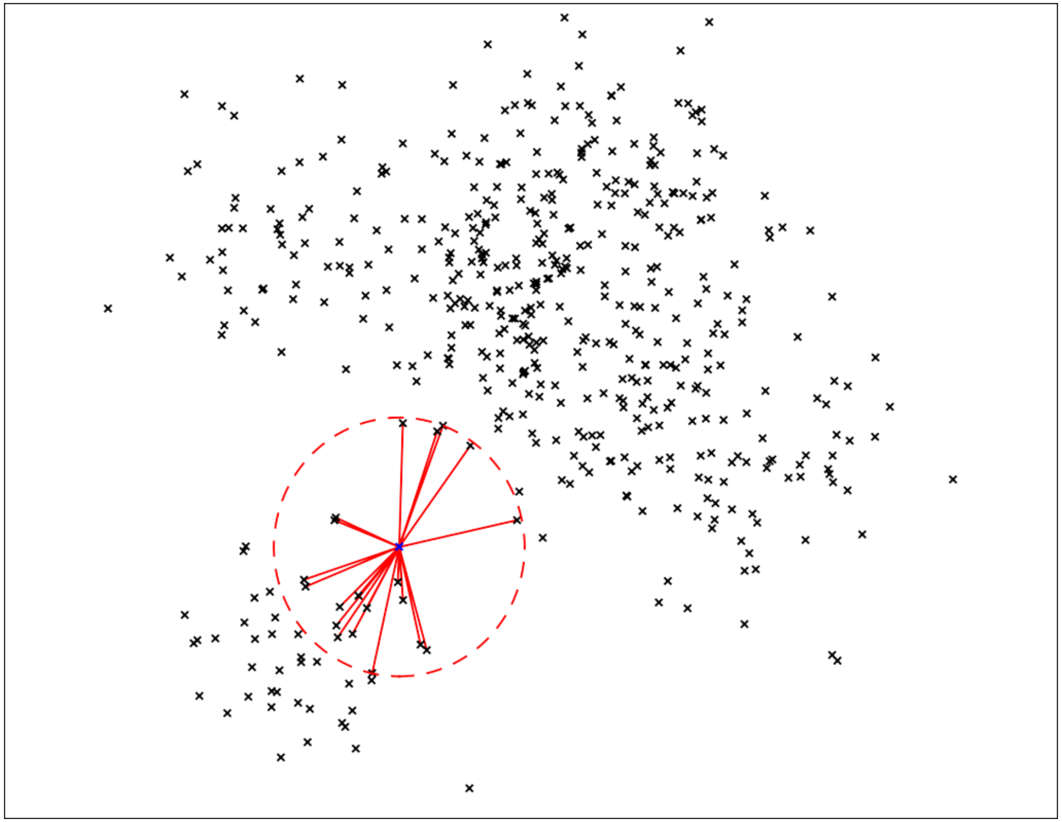
http://scikit-learn.org/stable/auto_examples/neighbors/plot_lof.html

AGENDA

k-Nearest Neighbor-based Novelty Detection

Harmeling et al. (2006)

- k-Nearest Neighbor-based Approach
  - ✓ Novelty score of an instance is computed based on the distance information to k nearest neighbors
  - ✓ Does not assume any prior probability distribution for the normal class



https://erikbern.com/2015/09/24/nearest-neighbor-methods-vector-models-part-1.html

k-Nearest Neighbor-based Novelty Detection

- Various distance information used for novelty score
  - ✓ Maximum distance to the k-th nearest neighbor

$$d^k_{max} = \kappa(\mathbf{x}) = ||\mathbf{x} - z_k(\mathbf{x})||$$

  - ✓ Average distance to the k-nearest neighbors

$$d^k_{avg} = \gamma(\mathbf{x}) = \frac{1}{k}\sum_{j=1}^{k}||\mathbf{x} - z_j(\mathbf{x})||$$

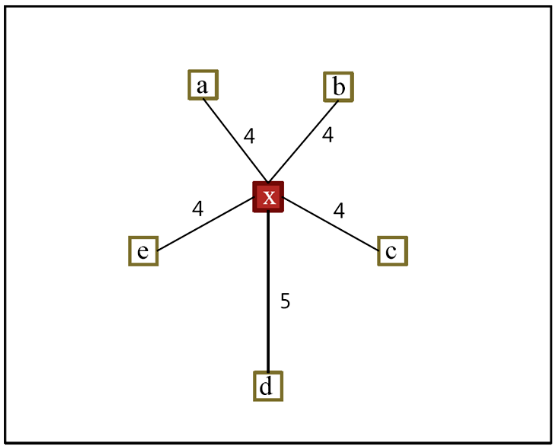
  - ✓ Distance to the mean of the k-nearest neighbors

$$d^k_{mean} = \delta(\mathbf{x}) = \left|\left|\mathbf{x} - \frac{1}{k}\sum_{j=1}^{k} z_j(\mathbf{x})\right|\right|$$

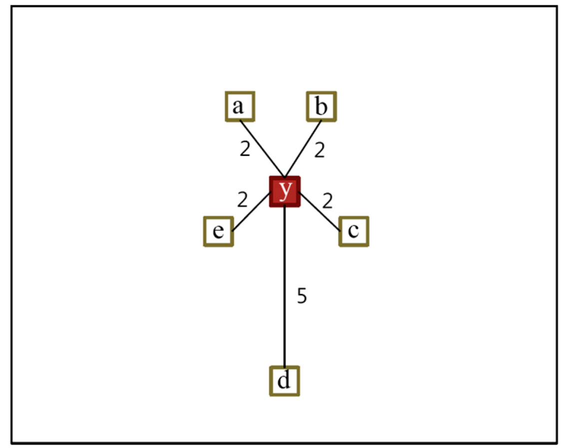
k-Nearest Neighbor-based Novelty Detection

Kang and Cho (2009)

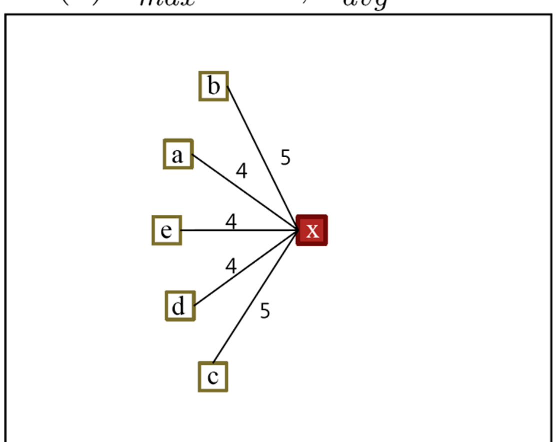
- Various distance information used for novelty score
  - ✓ Comparison among the maximum, average, and mean distance



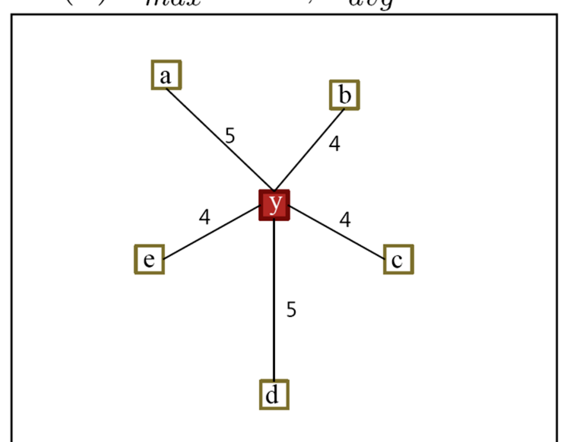
(a) $d^5_{max} = 5.0,\ d^5_{avg} = 4.2.$



(b) $d^5_{max} = 5.0,\ d^5_{avg} = 2.6.$



(c) $d^5_{avg} = 4.4,\ d^5_{mean} = 3.3.$



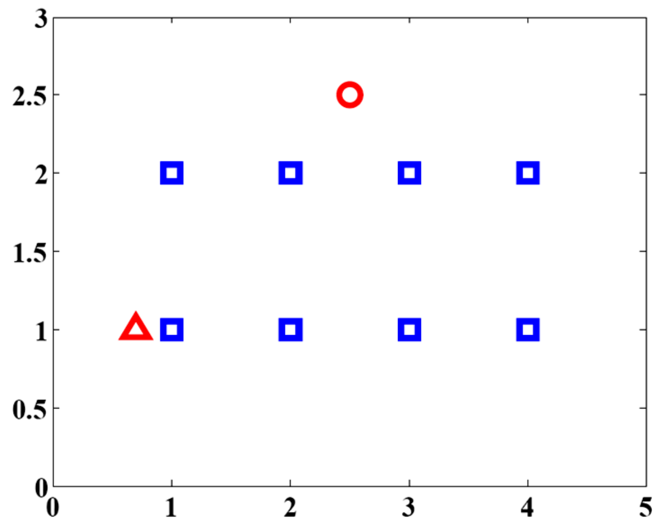
(d) $d^5_{avg} = 4.4,\ d^5_{mean} = 2.1.$

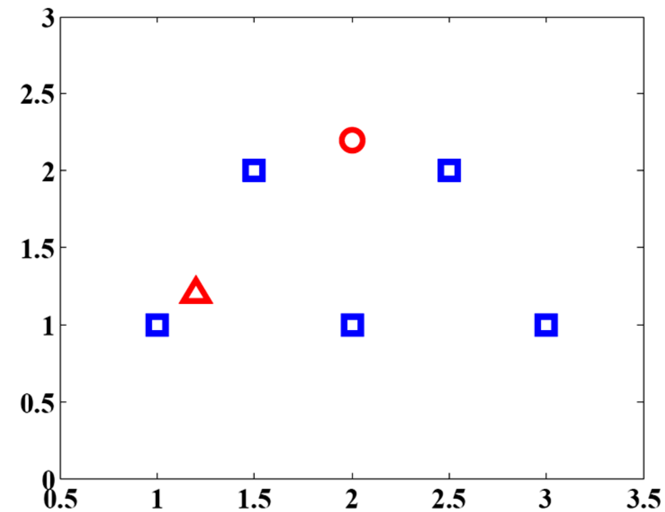
k-Nearest Neighbor-based Novelty Detection

Kang and Cho (2009)

- Counter example of the previous novelty scores
  - ✓ Which one should be identified as novel?

A





B

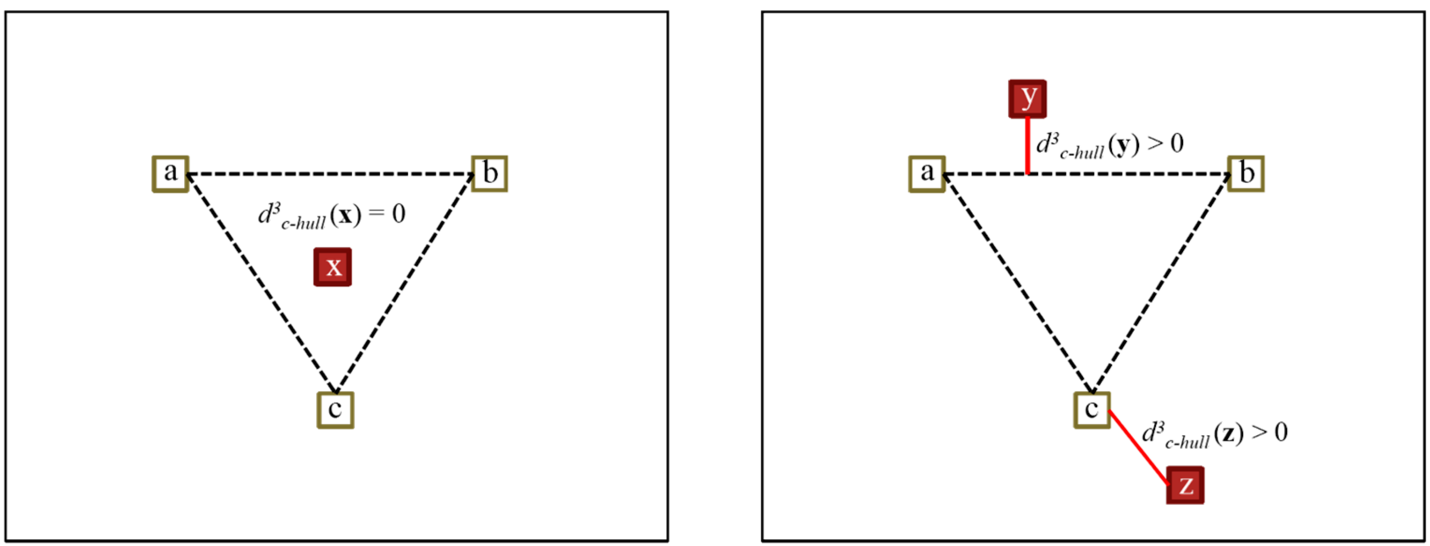
		d^k_{max}	d^k_{avg}	d^k_{mean}
A (k=4)	Circle	1.58	1.14	0.50
	Triangle	1.64	1.07	0.94
B (k=5)	Circle	1.56	1.08	0.80
	Triangle	1.86	1.09	0.88

k-Nearest Neighbor-based Novelty Detection

- Consider additional factor
  - ✓ whether the new instance is located inside the convex hull of its neighbors

$$\min_{\mathbf{w}} \left(d^k_{c-hull}(\mathbf{x})\right)^2 = \left|\left|\mathbf{x}_{new} - \sum_{j=1}^{k} \mathbf{w}_i z_j(\mathbf{x})\right|\right|^2$$

$$s.t. \sum_{i=1}^{k} \mathbf{w}_i = 1, \quad \mathbf{w}_i \geq 0, \ \forall i.$$



k-Nearest Neighbor-based Novelty Detection

- Combine the average distance and convex distance
  - ✓ Average distance to the k-nearest neighbors

$$d_{avg}^{k} = \frac{1}{k}\sum_{j=1}^{k}||\mathbf{x} - z_j(\mathbf{x})||$$

  - ✓ Convex distance to its k-nearest neighbors

$$d_{c-hull}^{k} = \left|\left|\mathbf{x} - \sum_{j=1}^{k}\mathbf{w}_i z_j(\mathbf{x})\right|\right|$$

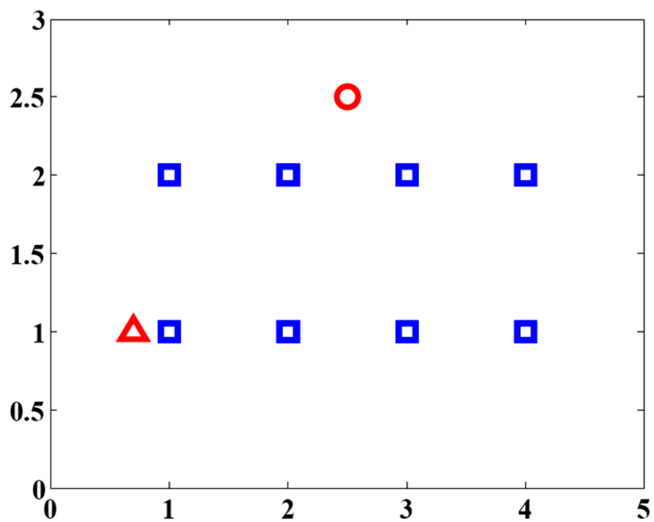
  - ✓ Put the penalty term using the convex distance for those instances located outside the convex hull of its k-nearest neighbors

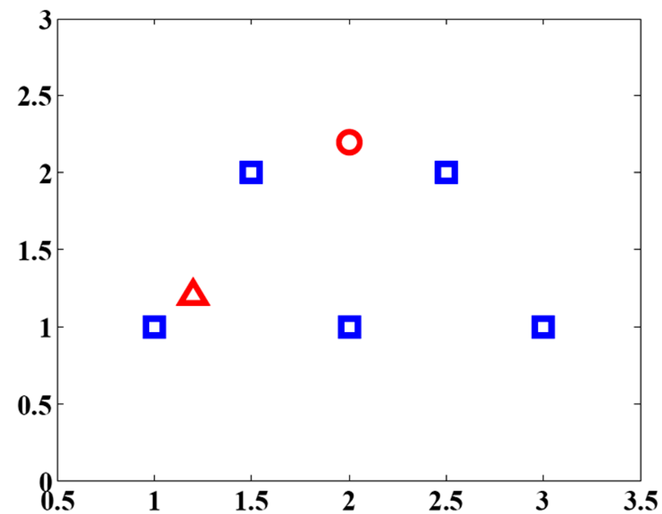
$$d_{hybrid}^{k} = d_{avg}^{k} \times \left(\frac{2}{1 + exp(-d_{c-hull}^{k})}\right)$$

k-Nearest Neighbor-based Novelty Detection

- Counter example revisited

A

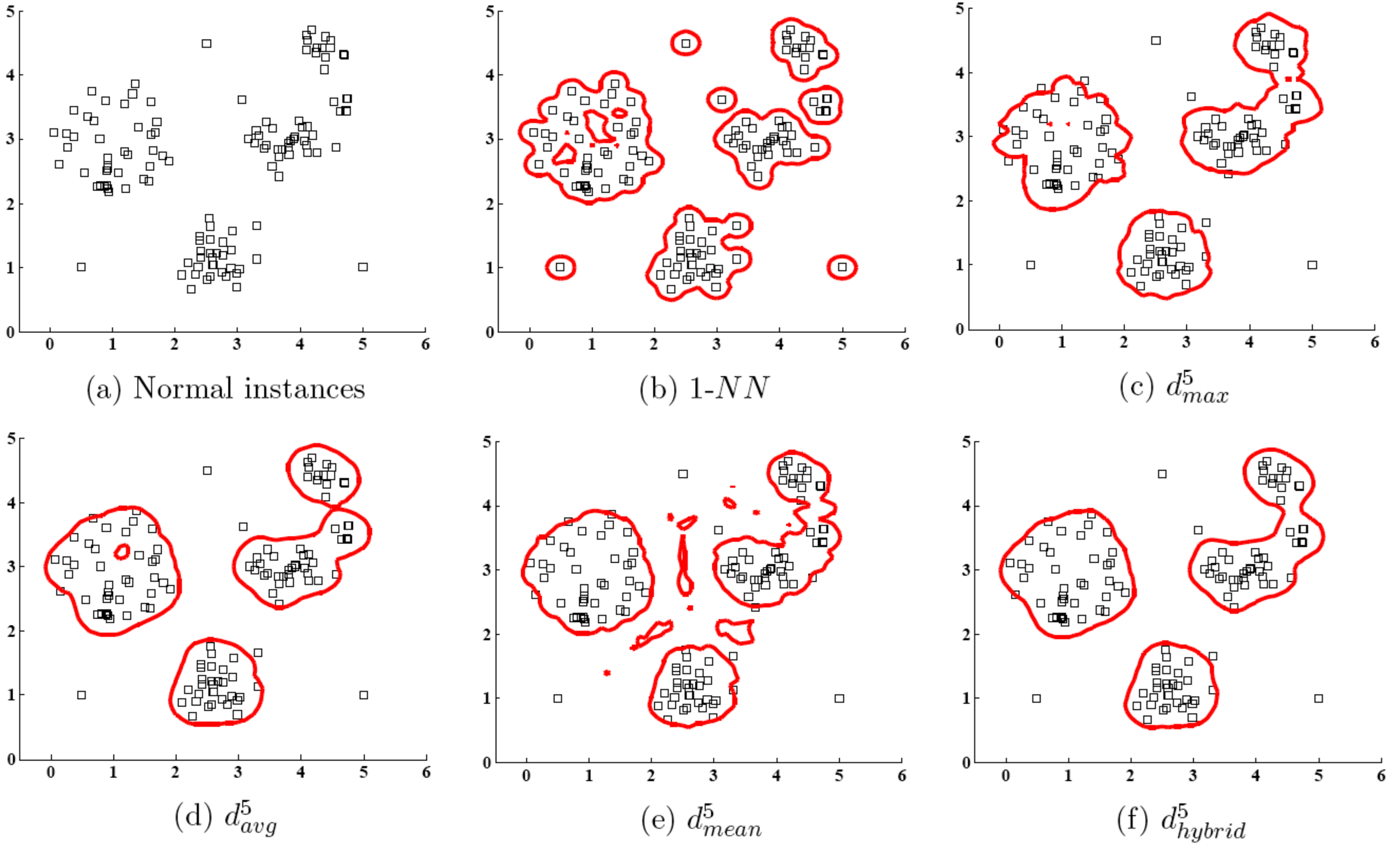




B

		d^k_{max}	d^k_{avg}	d^k_{mean}	d^k_{hybrid}
A (k=4)	Circle	1.58	1.14	0.50	1.42
	Triangle	1.64	1.07	0.94	1.18
B (k=5)	Circle	1.56	1.08	0.80	1.18
	Triangle	1.86	1.09	0.88	1.09

k-Nearest Neighbor-based Novelty Detection



k-Nearest Neighbor-based Novelty Detection

- Experiment
  - ✓ Datasets

No.	Name	Source	Class	Dim.	TrN_n	TsN_n	TsN_o
1	`Banana`	Rätch	-1	2	216	2,708	271
2	`Titanic`	Rätch	-1	3	100	1,390	139
3	`Liver`	UCI	healthy	6	73	72	7
4	`Ecoli`	UCI	cp	7	72	71	7
5	`Yeast`	UCI	0	8	232	231	23
6	`Pima`	UCI	0	8	250	250	25
7	`Diabetes`	Rätch	-1	8	304	196	20
8	`Glass`	UCI	1	9	35	35	4
9	`Breast`	Rätch	-1	9	142	54	5
10	`Flare`	Rätch	-1	9	300	178	18
11	`Heart`	Rätch	-1	13	94	56	6
12	`Image`	Rätch	-1	18	554	436	44
13	`Twonorm`	Rätch	-1	20	198	3,499	350
14	`German`	Rätch	-1	20	489	211	21
15	`Waveform`	Rätch	-1	21	268	3,085	308
16	`Parkinsons`	UCI	parkinsons	22	74	73	7
17	`Ionosphere`	UCI	0	33	113	112	11
18	`Spectf`	UCI	0	44	28	27	3
19	`Sonar`	UCI	mine	60	56	55	6
20	`Ozone`	UCI	non-ozone	72	29	28	3
21	`Arrhythmia`	UCI	normal	258	119	118	12

k-Nearest Neighbor-based Novelty Detection

- Performance (in terms of the Integrated Error)

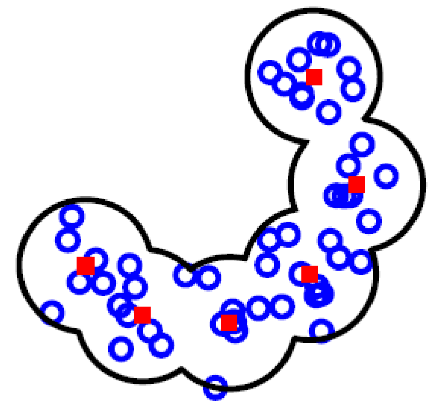
Data	Dim.	TrN$_n$	Gauss	MoG	Parzen	1-SVM	KMC	KCC	HC	PCA	d^k_{max}	d^k_{avg}	d^k_{mean}	1-NN	MST-CD	d^k_{hybrid}
Titanic	3	100	19.12	19.12	18.50	17.27	21.12	21.26	22.80	22.48	3.64	3.53	10.00	8.73	**1.33***	**1.33***
Liver	6	73	44.41	45.04	41.11	38.82	41.90	43.41	40.91	40.68	40.00	38.85	38.96	39.81	39.14	**38.18**
Ecoli	7	72	3.61	2.58	3.14	2.35	2.45	3.38	3.88	20.12	2.22	2.13	2.84	3.94	2.67	**2.11**
Glass	9	35	18.82	18.29	22.25	17.43	18.61	22.61	24.42	22.21	13.86	12.25	12.36	18.93	11.54	**11.39**
Breast	9	142	35.83	31.51	32.04	29.64	34.68	40.68	32.80	31.24	29.58	28.84	29.53	34.62	33.18	**26.99***
Banana	2	216	54.91	8.56	7.96	8.30	16.93	12.53	**7.65**	42.55	8.51	8.08	9.87	10.57	11.67	7.89
Yeast	8	232	31.55	28.98	27.99	26.58	28.78	33.25	27.32	31.47	25.81	24.54	25.87	27.79	26.50	**23.40**
Pima	8	250	29.86	33.55	26.04	27.50	29.60	32.69	28.46	33.28	24.82	24.57	27.68	28.17	27.72	**24.45**
Diabetes	8	304	30.61	34.68	27.35	26.60	28.80	35.31	26.45	31.32	23.70	23.29	25.68	26.66	28.21	**23.64**
Flare	9	300	23.19	23.19	24.82	15.40	29.67	26.65	25.57	26.76	10.49	9.74	17.09	5.62	**5.47**	6.14
Spectf	44	28	28.33	16.42	21.11	14.75	15.00	28.02	16.36	26.30	14.20	13.40	12.96	17.16	13.33	**11.67***
Sonar	60	56	41.59	37.27	34.32	33.80	41.55	40.06	40.07	42.32	39.65	34.67	32.12	33.73	**31.30**	32.62
Ozone	72	29	23.99	14.64	13.15	12.50	13.51	19.11	16.49	34.46	11.07	10.71	**9.76**	14.11	12.86	10.30
Arrhythmia	258	119	28.01	40.25	28.03	25.79	25.38	28.62	27.42	28.17	26.10	26.01	25.93	26.16	24.57	**23.93**
Heart	13	94	21.13	19.05	20.58	18.61	19.84	20.79	18.22	20.21	15.23	14.75	15.72	23.08	23.24	**14.30**
Image	18	554	13.11	13.61	11.79	10.38	23.22	30.13	31.21	15.87	13.80	11.99	10.32	10.53	**9.19***	11.04
Twonorm	20	198	9.83	11.80	11.62	9.48	8.82	12.38	**6.13***	9.62	9.62	10.02	10.79	12.87	12.62	10.11
German	20	489	38.16	36.99	37.24	35.72	39.23	42.79	40.56	37.73	34.72	33.95	34.59	37.88	36.35	**33.77**
Waveform	21	268	42.14	30.25	26.33	**22.65***	27.56	31.26	25.44	43.07	23.75	24.58	27.69	29.05	27.09	25.24
Parkinsons	22	74	32.71	46.35	32.14	**29.16**	32.65	32.66	32.79	34.60	36.95	32.54	31.63	34.22	30.68	30.30
Ionosphere	33	113	4.44	4.93	4.16	2.80	3.54	4.40	4.39	3.68	2.70	2.76	2.75	4.00	**2.70**	2.72

Clustering-based Approach

- K-Means clustering-based novelty detection
  - ✓ Novelty score of an instance is computed based on the distance information to the nearest centroid
  - ✓ Does not assume any prior probability distribution for the normal class

$$\mathcal{X} = C_1 \cup C_2 \ldots \cup C_K, \quad C_i \cap C_j = \phi, \quad i \neq j.$$

$$\arg\min_{\mathbf{C}} \sum_{i=1}^{K} \sum_{\mathbf{x}_j \in C_i} ||\mathbf{x}_j - \mathbf{c}_i||^2$$

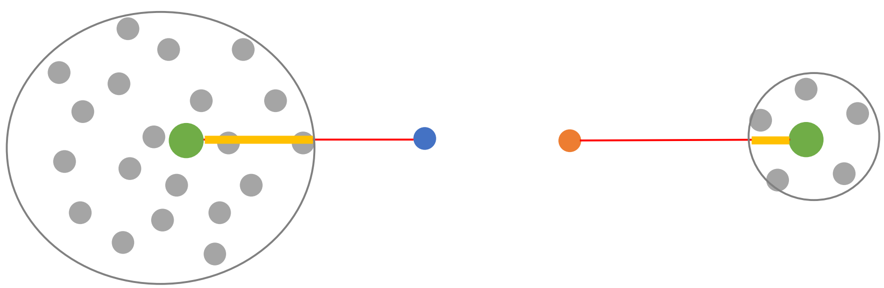


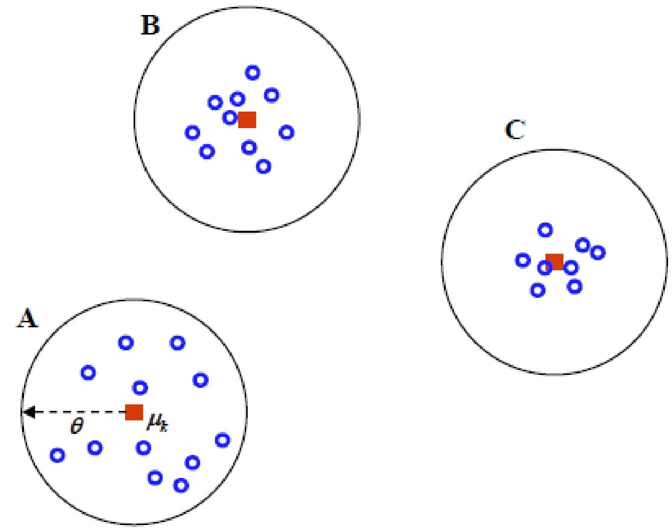
  - ✓ EM algorithm for K-Means clustering

1: Select K points as the initial centroids.
2: **repeat**
3: Form K clusters by assigning all points to the closest centroid.
4: Recompute the centroid of each cluster.
5: **until** The centroids don't change

Clustering-based Approach

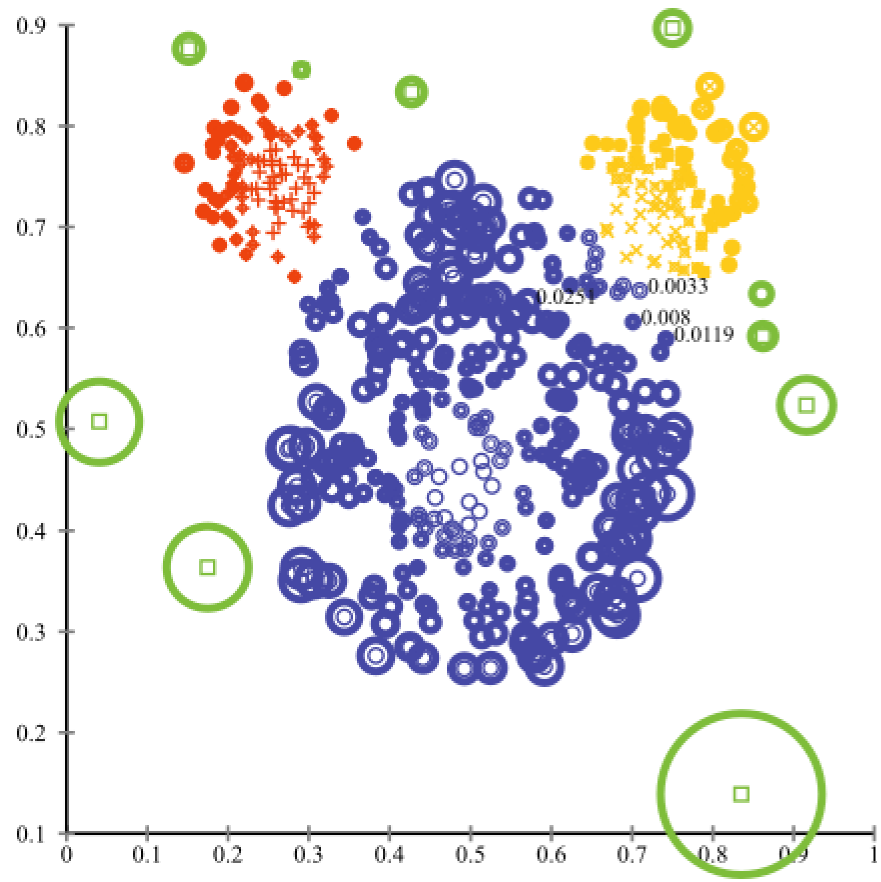
- Clustering-based Approach
  - ✓ Two novelty scores by KMC
    - ▪ Absolute distance to the nearest centroid
    - ▪ Relative distance to the nearest centroid





Clustering-based Approach

- KMC-based novelty score: Example



Principal Component Analysis-based Novelty Detection

- PCA revisited
  - ✓ Purpose: maximize the variance after projection

$$\max \quad \mathbf{w}^T \mathbf{S} \mathbf{w}$$
$$s.t. \quad \mathbf{w}^T \mathbf{w} = 1$$

  - ✓ Solution

$$L = \mathbf{w}^T \mathbf{S} \mathbf{w} - \lambda(\mathbf{w}^T \mathbf{w} - 1)$$

$$\frac{\partial L}{\partial \mathbf{w}} = 0 \Rightarrow \mathbf{S}\mathbf{w} - \lambda \mathbf{w} = 0 \;\Rightarrow (\mathbf{S} - \lambda \mathbf{I})\mathbf{w} = 0$$

Principal Component Analysis-based Novelty Detection

- PCA as a novelty detector
  - ✓ Novelty score: the amount of reconstruction loss from the projected space into the original space

$$\underset{(d \text{ by } n)}{\mathbf{X}} \xrightarrow{\text{Projection}} \underset{(1 \text{ by } d)\ (d \text{ by } n)}{\mathbf{w}^T\mathbf{X}} \xrightarrow{\text{Reconstruction}} \underset{(d \text{ by } 1)(1 \text{ by } d)\ (d \text{ by } n)}{\mathbf{w}\mathbf{w}^T\mathbf{X}}$$

$\mathbf{x}_1$	0.69	-1.31	0.39	0.09	1.29	0.49	0.19	-0.81	-0.31	-0.71
$\mathbf{x}_2$	0.49	-1.21	0.99	0.29	1.09	0.79	-0.31	-0.81	-0.31	-1.01
$\mathbf{z}_1$	0.83	-1.78	0.99	0.27	1.68	0.91	-0.10	-1.14	-0.44	-1.22
$\mathbf{x}'_1$	0.56	-1.21	0.67	0.19	1.14	0.62	-0.07	-0.78	-0.30	-0.83
$\mathbf{x}'_2$	0.61	-1.31	0.73	0.20	1.23	0.67	-0.07	-0.84	-0.32	-0.90

$\mathbf{w}^T\mathbf{X}$

$\mathbf{w}\mathbf{w}^T\mathbf{X}$

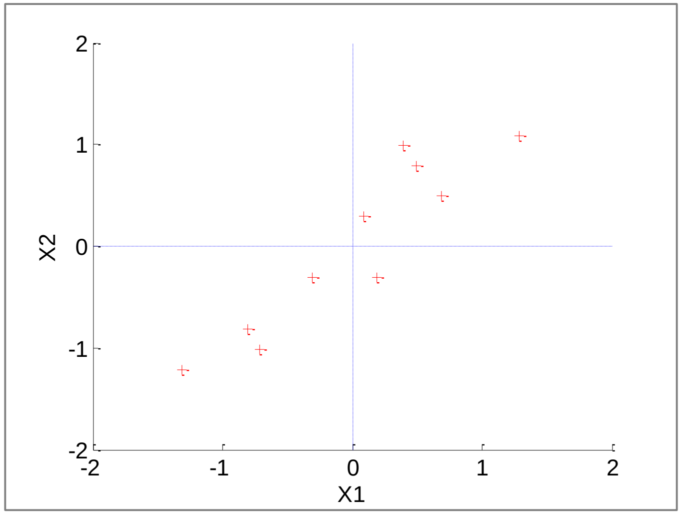
Principal Component Analysis-based Novelty Detection

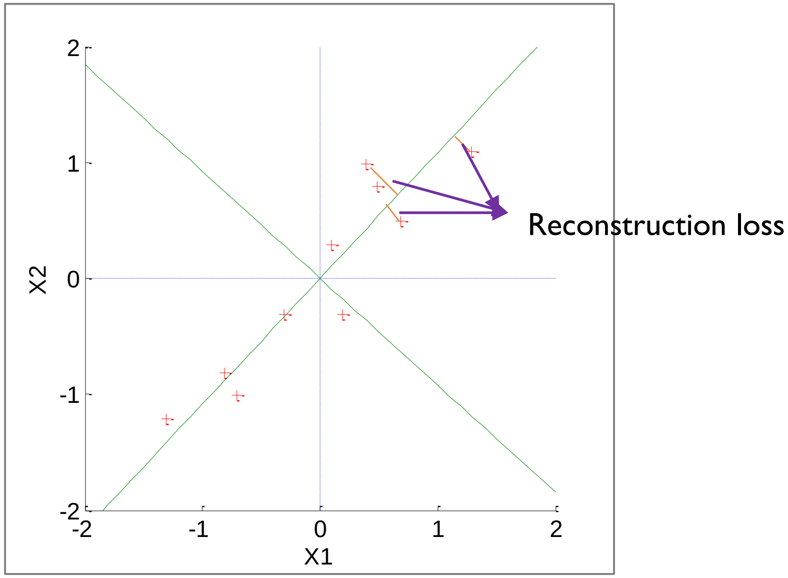
- PCA as a novelty detector
  - ✓ Compute the reconstruction loss

$$\text{error}(\boldsymbol{x}) = \left\|\mathbf{x} - \mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{x}\right\|^{2} = \left(\mathbf{x} - \mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{x}\right)^{\mathrm{T}}\left(\mathbf{x} - \mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{x}\right)$$

$$= \mathbf{x}^{\mathrm{T}}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{x} + \mathbf{x}^{\mathrm{T}}\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{x}$$

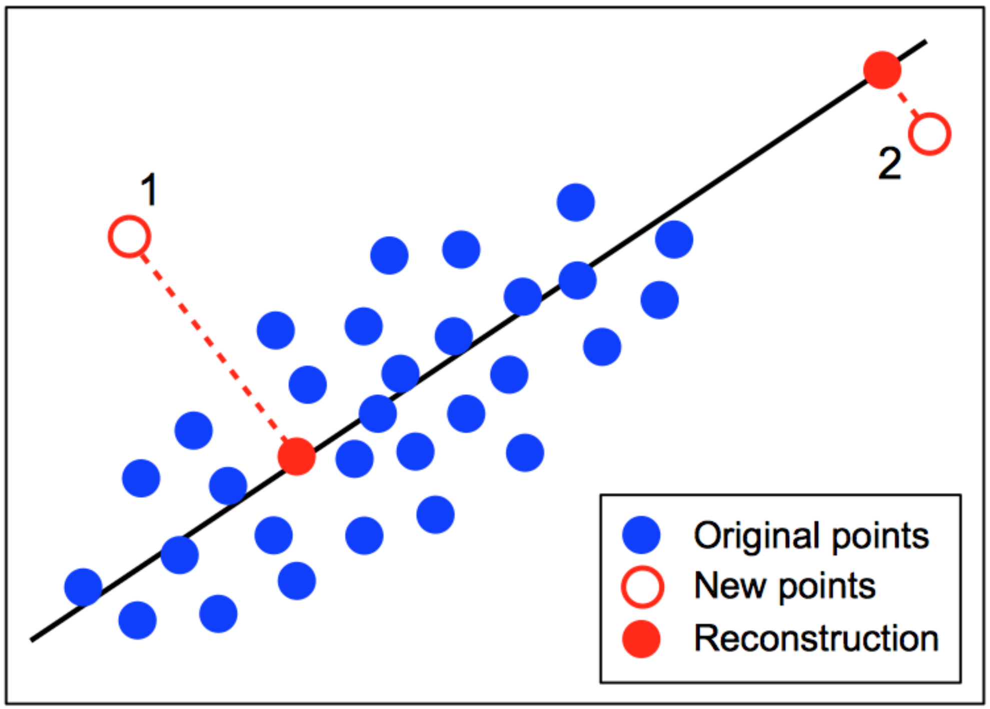
$$= \mathbf{x}^{\mathrm{T}}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{x} = \|\mathbf{x}\|^{2} - \left\|\mathbf{w}^{\mathrm{T}}\mathbf{x}\right\|^{2}$$

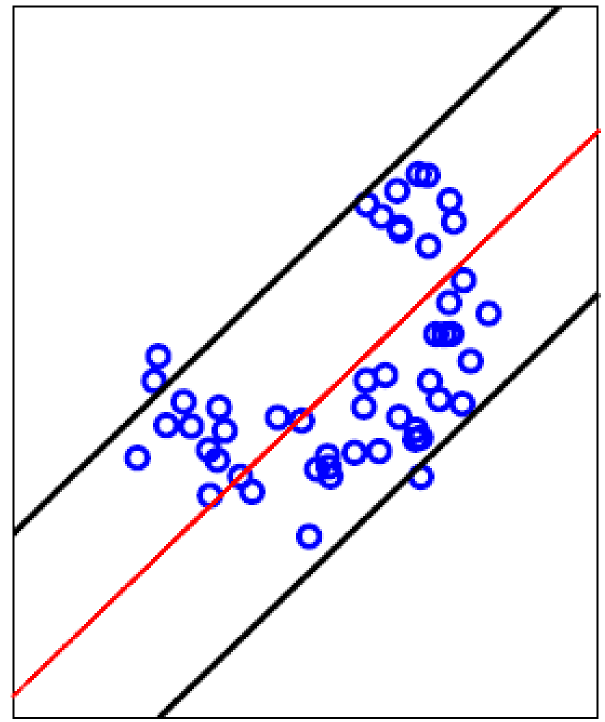




Principal Component Analysis-based Novelty Detection

- PCA as a novelty detector
  - ✓ Graphical interpretation



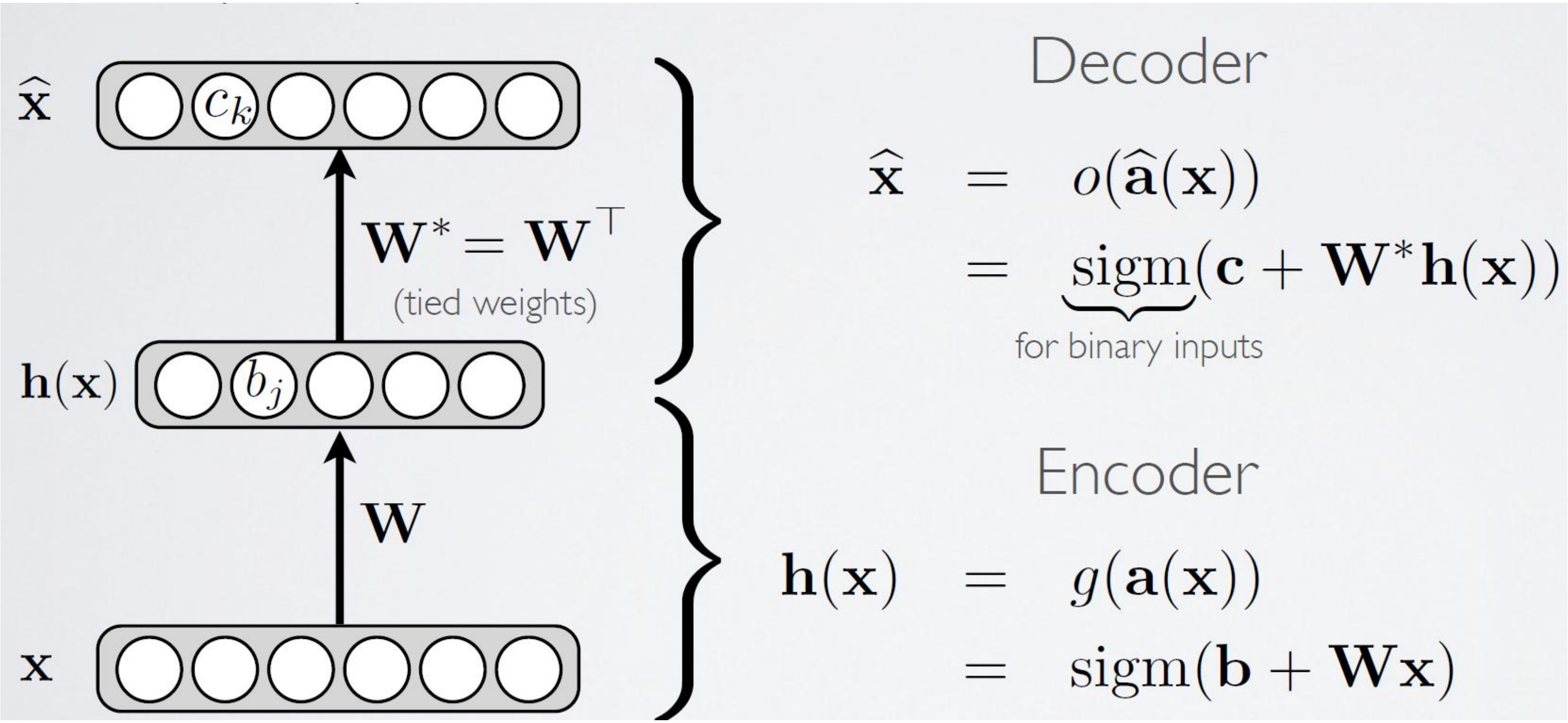


https://stats.stackexchange.com/questions/259806/anomaly-detection-using-pca-reconstruction-error

AGENDA

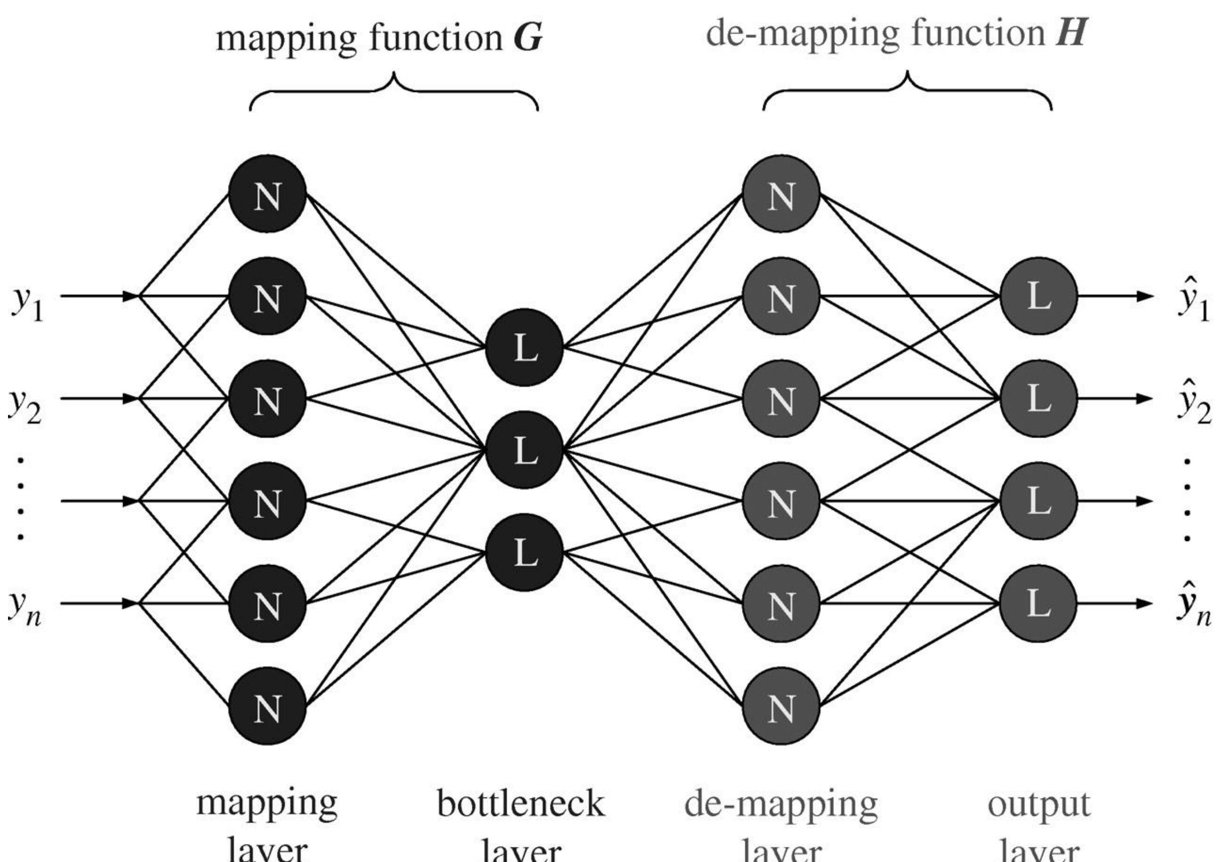
Auto-Encoder for Novelty Detection

- Auto-Encoder (Auto-Associative Neural Network)
  - ✓ Feed-forward neural network trained to reproduce its input at the output layer
    - Loss function: $l(f(\mathbf{x})) = \frac{1}{2}\sum_k (\widehat{x}_k - x_k)^2$



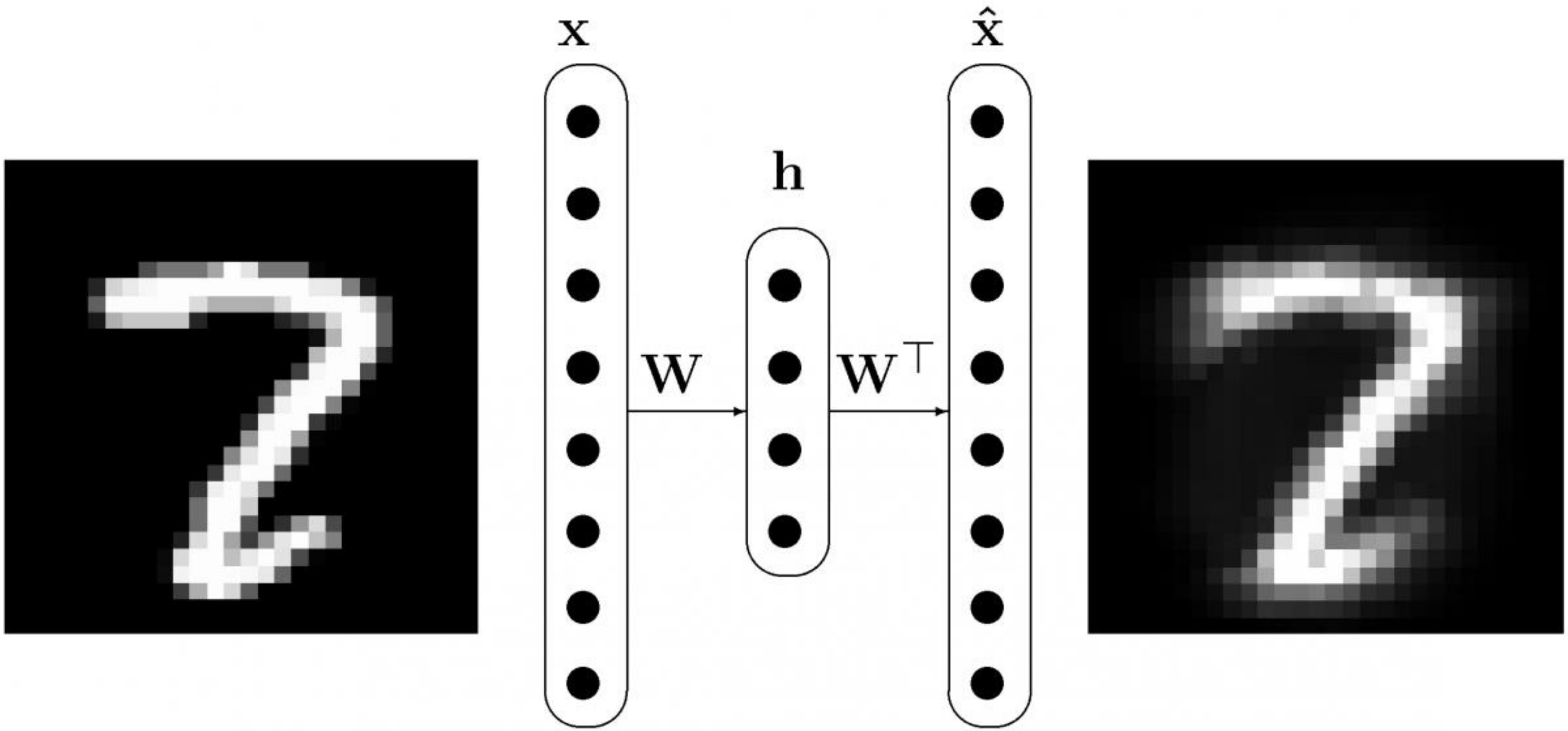
Auto-Encoder for Novelty Detection

- Auto Encoder (Auto-Associative Neural Network)
  - ✓ Feed-forward neural network trained to reproduce its input at the output layer
  - ✓ Overcomplete and Undercomplete hidden layers for AE



Auto-Encoder for Novelty Detection

- Auto Encoder (Auto-Associative Neural Network)
  - ✓ Example



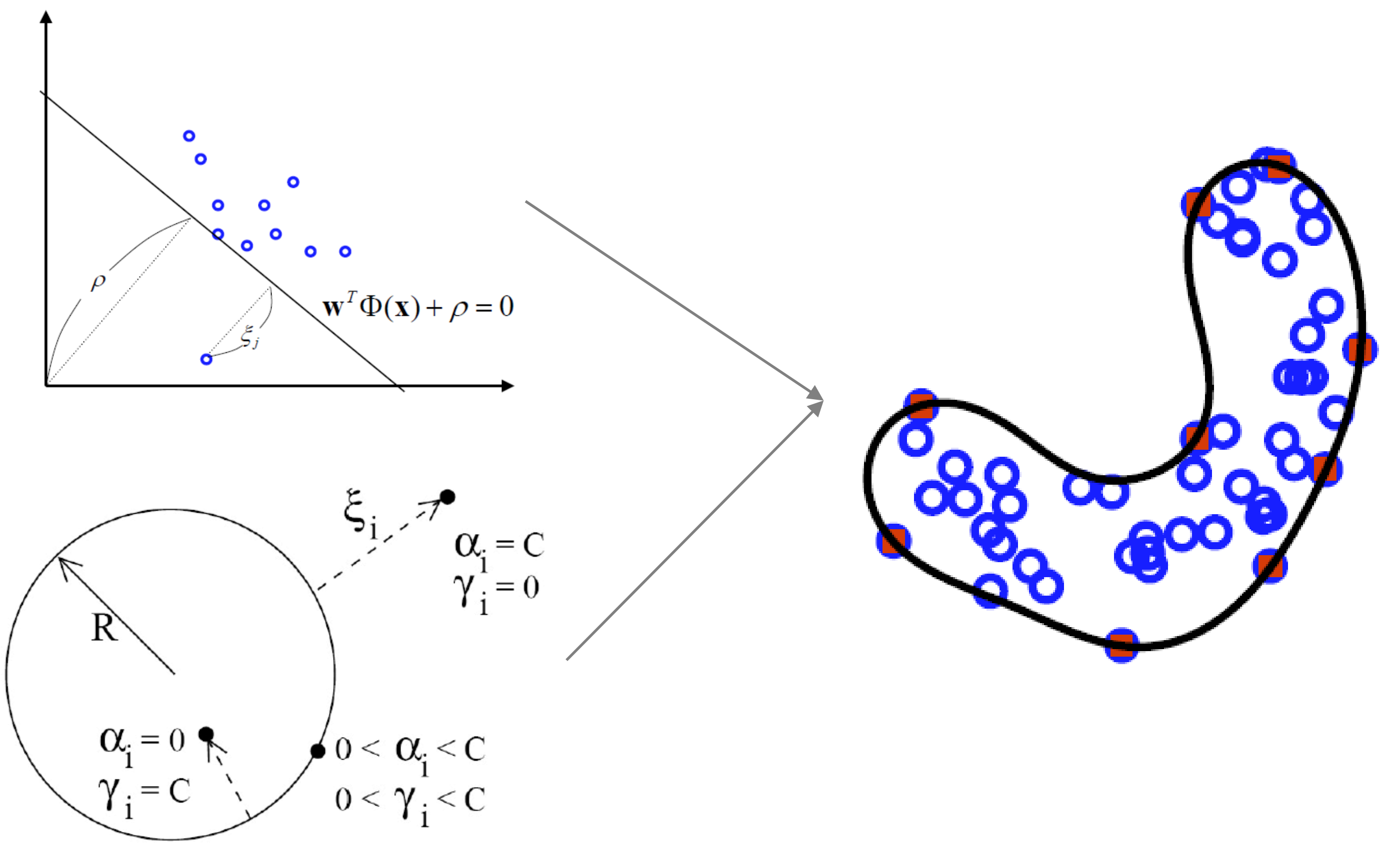
(a) Input (b) Neural Encoding (c) Reconstruction

Support Vector-based Novelty Detection

- Support vector-based novelty detection
  - ✓ Define boundaries of normal regions directly by finding function that separates the normal and abnormal observations

1-SVM

SVDD



One-Class Support Vector Machine

Scholkopf et al. (2001)

- One-class support vector machine (1-SVM)
  - ✓ Map the data into the feature space corresponding to the kernel and to separate them from the origin with maximum margin
    - Optimization problem

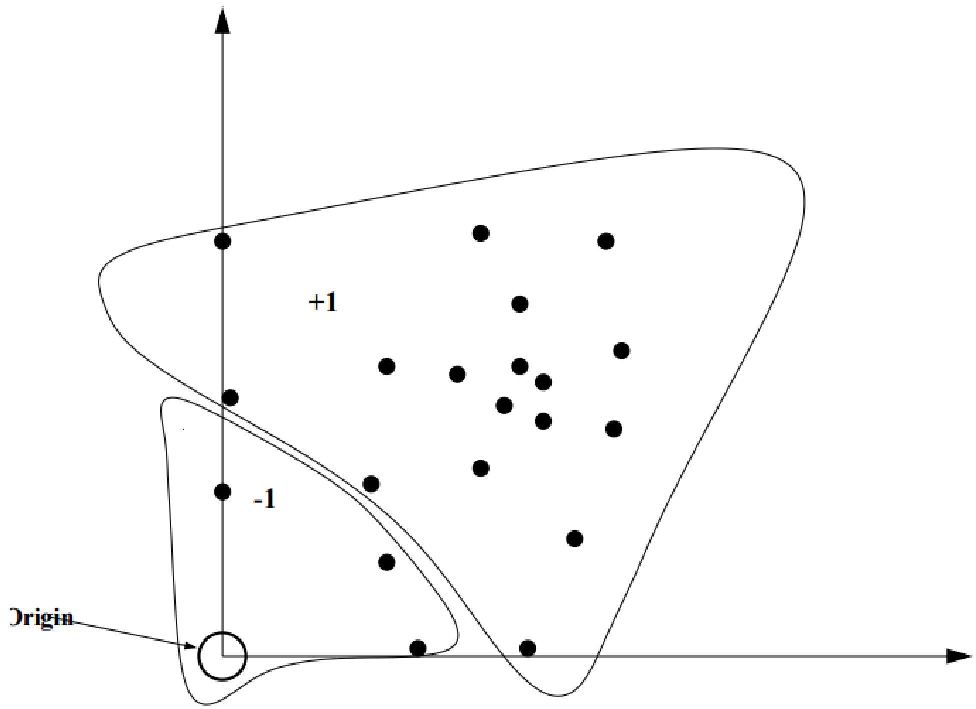
$$\min_{\mathbf{w}} \frac{1}{2}||\mathbf{w}||^2 + \frac{1}{\nu l}\sum_{i=1}^{l}\xi_i - \rho$$

$$s.t. \quad \mathbf{w}\cdot\Phi(\mathbf{x}_i) \geq \rho - \xi_i$$

$$i = 1, 2, \cdots, l, \quad \xi_i \geq 0$$

    - Decision function

$$f(\mathbf{x}_i) = sign\big(\mathbf{w}\cdot\Phi(\mathbf{x}_i) - \rho\big)$$



One-Class Support Vector Machine

- One-class support vector machine (1-SVM)
  - ✓ Primal Lagrangian problem (Minimize)

$$L = \frac{1}{2}||\mathbf{w}||^2 + \frac{1}{\nu l}\sum_{i=1}^{l}\xi_i - \rho - \sum_{i=1}^{l}\alpha_i\big(\mathbf{w}\cdot\Phi(\mathbf{x}_i) - \rho + \xi_i\big) - \sum_{i=1}^{l}\beta_i\xi_i$$

  - ✓ KKT condition

$$\frac{\partial L}{\partial \mathbf{w}} = \mathbf{w} - \sum_{i=1}^{l}\alpha_i\Phi(\mathbf{x}_i) = 0 \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{l}\alpha_i\Phi(\mathbf{x}_i)$$

$$\frac{\partial L}{\partial \xi_i} = \frac{1}{\nu l} - \alpha_i - \beta_i = 0 \quad \Rightarrow \quad \alpha_i = \frac{1}{\nu l} - \beta_i$$

$$\frac{\partial L}{\partial \rho} = -1 + \sum_{i=1}^{l}\alpha_i = 0 \quad \Rightarrow \quad \sum_{i=1}^{l}\alpha_i = 1$$

One-Class Support Vector Machine

- One-class support vector machine (1-SVM)
  - ✓ Dual Lagrangian problem (Maximize)

$$L = \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_j) + \frac{1}{\nu l}\sum_{i=1}^{l}\xi_i - \rho$$

$$- \sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_j) + \rho\sum_{i=1}^{l}\alpha_i - \sum_{i=1}^{l}\alpha_i\xi_i - \sum_{i=1}^{l}\beta_i\xi_i$$

  - ✓ We should solve

$$\min \ L = \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_j)$$

$$s.t. \quad \sum_{i=1}^{l}\alpha_i = 1, \quad 0 \leq \alpha_i \leq \frac{1}{\nu l}$$

One-Class Support Vector Machine

- One-class support vector machine (1-SVM)
  - ✓ Employ Kernel Trick for a non-linear mapping

$$\min \; L = \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_j)$$

$$s.t. \quad \sum_{i=1}^{l}\alpha_i = 1, \quad 0 \le \alpha_i \le \frac{1}{\nu l}$$

$$\min \; L = \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j K(\mathbf{x}_i, \mathbf{x}_j)$$

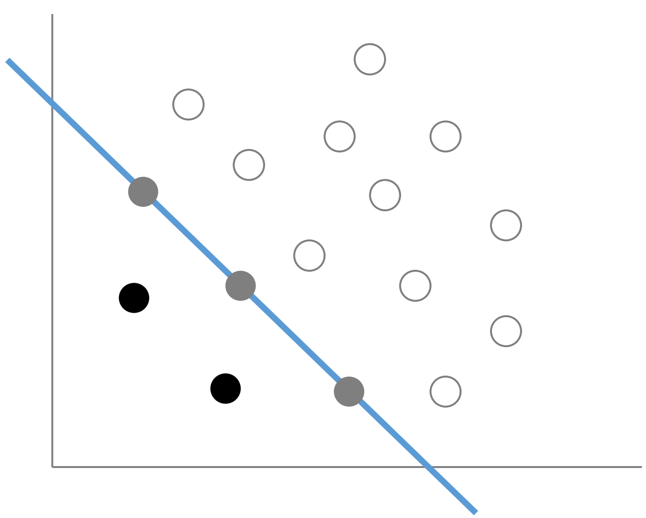
$$s.t. \quad \sum_{i=1}^{l}\alpha_i = 1, \quad 0 \le \alpha_i \le \frac{1}{\nu l}$$

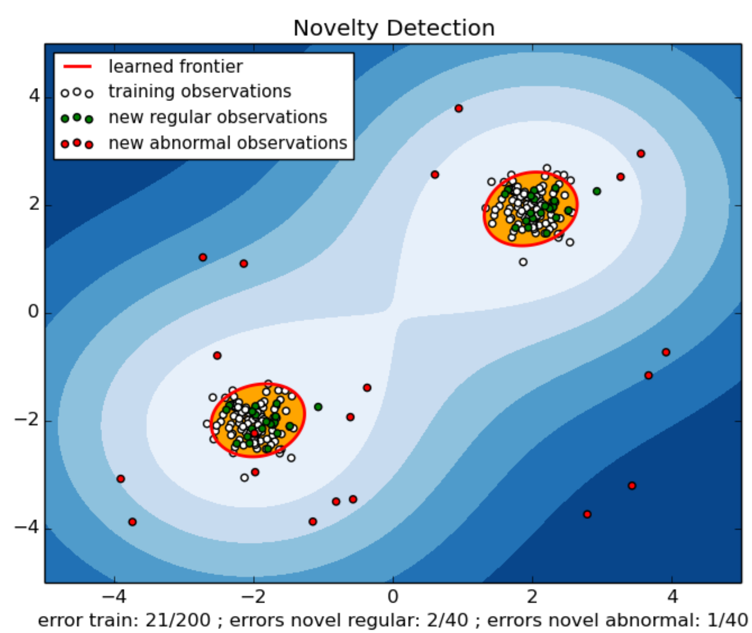
Some possible kernels $K(\cdot,\cdot)$:

$K(x, x_i) = x_i^T x$ (linear SVM)
$K(x, x_i) = (x_i^T x + \tau)^d$ (polynomial SVM of degree d)
$K(x, x_i) = \exp(-\|x - x_i\|_2^2/\sigma^2)$ (RBF kernel)
$K(x, x_i) = \tanh(\kappa\, x_i^T x + \theta)$ (MLP kernel)

One-Class Support Vector Machine

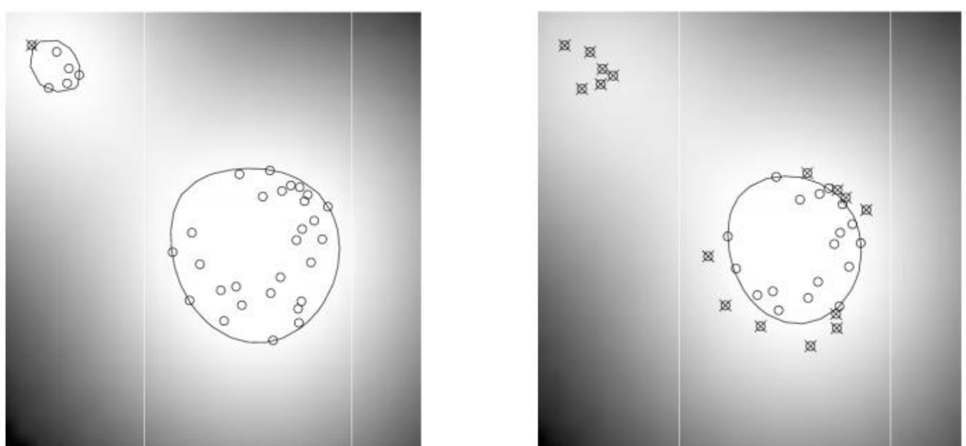
- One-class support vector machine (1-SVM)
  - ✓ Location of a point w.r.t. α_i
    - ○ ▪ Case 1: $\alpha_i = 0 \quad \Rightarrow$ a non-support vector
    - ● ▪ Case 2: $\alpha_i = \frac{1}{\nu l} \quad \Rightarrow \quad \beta_i = 0 \quad \Rightarrow \quad \xi_i > 0 \Rightarrow$ Support vector (outsider the hyperplane)
    - ● ▪ Case 3: $0 < \alpha_i < \frac{1}{\nu l} \quad \Rightarrow \quad \beta_i > 0 \quad \Rightarrow \quad \xi_i = 0 \Rightarrow$ Support vector (on the hyperplane)





One-Class Support Vector Machine

- One-class support vector machine (1-SVM)
  - ✓ The role of ν
    - The maximum possible value of $\alpha_i = \frac{1}{\nu l}$
    - At least νl support vectors exist
    - At most νl support vectors can be located outside the hyperplane
    - Thus, ν is the lower bound for the fraction of support vectors and the upper bound for the fraction of errors
  - ✓ The higher the ν, the more complex decision boundary is generated

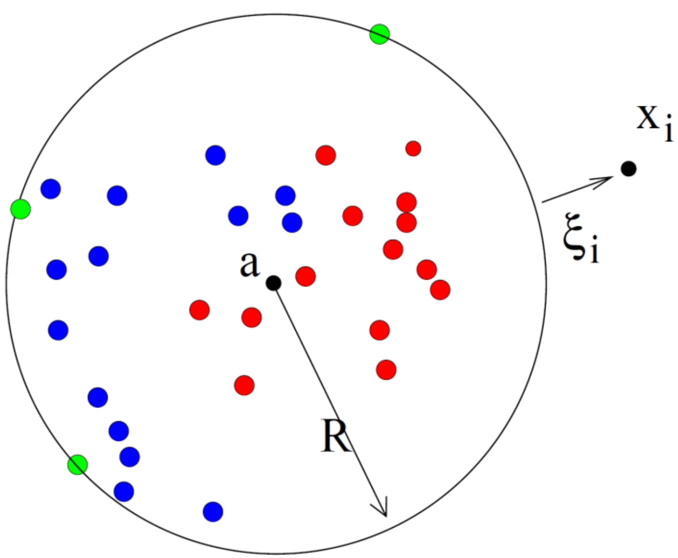


Support Vector Data Description

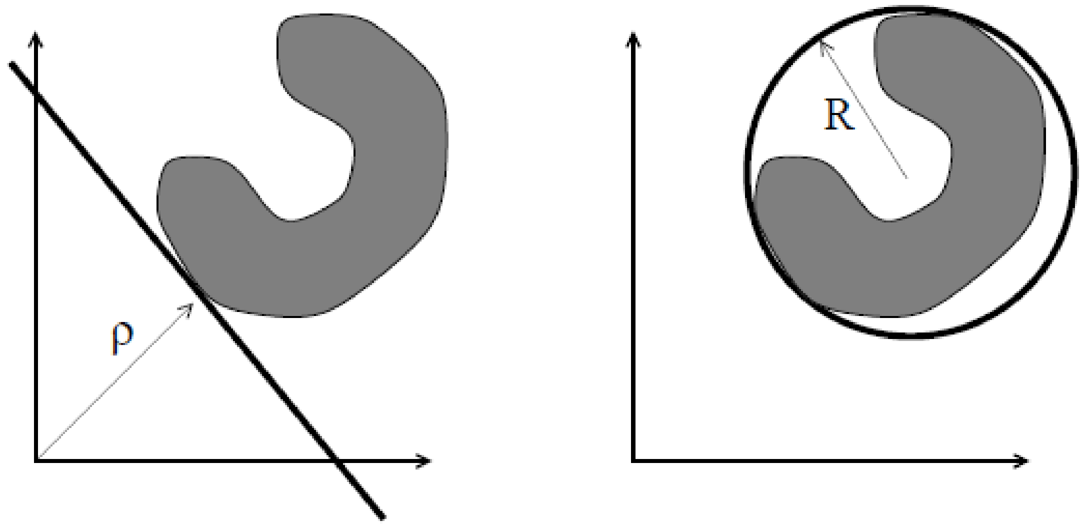
Tax and Duin (2004)

- Support Vector Data Description (SVDD)
  - ✓ Find a hypersphere enclosing all the normal instances in a feature space

SVDD



1-SVM vs. SVDD



Support Vector Data Description

- Support Vector Data Description (SVDD)
  - ✓ Find a hypersphere enclosing all the normal instances in a feature space
    - Optimization function

$$\min_{R,\mathbf{a},\xi_i} R^2 + C\sum_{i=1}^{l}\xi_i$$

$$s.t. \quad ||\Phi(\mathbf{x}_i) - \mathbf{a}||^2 \leq R^2 + \xi_i, \quad \xi_i \geq 0, \quad \forall i.$$

    - Decision function

$$f(\mathbf{x}) = sign\big(R^2 - ||\Phi(\mathbf{x}_i) - \mathbf{a}||^2\big)$$

Support Vector Data Description

- Support Vector Data Description (SVDD)
  - ✓ Find a hypersphere enclosing all the normal instances in a feature space
    - Primal Lagrangian problem (Minimization)

$$L = R^2 + C\sum_{i=1}^{l}\xi_i - \sum_{i=1}^{l}\alpha_i\Big(R^2 + \xi_i - (\Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x}_i) - 2\cdot\mathbf{a}\cdot\Phi(\mathbf{x}_i) + \mathbf{a}\cdot\mathbf{a})\Big) - \sum_{i=1}^{l}\beta_i\xi_i$$

$$\alpha_i \geq 0, \quad \beta_i \geq 0$$

    - KKT condition

$$\frac{\partial L}{\partial R} = 2R - 2R\sum_{i=1}^{l}\alpha_i = 0 \quad \Rightarrow \sum_{i=1}^{l}\alpha_i = 1$$

$$\frac{\partial L}{\partial \mathbf{a}} = 2\sum_{i=1}^{l}\alpha_i\cdot\Phi(\mathbf{x}_i) - 2\mathbf{a}\sum_{i=1}^{l}\alpha_i = 0 \quad \Rightarrow \quad \mathbf{a} = \sum_{i=1}^{l}\alpha_i\cdot\Phi(\mathbf{x}_i)$$

$$\frac{\partial L}{\xi_i} = C - \alpha_i - \beta_i = 0 \quad \forall i$$

Support Vector Data Description

- Support Vector Data Description (SVDD)
  - ✓ Find a hypersphere enclosing all the normal instances in a feature space
    - Dual Lagrangian problem (Maximization)

$$L = R^2 + C\sum_{i=1}^{l}\xi_i - \sum_{i=1}^{l}\alpha_i\Big(R^2+\xi_i-(\Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x}_i)-2\cdot\mathbf{a}\cdot\Phi(\mathbf{x}_i)+\mathbf{a}\cdot\mathbf{a})\Big)-\sum_{i=1}^{l}\beta_i\xi_i$$

$$L = R^2 - R^2\sum_{i=1}^{l}\alpha_i + \sum_{i=1}^{l}\xi_i(C-\alpha_i-\beta_i)$$

$$+\sum_{i=1}^{l}\alpha_i\Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x}_i) - 2\sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_j) + \sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_j)$$

$$L = \sum_{i=1}^{l}\alpha_i\Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x}_i) - \sum_{i=1}^{l}\sum_{j=1}^{l}\alpha_i\alpha_j\Phi(\mathbf{x}_i)\Phi(\mathbf{x}_j) \qquad (0 \le \alpha_i \le C)$$

Support Vector Data Description

- Support Vector Data Description (SVDD)
  - ✓ Find a hypersphere enclosing all the normal instances in a feature space
    - Dual Lagrangian problem (Maximization)

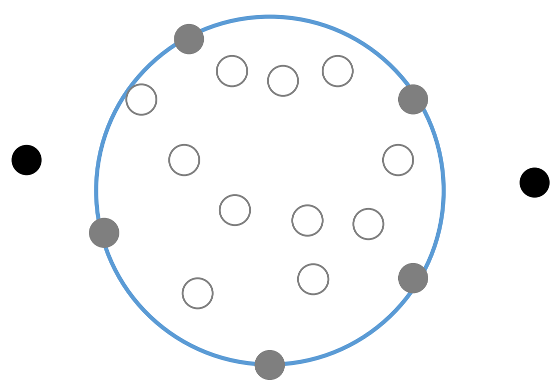
$$L = \sum_{i=1}^{l} \alpha_i \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_i) - \sum_{i=1}^{l} \sum_{j=1}^{l} \alpha_i \alpha_j \Phi(\mathbf{x}_i) \Phi(\mathbf{x}_j) \quad (0 \leq \alpha_i \leq C)$$

    - Dual Lagrangian problem (Minimization)

$$L = \sum_{i=1}^{l} \sum_{j=1}^{l} \alpha_i \alpha_j \Phi(\mathbf{x}_i) \Phi(\mathbf{x}_j) - \sum_{i=1}^{l} \alpha_i \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_i) \quad (0 \leq \alpha_i \leq C)$$

Support Vector Data Description

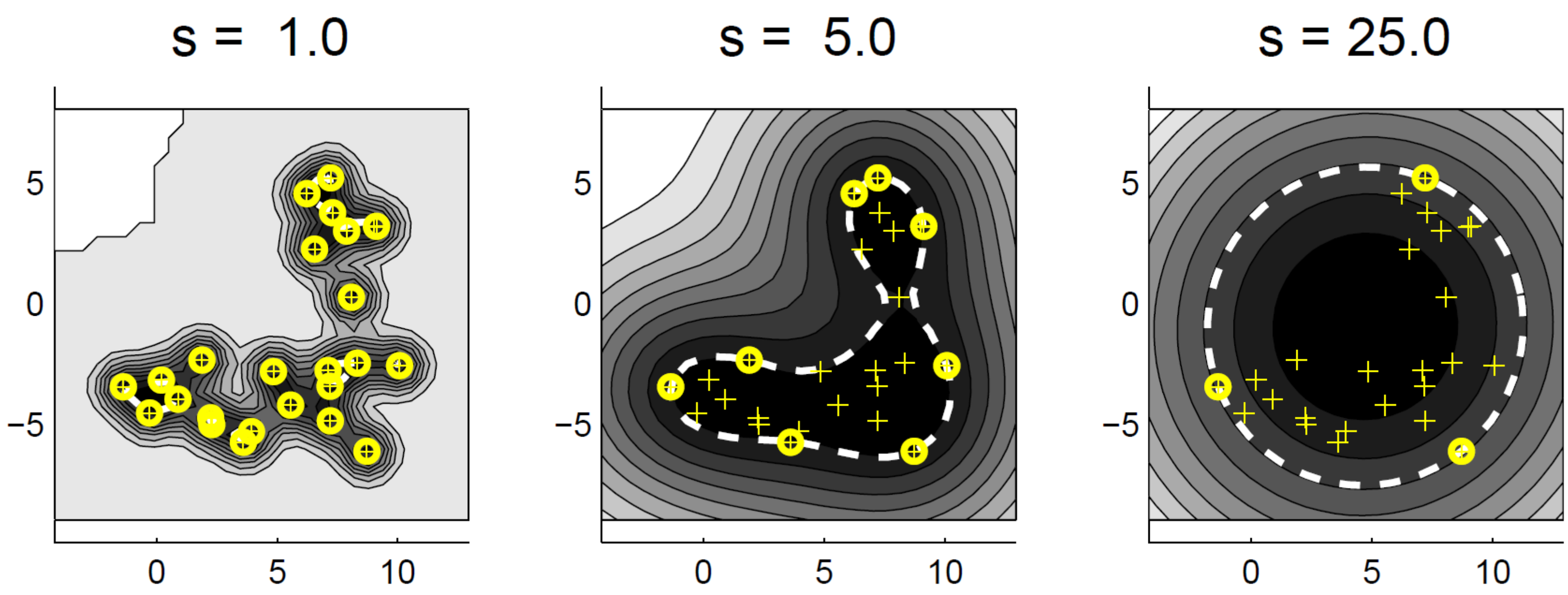
- Support Vector Data Description (SVDD)
  - ✓ Location of a point w.r.t. α_i
    - Case 1: $\alpha_i = 0 \quad \Rightarrow$ a non-support vector
    - Case 2: $\alpha_i = C \quad \Rightarrow \quad \beta_i = 0 \quad \Rightarrow \quad \xi_i > 0 \Rightarrow$ Support vector (outsider the hypersphere)
    - Case 3: $0 < \alpha_i < C \quad \Rightarrow \quad \beta_i > 0 \quad \Rightarrow \quad \xi_i = 0 \Rightarrow$ Support vector (on the hypersphere)



Support Vector Data Description

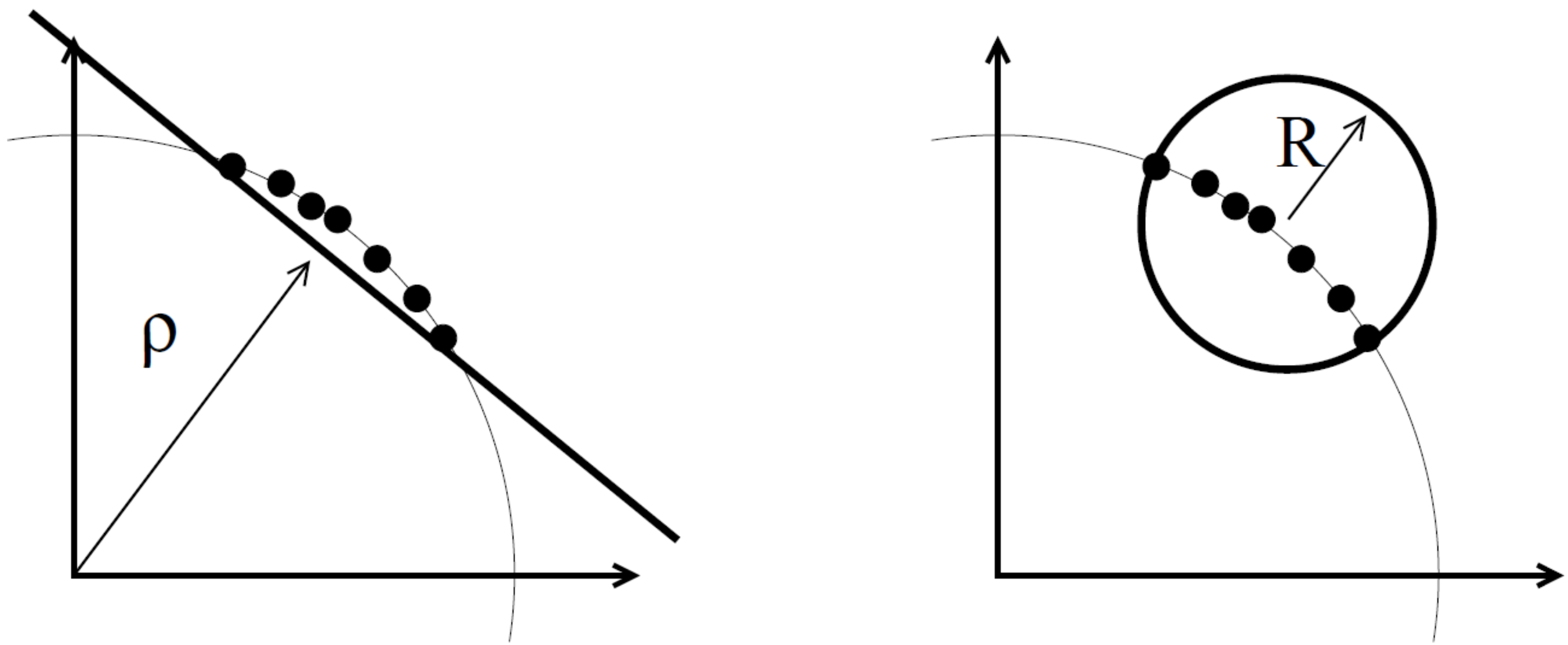
- Support Vector Data Description (SVDD)
  - ✓ SVDD with Gaussian (RBF) kernels

$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(\frac{-\|\mathbf{x}_i - \mathbf{x}_j\|^2}{s^2}\right)$$



Support Vector Data Description

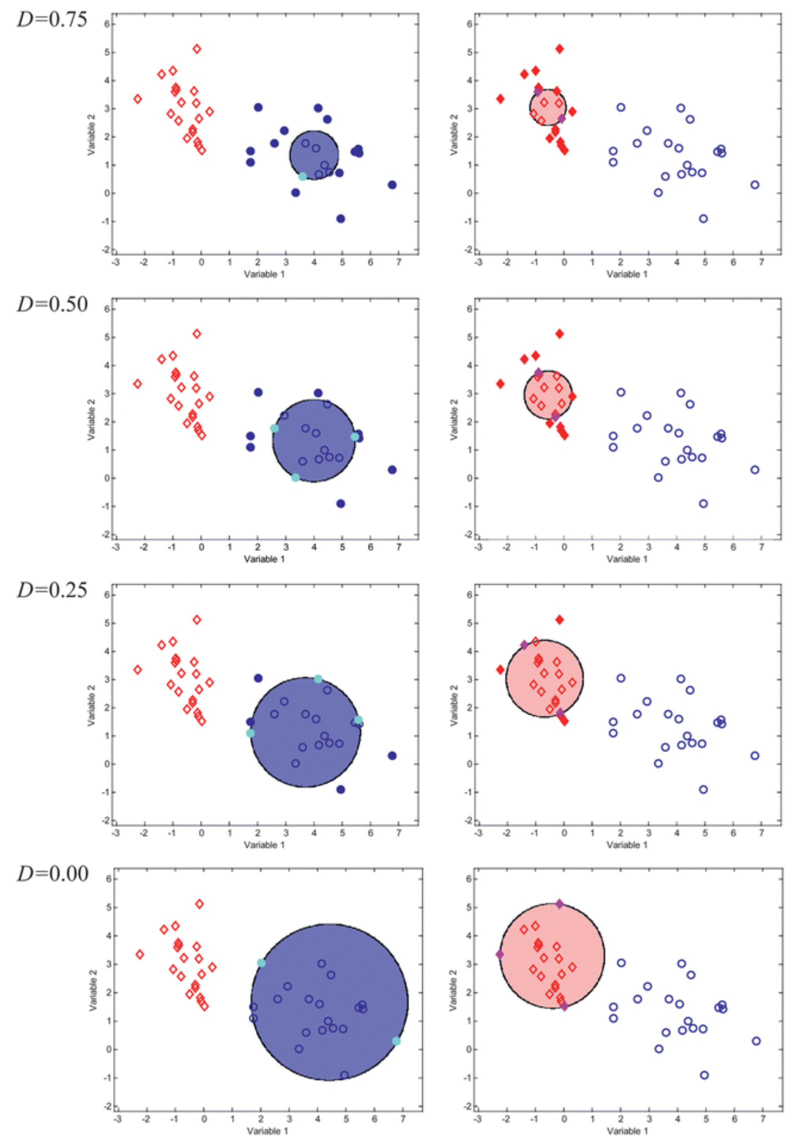
- Support Vector Data Description (SVDD)
  - ✓ When all data is normalized to unit norm vector, SVDD and 1-SVM are equivalent



  - For the detailed proof, please refer to Tax (2001) pp. 39-41.

Support Vector Data Description

- Support Vector Data Description (SVDD)
  - ✓ As in 1-SVM, υ-SVDD can also be formulated
  - ✓ D in the right figure is υ

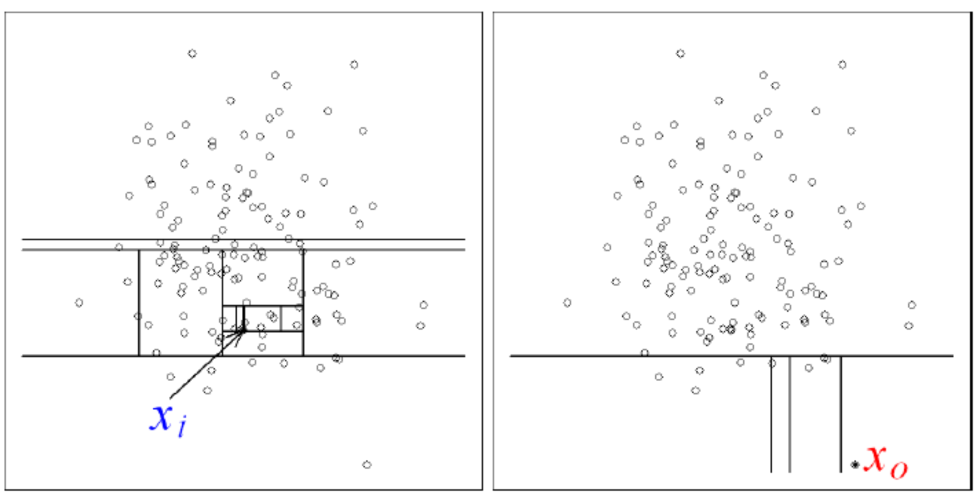


http://pubs.rsc.org/-/content/articlehtml/2010/an/b918972f

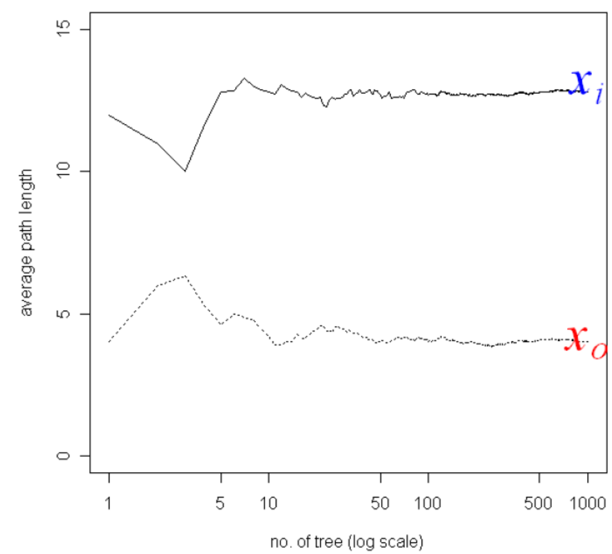
Isolation Forest

Liu et al. (2008, 2012)

- Motivation: Few and Different
  - ✓ The minority consists of fewer instances
  - ✓ They have attribute-values, which are very different from those of normal instances
- A tree structure can be constructed effectively to isolate every single instances
  - ✓ Novel instances are isolated closer to the root of the tree
  - ✓ Normal instances are isolated at the deeper end of the tree

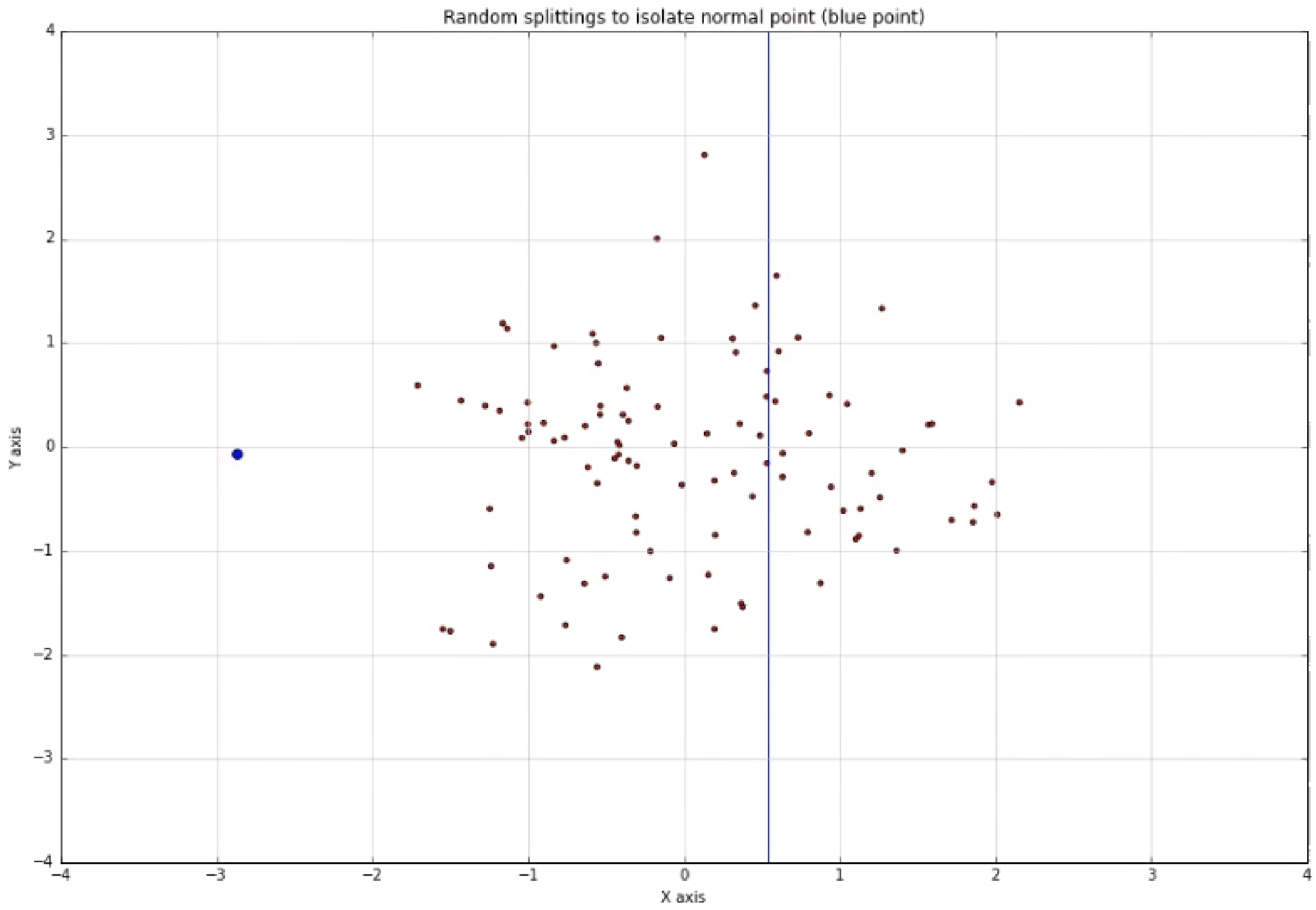


(a) Isolating x_i (b) Isolating x_o



Isolation Forest

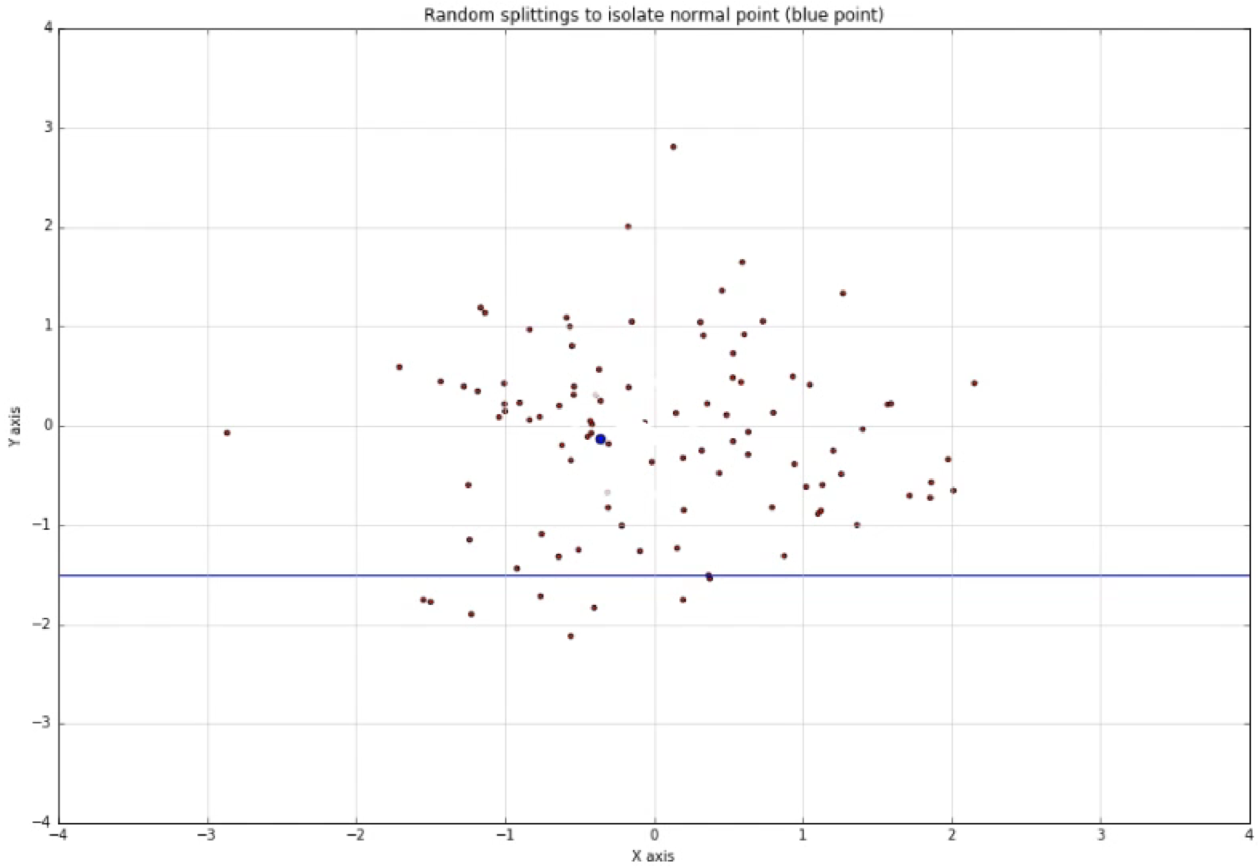
- Isolating a normal instance



https://blog.easysol.net/using-isolation-forests-anamoly-detection/

Isolation Forest

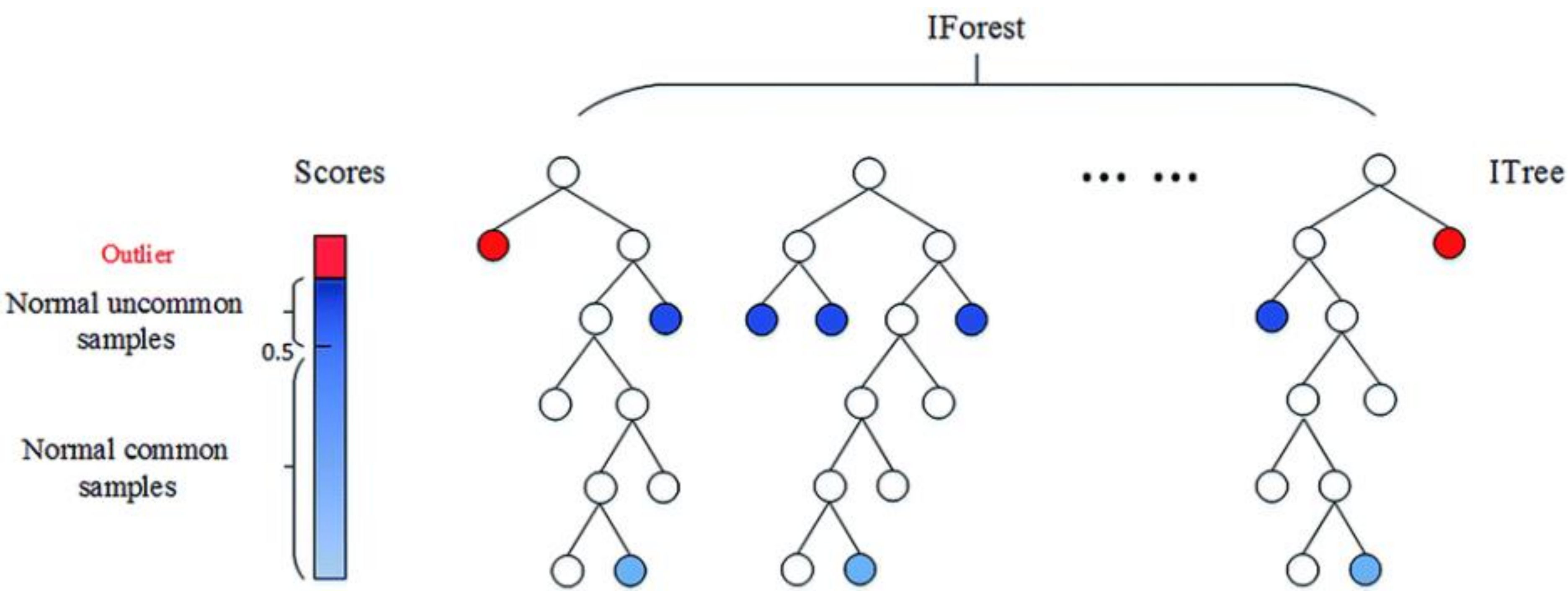
- Isolating an abnormal instance



https://blog.easysol.net/using-isolation-forests-anamoly-detection/

Isolation Forest

- The isolation characteristics of tree forms the basis of the method to detect novel instances
    - ✓ The average path to the terminal node can be used as a novelty score of an instance



Isolation Forest

- Definition: Isolation Tree (iTree)
  - ✓ Given a sample of data X of n instances, the dataset X is recursively divided by randomly selected attribute q with a split value p, until either
    - The tree reaches a height limit
    - $|X| = 1$
    - All instances in X have the same value
- Definition: Path Length
  - ✓ The path length h(x) of an instance x is measured by the number of edges x traverses an iTree from the root node to the terminal node in which the instance x is located
  - ✓ h(x) is normalized by the average path length of h(x) given n
    - $c(n) = 2H(n-1)-(2(n-1)/n)$ ($H(i) = \ln(i) + 0.5772156649$ (Euler's constant))

Isolation Forest

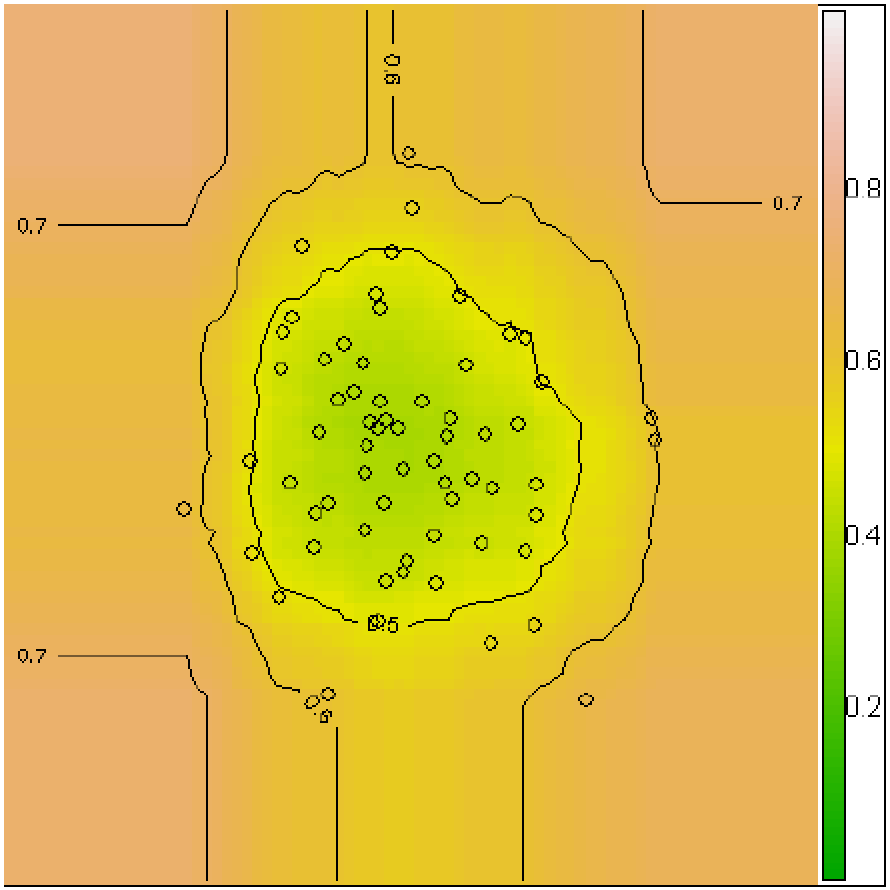
- Definition: Novelty score
  - ✓ The path length h(x) of an instance x is measured by the number of edges x traverses an iTree from the root node to the terminal node in which the instance x is located
  - ✓ h(x) is normalized by the average path length of h(x) given n
    - c(n) = 2H(n-1)-(2(n-1)/n) (H(i) = ln(i) + 0.5772156649 (Euler's constant))
  - ✓ The novelty score s of an instance x is defined by

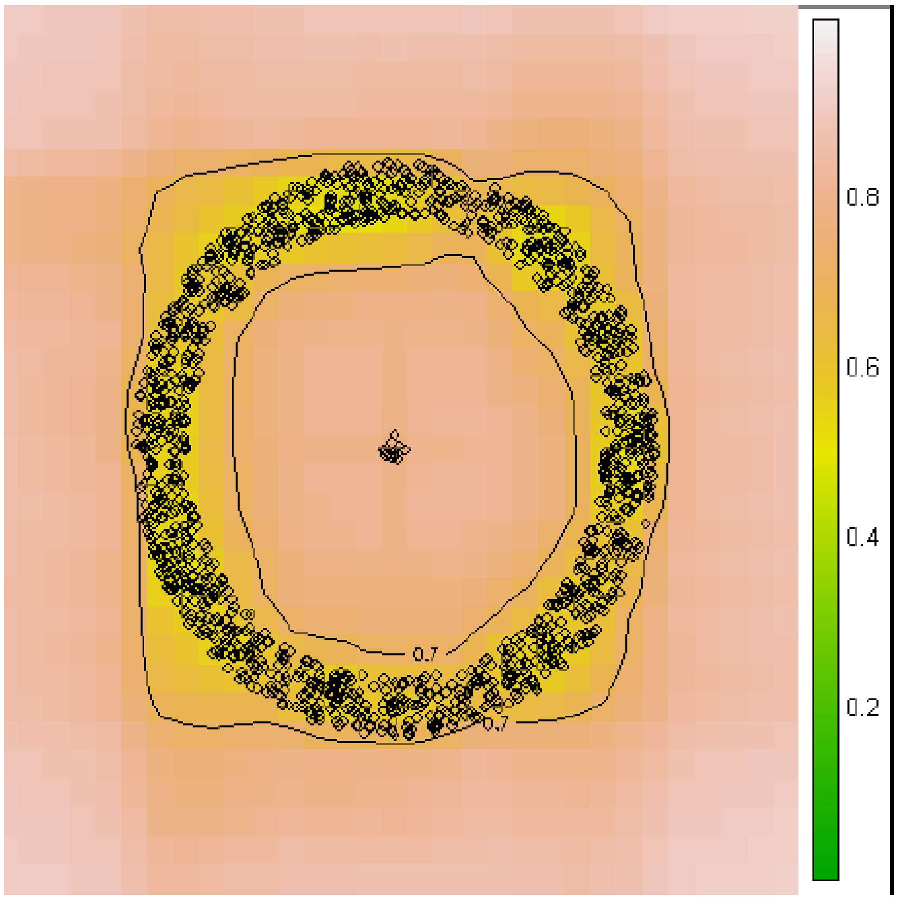
$$s(x, n) = 2^{-\frac{E(h(x))}{c(n)}}$$

- When $E(h(x)) \rightarrow c(n), \quad s \rightarrow 0.5$
- When $E(h(x)) \rightarrow 0, \quad s \rightarrow 1$
- When $E(h(x)) \rightarrow n-1, \quad s \rightarrow 0$

Isolation Forest

- Novelty score contour





Isolation Forest

- Training Isolation Forest
  - ✓ Randomly sample datasets
  - ✓ Construct iTree
  - ✓ Compute the path length

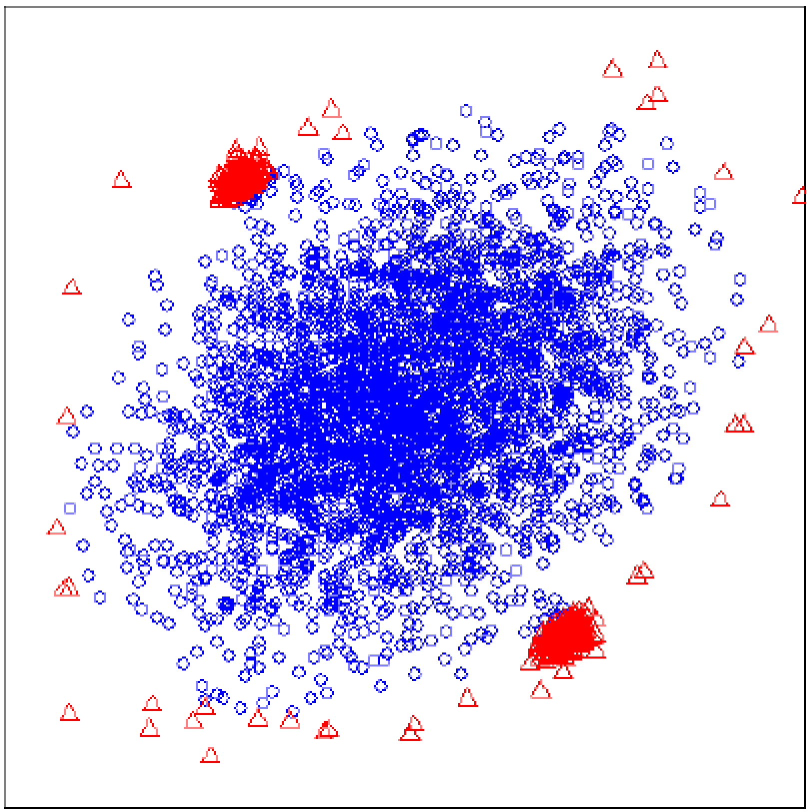
Algorithm 1 : $iForest(X, t, \psi)$

Inputs: X - input data, t - number of trees, ψ - subsampling size
Output: a set of t $iTrees$

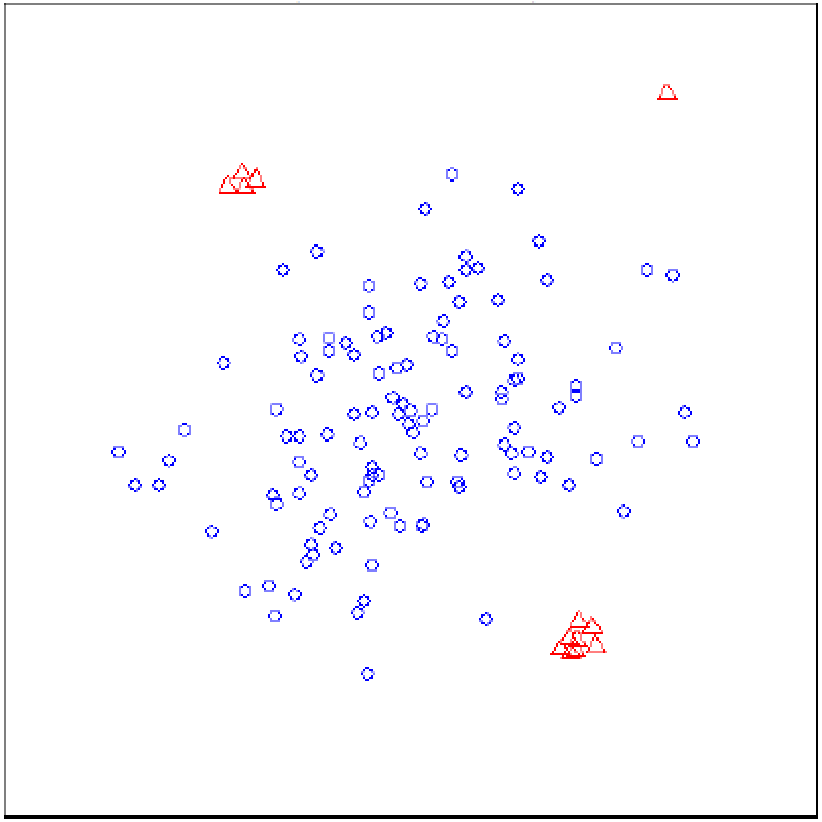
1: **Initialize** $Forest$
2: **for** $i = 1$ to t **do**
3: $\quad X' \leftarrow sample(X, \psi)$
4: $\quad Forest \leftarrow Forest \cup iTree(X')$
5: **end for**
6: **return** $Forest$

Isolation Forest

- Training Isolation Forest
  - ✓ Randomly sample datasets: 256 is generally enough



(a) Original sample
(4096 instances)



(b) Sub-sample
(128 instances)

Isolation Forest

- Training Isolation Forest
  - ✓ Construct iTree

Algorithm 2 : $iTree(X')$

Inputs: X' - input data
Output: an iTree

if X' cannot be divided **then**
  return $exNode\{Size \leftarrow |X'|\}$
else
  let Q be a list of attributes in X'
  randomly select an attribute $q \in Q$
  randomly select a split point p between the max and min values of attribute q in X'
  $X_l \leftarrow filter(X', q < p)$
  $X_r \leftarrow filter(X', q \geq p)$
  return $inNode\{Left \leftarrow iTree(X_l),$
    $Right \leftarrow iTree(X_r),$
    $SplitAtt \leftarrow q,$
    $SplitValue \leftarrow p\}$
end if

Isolation Forest

- Training Isolation Forest
  - ✓ Compute the path length

Algorithm 3 : $PathLength(x, T, hlim, e)$

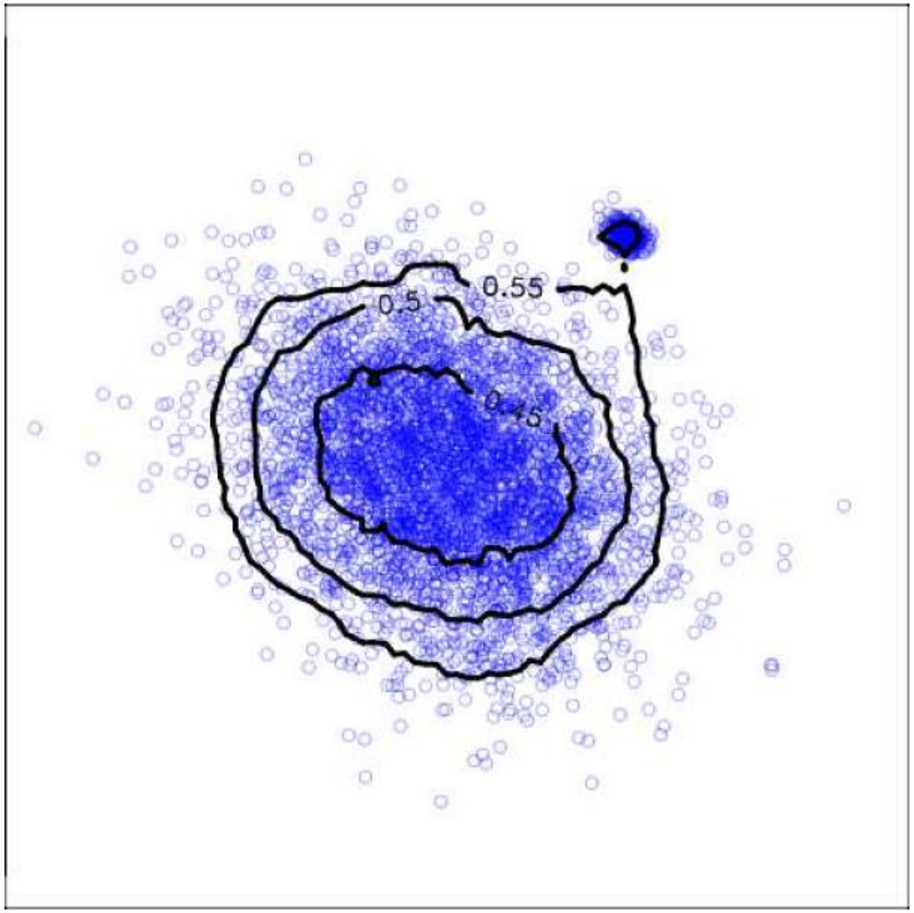
Inputs : x - an instance, T - an iTree, $hlim$ - height limit, e - current path length; to be initialized to zero when first called

Output: path length of x

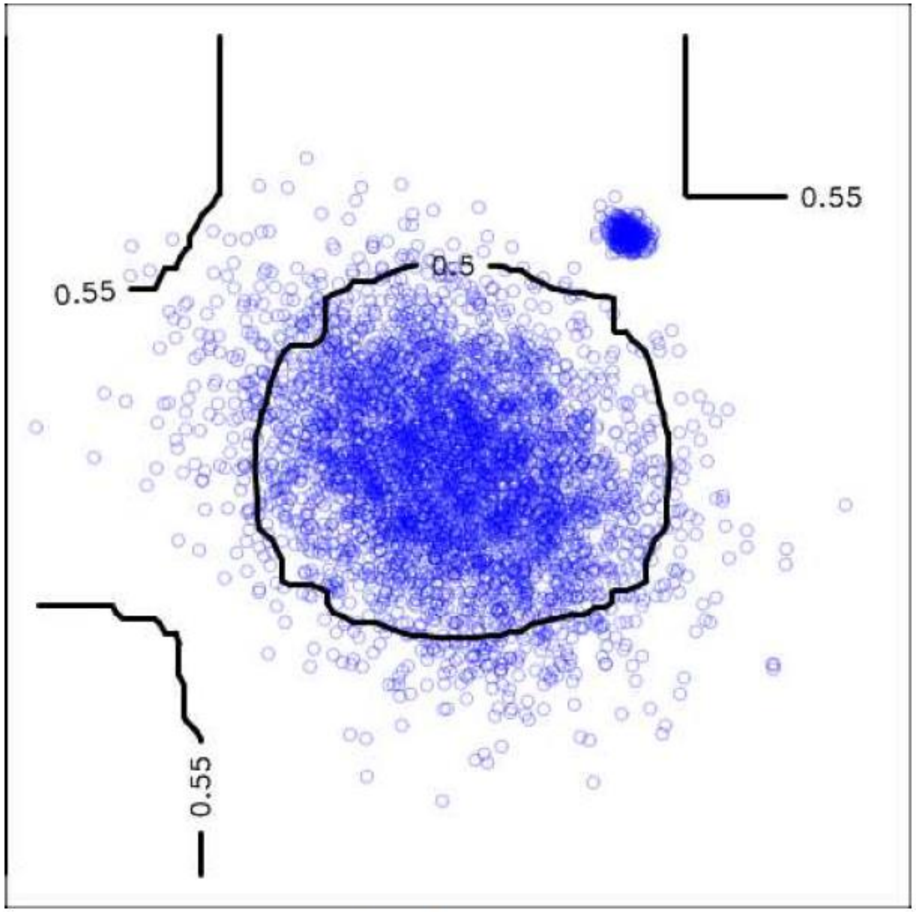
if T is an external node or $e \geq hlim$ **then**
    return $e + c(T.size)$ $\{c(.)$ is defined in Equation 1$\}$
end if
$a \leftarrow T.splitAtt$
if $x_a < T.splitValue$ **then**
    return $PathLength(x, T.left, hlim, e + 1)$
else $\{x_a \geq T.splitValue\}$
    return $PathLength(x, T.right, hlim, e + 1)$
end if

Isolation Forest

- Effect of the height limit



(a) $hlim = 6$,



(b) $hlim = 1$,

Isolation Forest

- Empirical evaluation
  - ✓ Datasets

	n	d	anomaly class
Http (KDDCUP99)	567497	3	attack (0.4%)
ForestCover	286048	10	class 4 (0.9%) vs. class 2
Mulcross	262144	4	2 clusters (10%)
Smtp (KDDCUP99)	95156	3	attack (0.03%)
Shuttle	49097	9	classes 2,3,5,6,7 (7%)
Mammography	11183	6	class 1 (2%)
Annthyroid	6832	6	classes 1, 2 (7%)
Satellite	6435	36	3 smallest classes (32%)
Pima	768	8	pos (35%)
Breastw	683	9	malignant (35%)
Arrhythmia	452	274	classes 03,04,05,07, 08,09,14,15 (15%)
Ionosphere	351	32	bad (36%)
hbk	75	4	14 points (19%)
wood	20	6	6 instances (30%)

Isolation Forest

- Empirical evaluation
  - ✓ Performance (in terms of AUROC)

	AUC				
	*i*Forest	ORCA	SVM	LOF	RF
Http (KDDCUP99)	**1.00**	0.36	0.90	*	**
ForestCover	0.87	0.83	**0.90**	0.57	**
Mulcross	**0.96**	0.33	0.59	0.59	**
Smtp (KDDCUP99)	**0.89**	0.80	0.78	0.32	**
Shuttle	**1.00**	0.60	0.79	0.55	**
Mammography	**0.84**	0.77	0.65	0.67	**
Annthyroid	**0.84**	0.68	0.63	0.72	**
Satellite	**0.73**	0.65	0.61	0.52	**
Pima	0.67	**0.71**	0.55	0.49	0.65
Breastw	**0.98**	**0.98**	0.66	0.37	0.97
Arrhythmia	**0.81**	0.78	0.71	0.73	0.60
Ionosphere	0.83	**0.92**	0.71	0.89	0.85

(a) AUC performance

Isolation Forest

- Empirical evaluation
  - ✓ Performance (in terms of computational complexity)

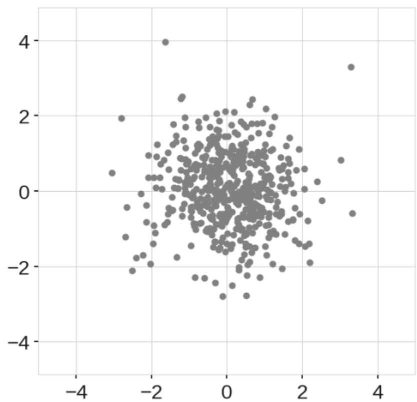
	Time (seconds)						
	*i*Forest			ORCA	SVM	LOF	RF
	Train	Eval.	Total				
Http	0.25	15.33	**15.58**	9487.47	35872.09	*	**
ForestCover	0.76	15.57	**16.33**	6995.17	9737.81	224380.19	**
Mulcross	0.26	12.26	**12.52**	2512.20	7342.54	156044.13	**
Smtp	0.14	2.58	**2.72**	267.45	986.84	24280.65	**
Shuttle	0.30	2.83	**3.13**	156.66	332.09	7489.74	**
Mammography	0.16	0.50	**0.66**	4.49	10.8	14647.00	**
Annthyroid	0.15	0.36	**0.51**	2.32	4.18	72.02	**
Satellite	0.46	1.17	**1.63**	8.51	8.97	217.39	**
Pima	0.17	0.11	0.28	**0.06**	**0.06**	1.14	4.98
Breastw	0.17	0.11	0.28	**0.04**	0.07	1.77	3.10
Arrhythmia	2.12	0.86	2.98	**0.49**	0.15	6.35	2.32
Ionosphere	0.33	0.15	0.48	**0.04**	0.04	0.64	0.83

(b) Actual processing time

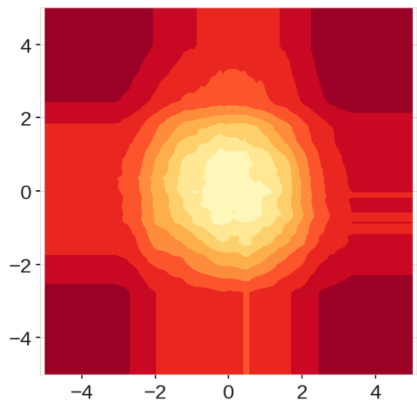
Extended Isolation Forests

Hariri et al. (2018)

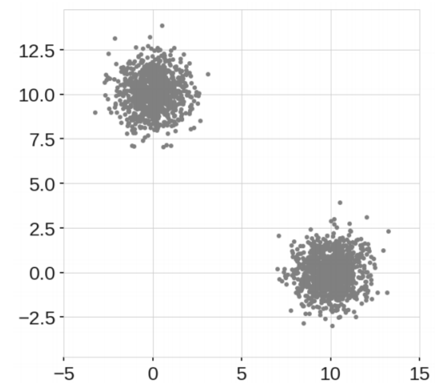
- Motivation



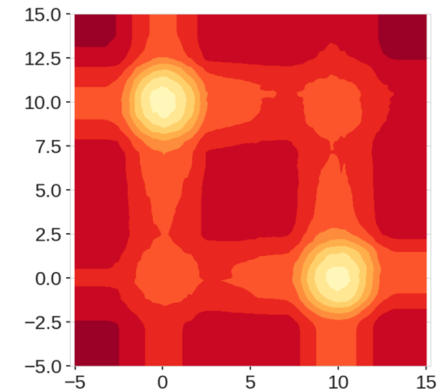
(a) Normally Distributed Data



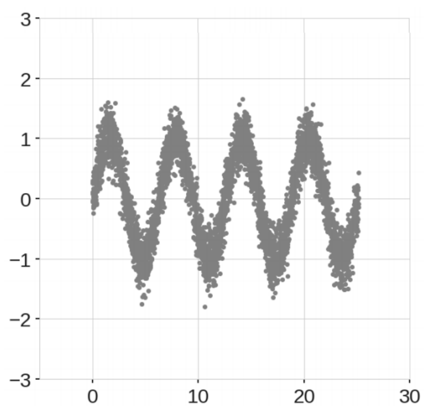
(b) Anomaly Score Map



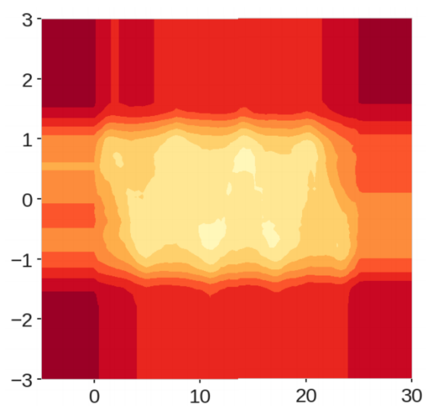
(a) Two normally distributed clusters



(b) Anomaly Score Map



(a) Sinusoidal data points with Gaussian noise.



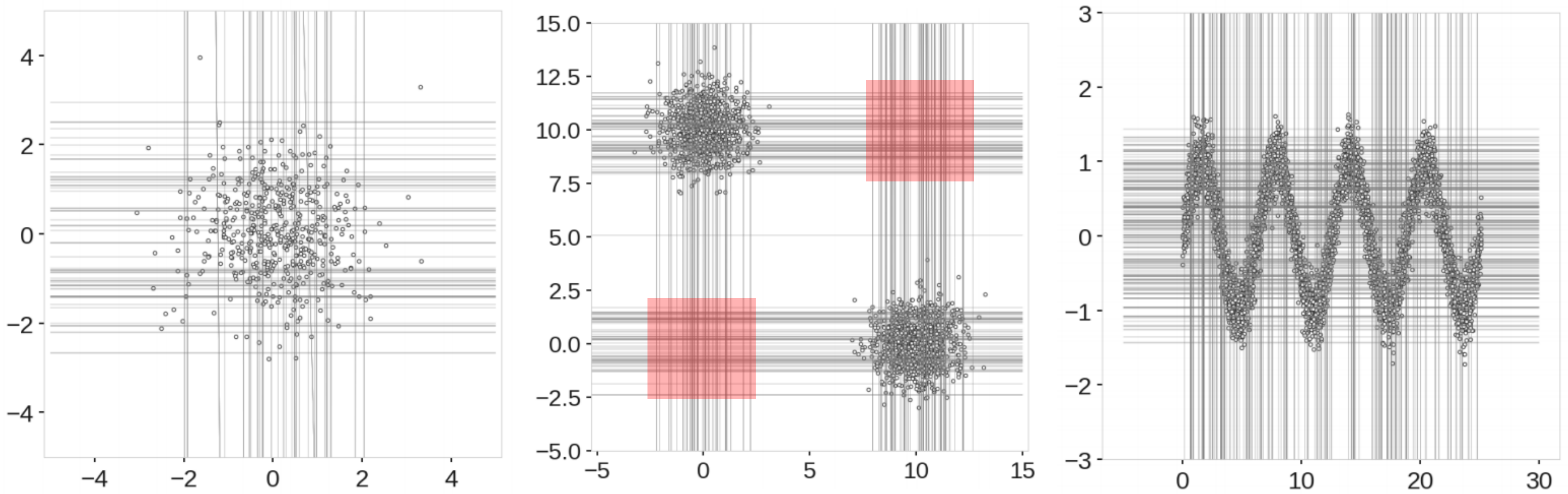
(b) Anomaly Score Map

Standard Isolation Forest
cannot work well for this dataset

Extended Isolation Forests

- Contribution

But as we have seen, the branch cuts are always either horizontal or vertical, and this introduces a bias and artifacts in the anomaly score map. There is no fundamental reason in the algorithm that requires this restriction, and so at each branching point, we can select a branch cut that has a random "slope".

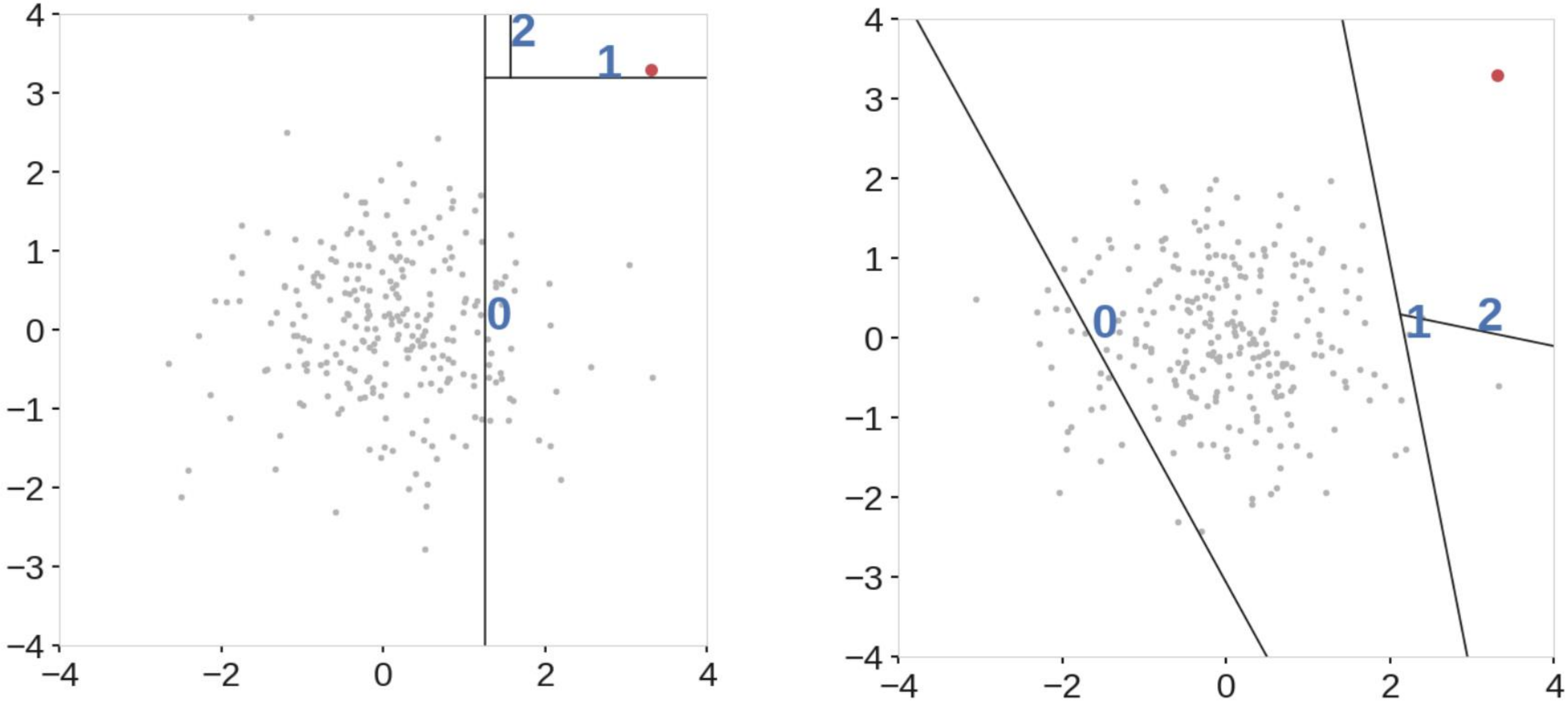


Extended Isolation Forests

- Illustrative example

Standard Isolation Forest

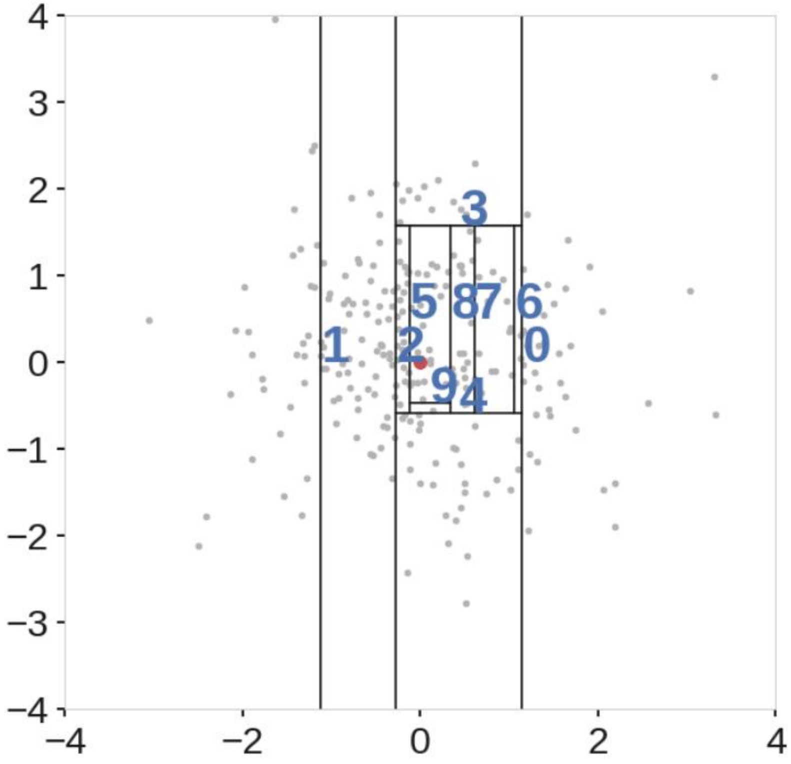
Extended Isolation Forest



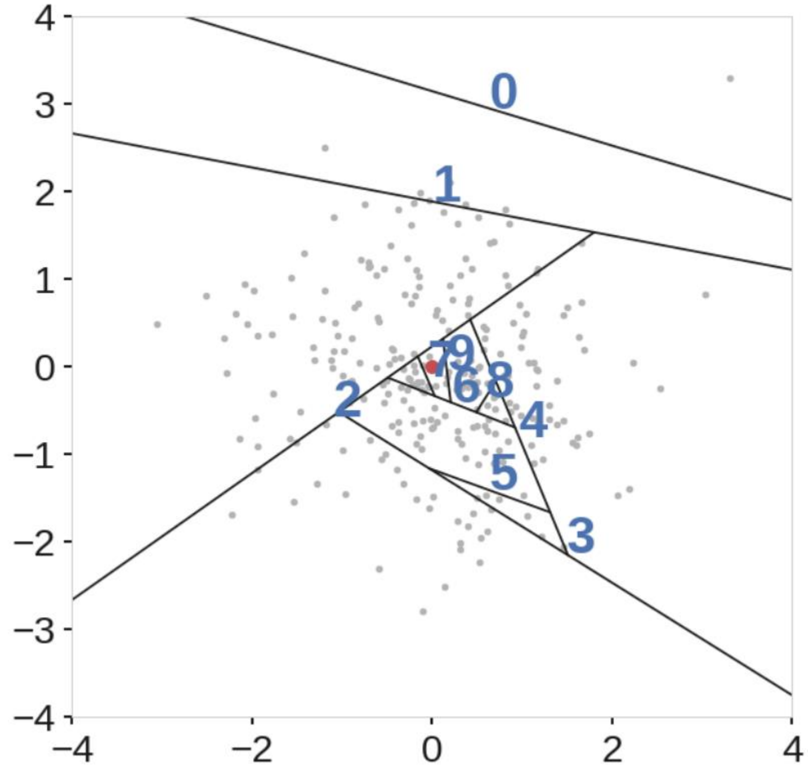
Extended Isolation Forests

- Illustrative example

Standard Isolation Forest



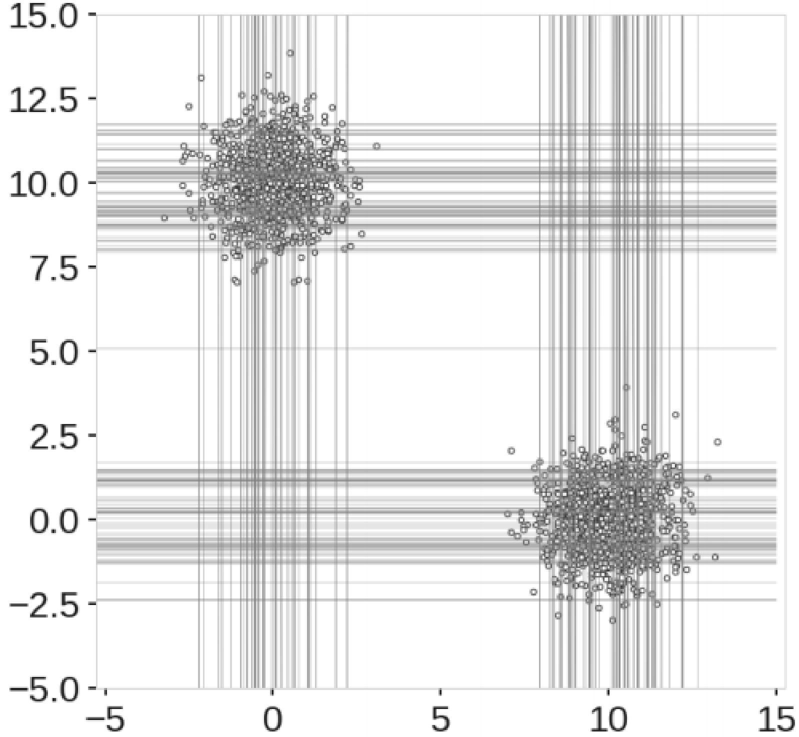
Extended Isolation Forest



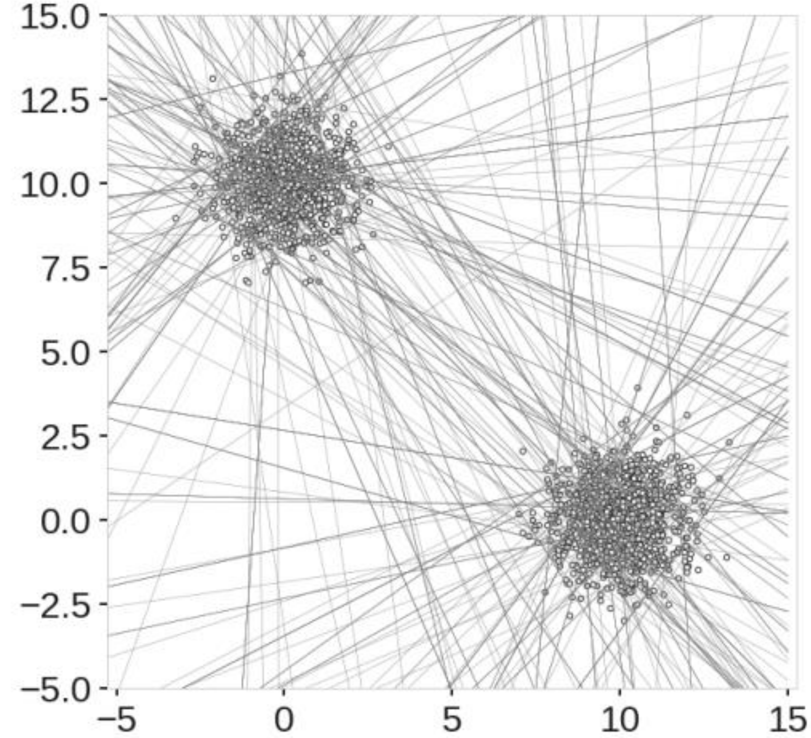
Extended Isolation Forests

- How are the biases reduced?

Standard Isolation Forest



Extended Isolation Forest



Extended Isolation Forests

- Algorithm

Algorithm 2 $iTree(X, e, l)$

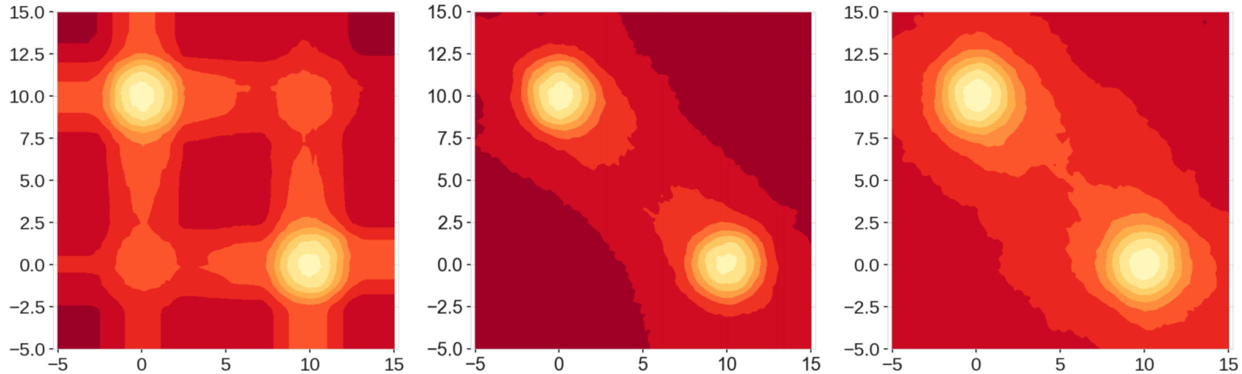
Input: X - input data, e - current tree height, l - height limit

Output: an iTree

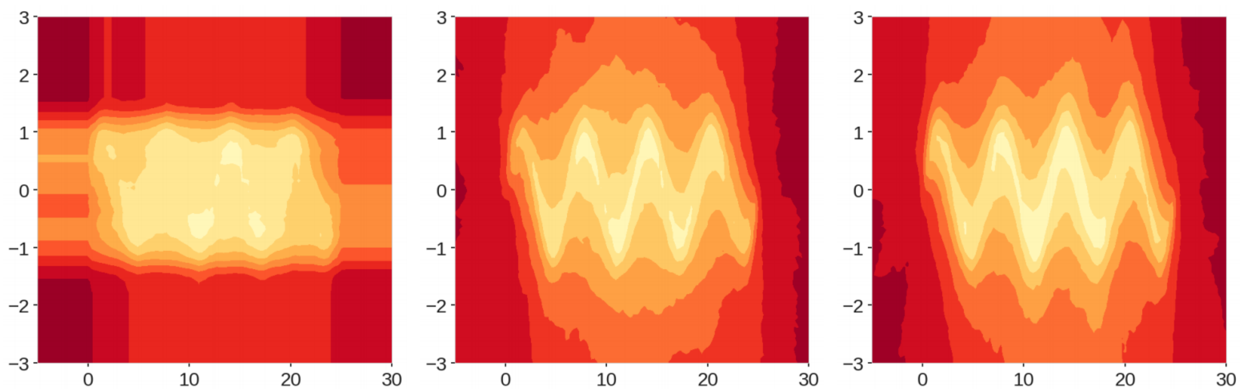
```
if e ≥ l or |X| ≤ 1 then
    return exNode{Size ← |X|}
else
    randomly select a normal vector n ∈ ℝ^|X| by drawing each coordinate of n⃗ from a uniform distribution.
    randomly select an intercept point p ∈ ℝ^|X| in the range of X
    set coordinates of n to zero according to extension level
    X_l ← filter(X, (X − p) · n ≤ 0)
    X_r ← filter(X, (X − p) · n > 0)
    return inNode{ Left ← iTree(X_l, e + 1, l),
                   Right ← iTree(X_r, e + 1, l),
                   Normal ← n,
                   Intercept ← p}
end if
```

Extended Isolation Forests

- Anomaly score distribution



(a) Standard IF (b) Rotated IF (c) Extended IF

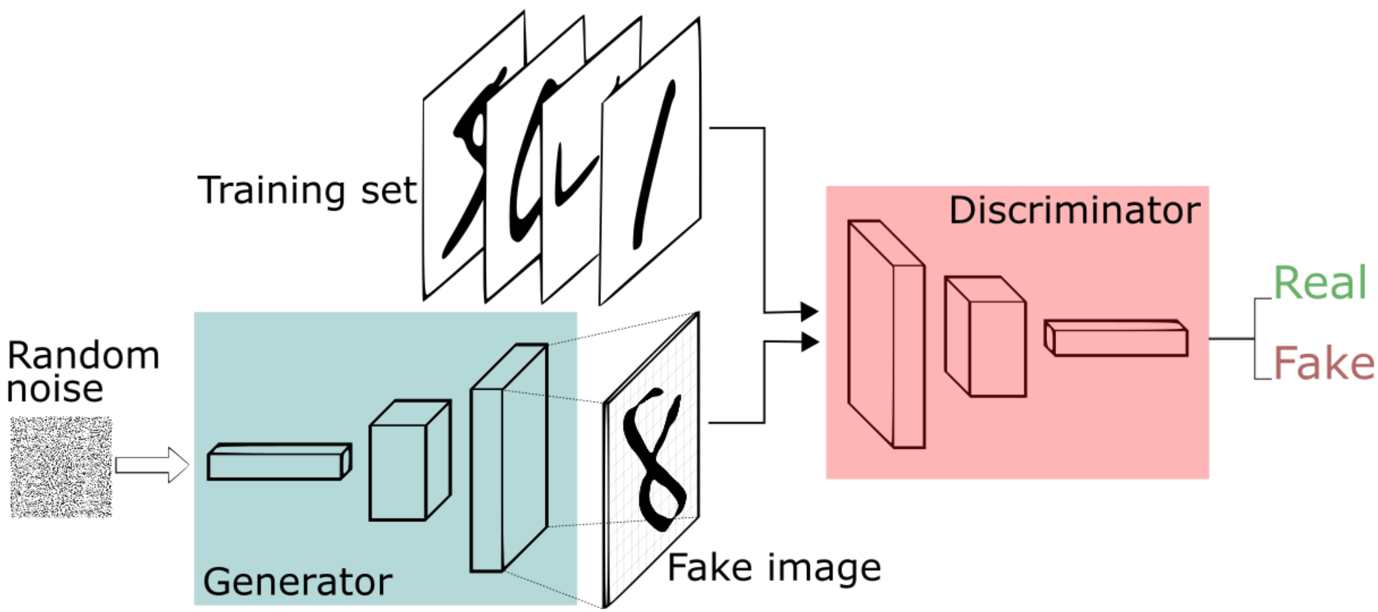


(a) Generic IF (b) Rotated IF (c) Extended IF

AnoGAN

Schlegl et al. (2017)

- AnoGAN
  - ✓ Original Generative Adversarial Network (GAN)

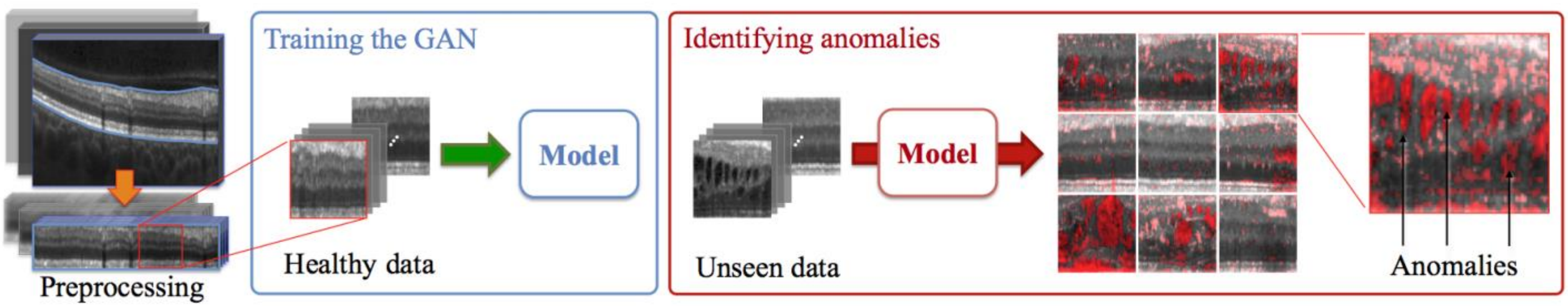


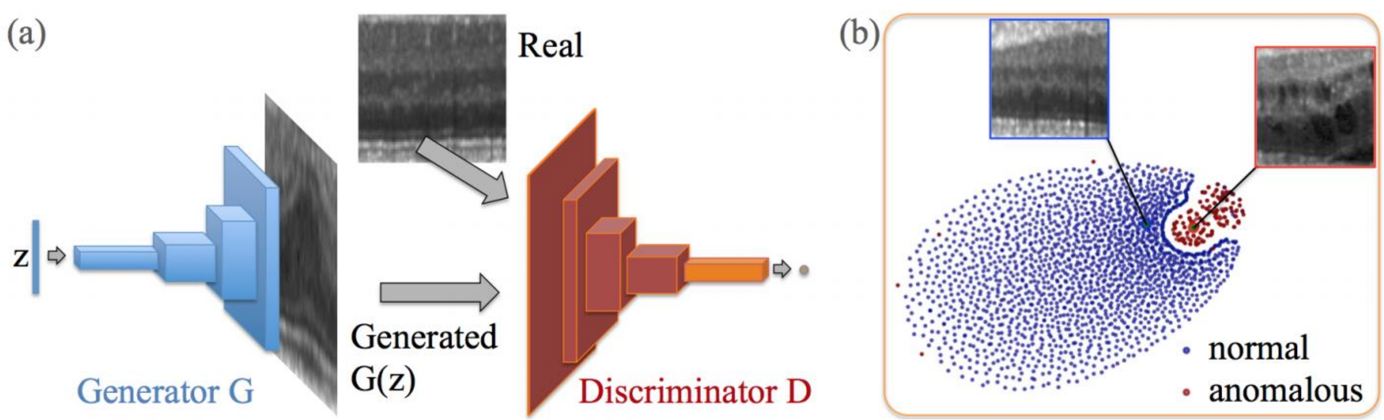
  - ▪ Loss function: $E_x[log(D(x))] + E_z[log(1 - D(G(z)))]$
    - Discriminator tries to maximize it
    - Generator tries to minimize it

AnoGAN

Schlegl et al. (2017)

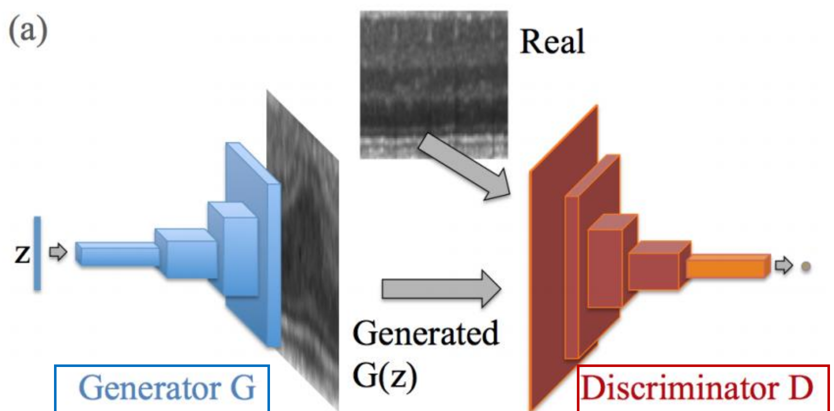
- AnoGAN





AnoGAN

- AnoGAN
  - ✓ Training: Train a GAN with normal data (medical images in the original paper)
    - Train the parameters of Generator G and Discriminator D

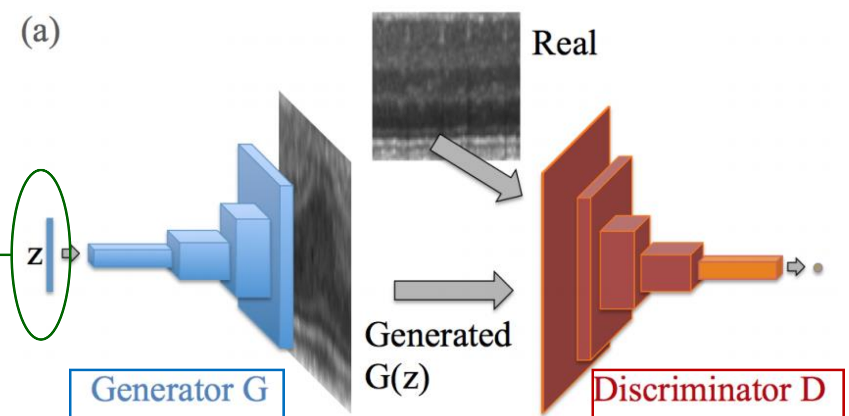


These two models are trained

AnoGAN

- AnoGAN
  - ✓ Test: Update the latent vector z to generate a similar image of the given image and to fool the discriminator
    - Train the latent vector
    - Parameters of Generate G and Discriminator D are fixed in this step

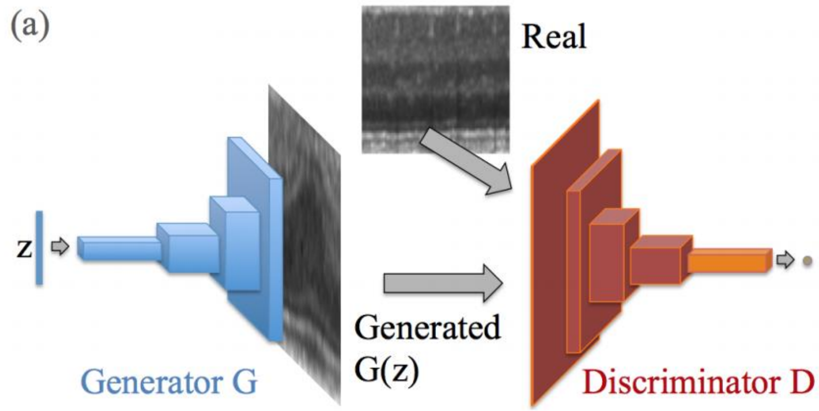
This latent vector is updated to generate a fake image as similar as possible to the test image



They are fixed

AnoGAN

- AnoGAN



✓ Two types of loss functions are used

- Generation loss: $\mathrm{L_R}(\mathrm{z}_\gamma) = \sum|\mathrm{x} - \mathrm{G}(\mathrm{z}_\gamma)|$
- Discrimination loss: $\mathrm{L_D}(\mathrm{z}_\gamma) = \sum\left|\mathrm{f}(\mathrm{x}) - \mathrm{f}\left(\mathrm{G}(\mathrm{z}_\gamma)\right)\right|$

✓ Total loss: $\mathrm{L}(\mathrm{z}_\gamma) = (1-\lambda)\cdot\mathrm{L_R}(\mathrm{z}_\gamma) + \lambda\cdot\mathrm{L_D}(\mathrm{z}_\gamma)$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Other materials

- Pages 28-33 & 36: http://research.cs.tamu.edu/prism/lectures/pr/pr_l7.pdf
- Figures in Auto-encoder section: https://dl.dropboxusercontent.com/u/19557502/6_01_definition.pdf
- Gramfort, A. (2016). Anomaly/Novelty detection with scikit-learn: https://www.slideshare.net/agramfort/anomalynovelty-detection-with-scikitlearn