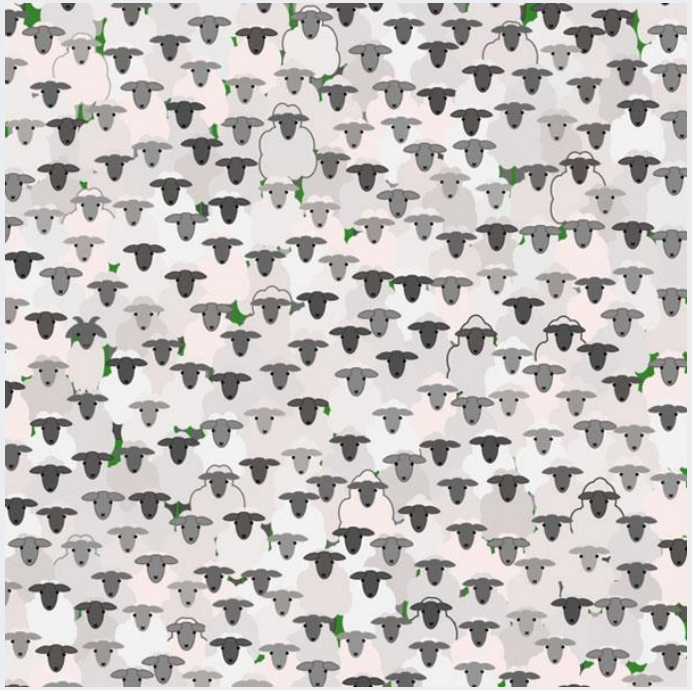

Lecture 3: Novelty Detection

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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

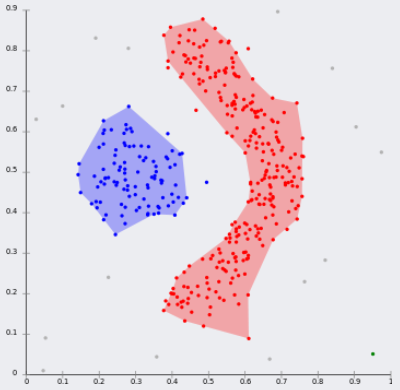
Unsupervised Learning

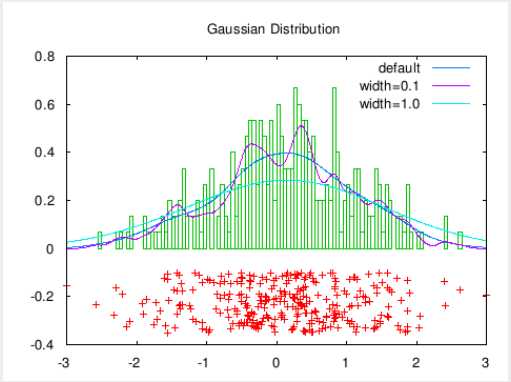
A given dataset **X**

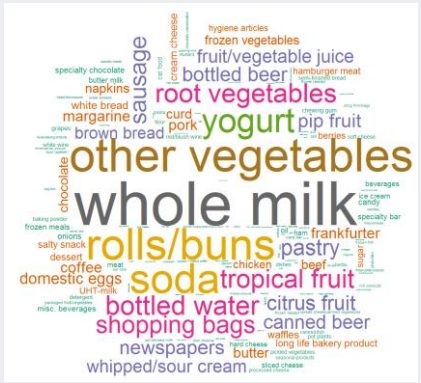
	Var. 1	Var. 2	...	Var. d
Ins. 1	..	..	...	..
Ins. 2	..	..	...	..
...	...	...	...	...
Ins. N	..	..	..	..

[Unsupervised learning]

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







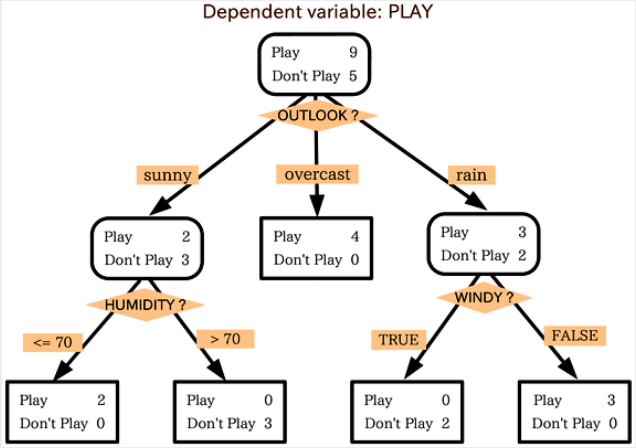
Unsupervised Learning

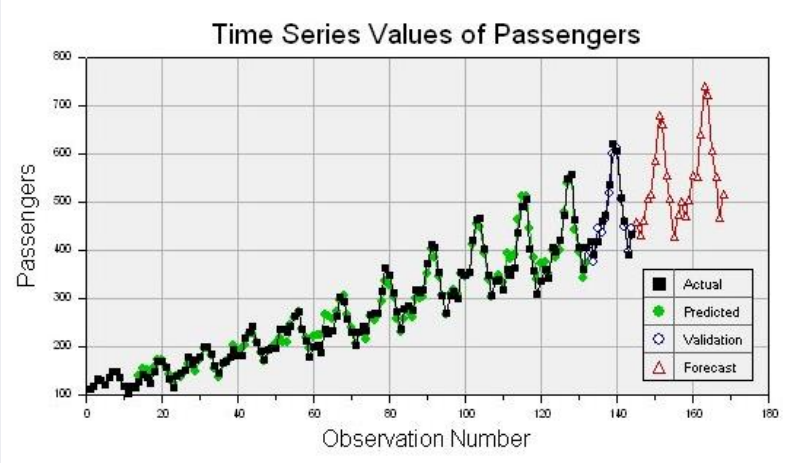
A given dataset **X** & **Y**

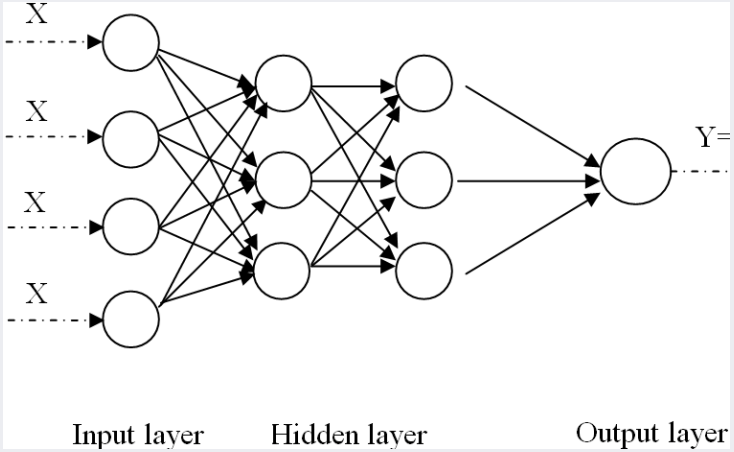
	Var. 1	Var. 2	...	Var. d		Y
Ins. 1	..	..	...	..		..
Ins. 2	..	..	...	..	$y = f(x)$	..
...	...	...	...	...		...
Ins. N	..	..	..	..		..

[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

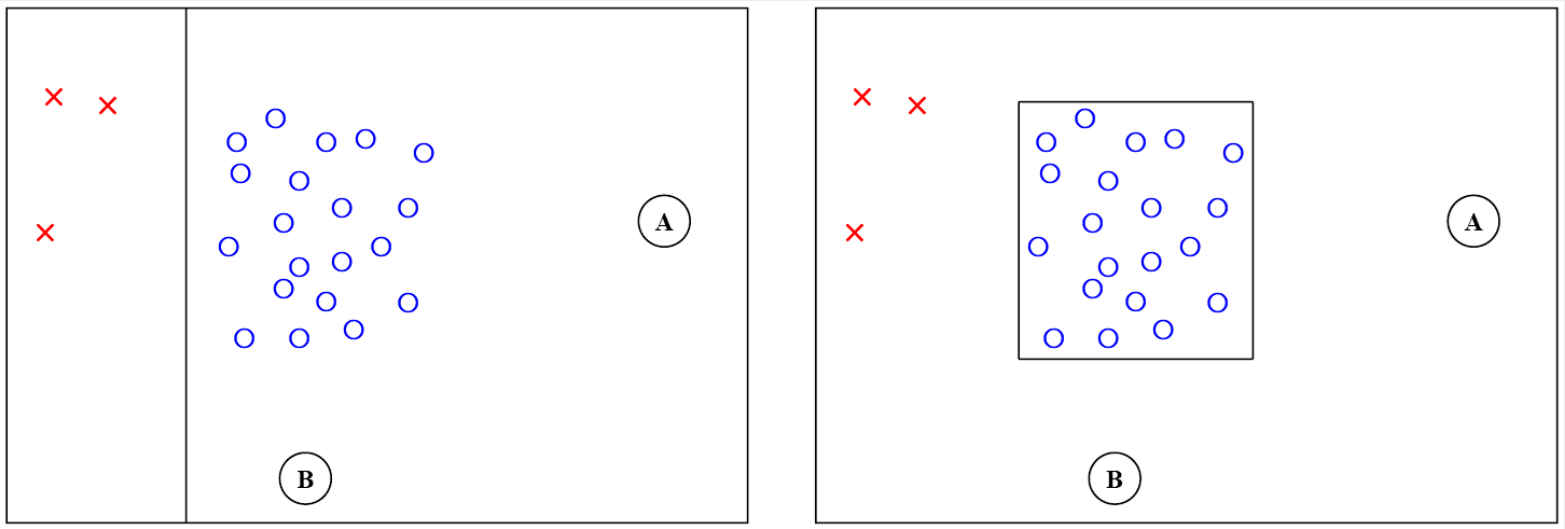
- Applications
  - ✓ Industrial monitoring
  - ✓ IT security
  - ✓ Healthcare informatics
  - ✓ Sensor network
  - ✓ Computer vision
  - ✓ Credit card fraud detection
  - ✓ Telecom fraud detection
  - ✓ Customer segmentation/Medical analysis

Supervised Learning: Novelty Detection

- Classification vs. Novelty Detection

Supervised Learning: Novelty Detection

- Classification vs. Novelty Detection

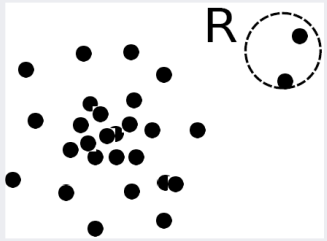


Binary classification

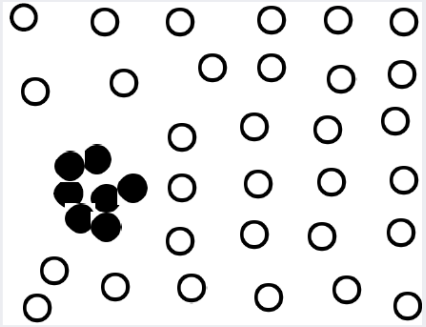
Novelty detection

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 attack

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

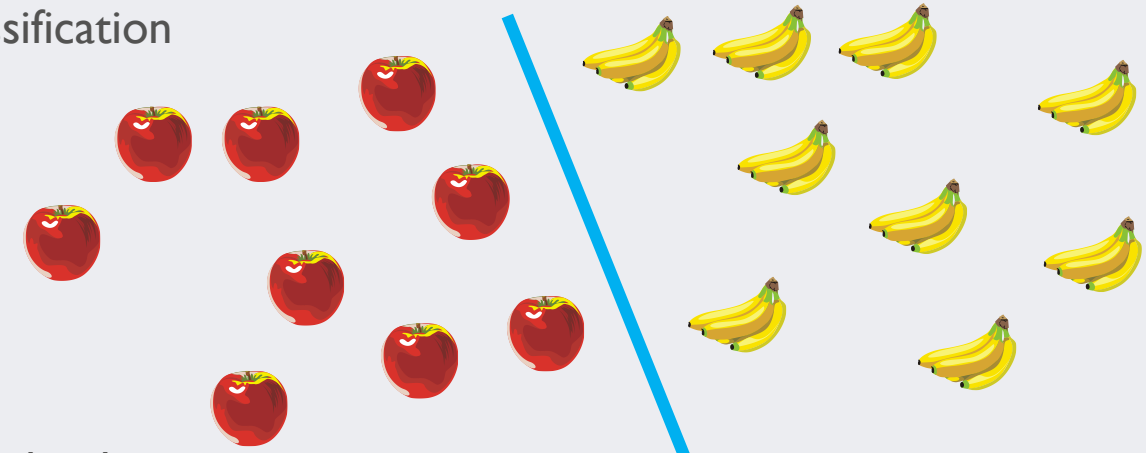
○ 문의사항

- 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?

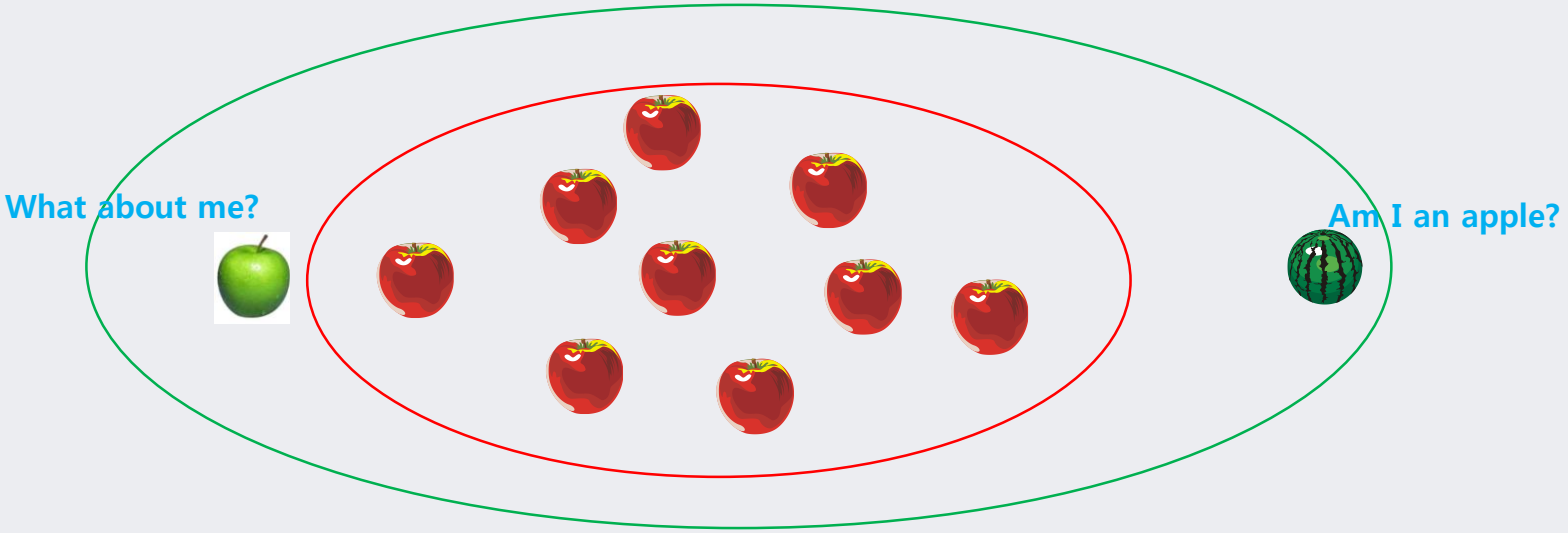
Supervised Learning: Novelty Detection

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

✓ Classification

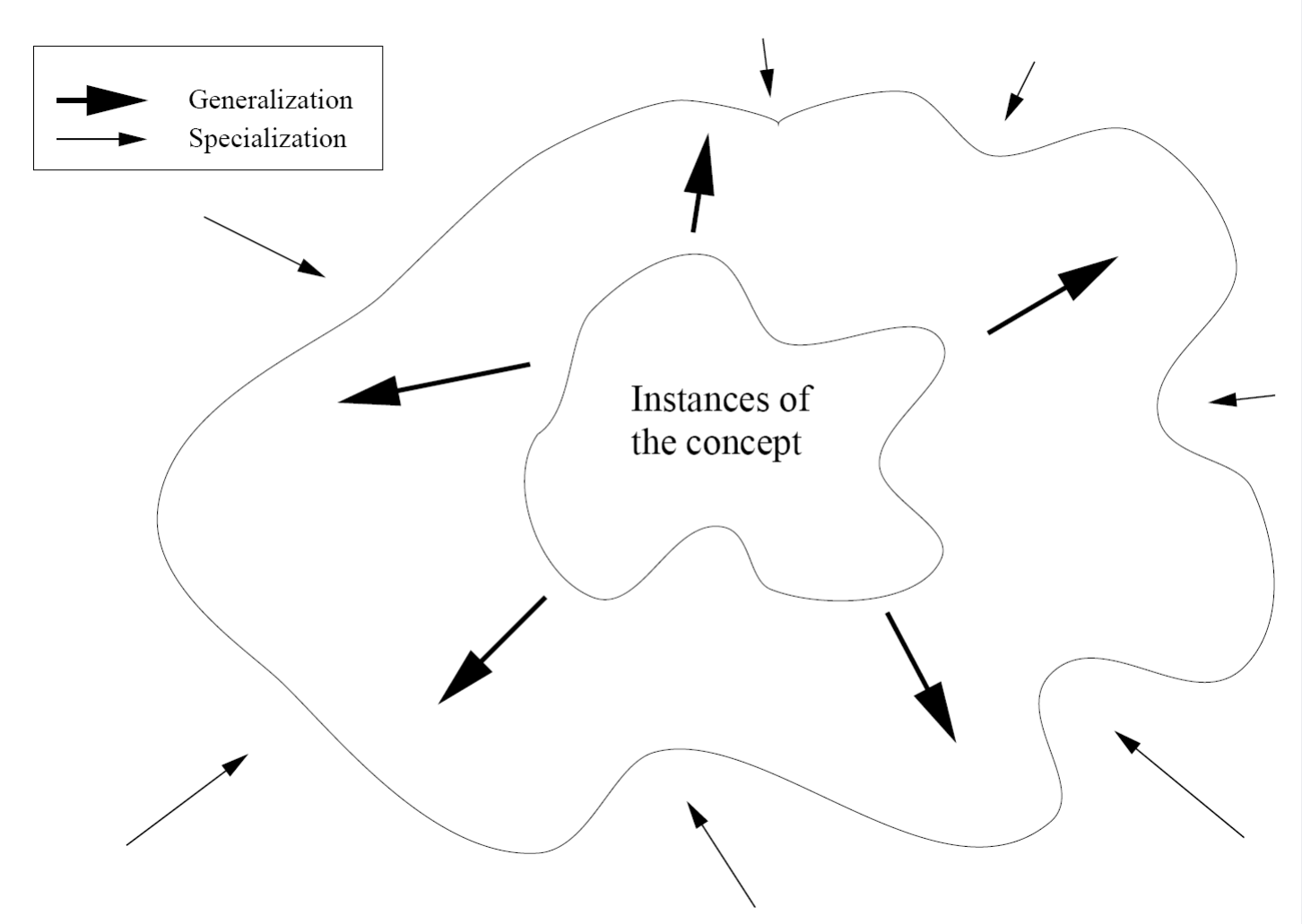


✓ Novelty detection



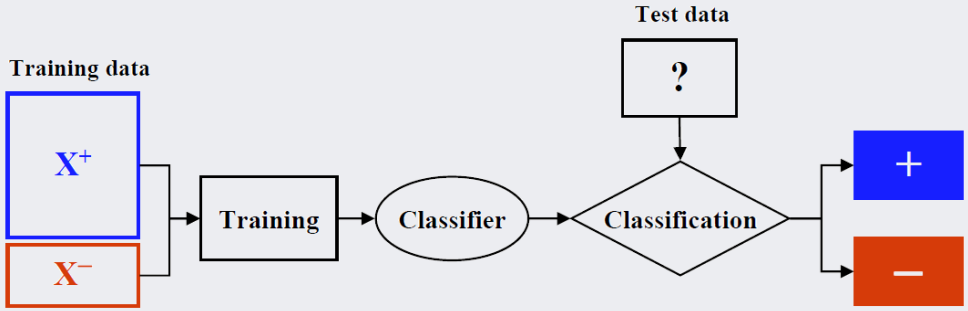
Supervised Learning: Novelty Detection

- Generalization vs. Specialization

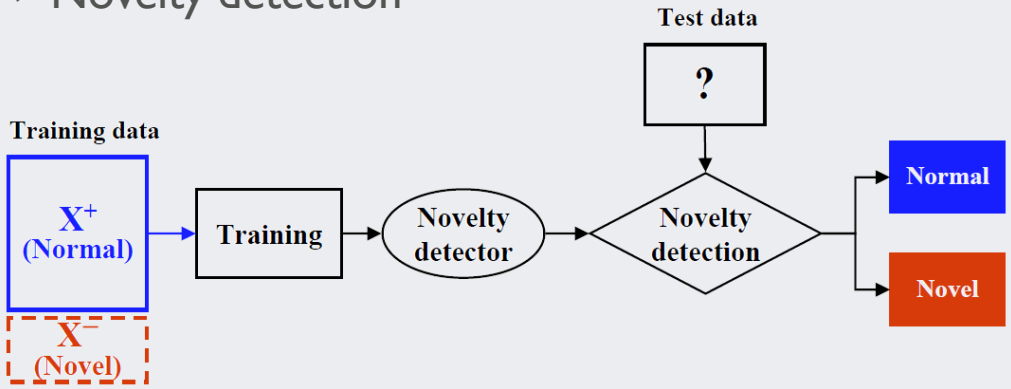


ND Approach

- 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

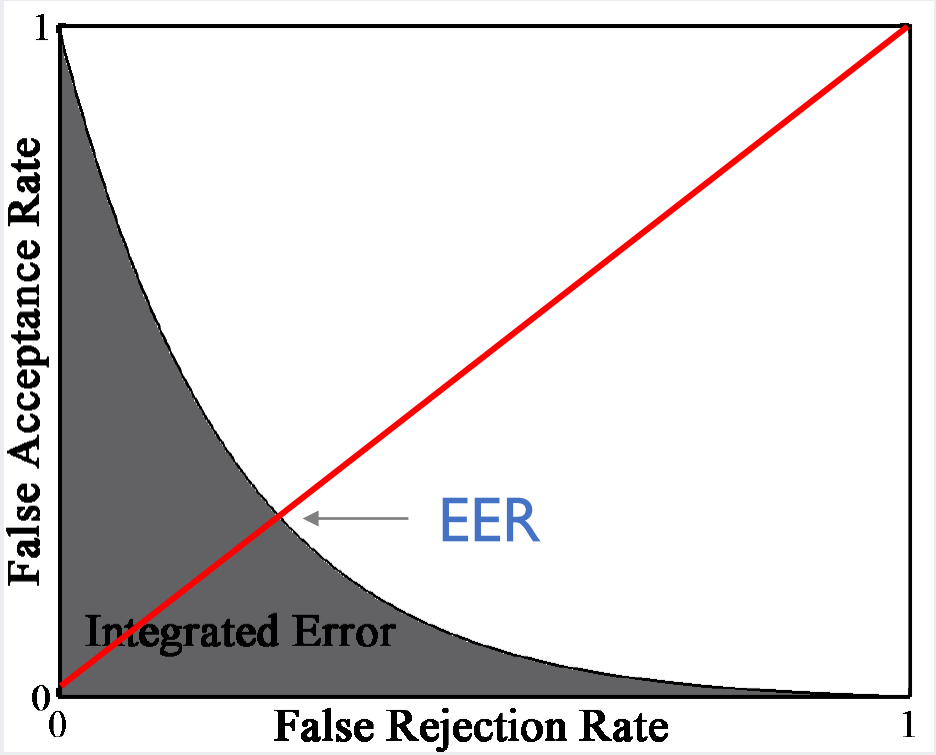
		Predicted class	
		Novel	Normal
Actual class	Novel	A	B
	Normal	C	D

  - ✓ 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

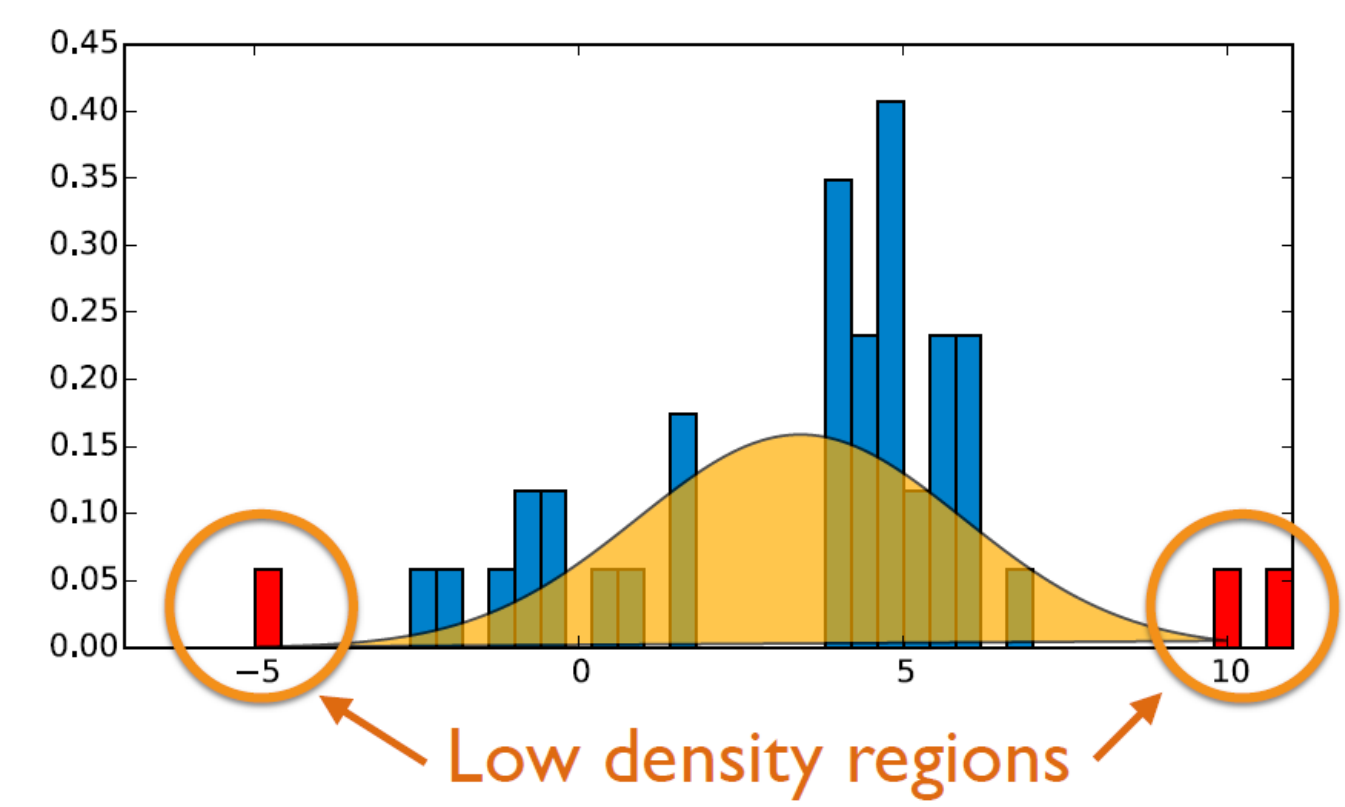


AGENDA

Density-based Novelty Detection

Gramfort (2006)

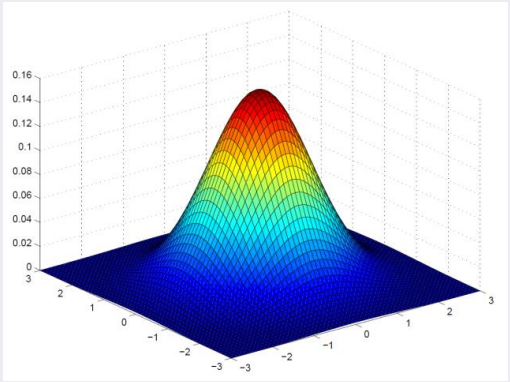
- Purpose
  - ✓ Estimate the data-driven density function
  - ✓ If a new instance has a low probability according the trained density function, it will be identified as novel



Density-based Novelty Detection

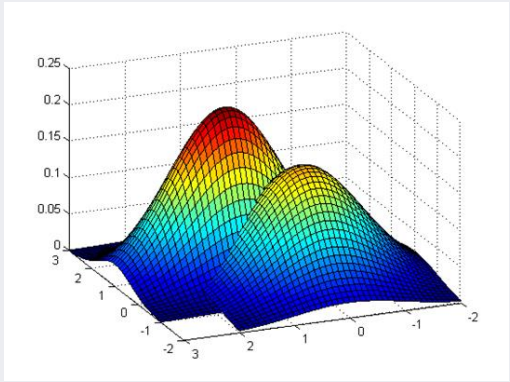
- Purpose
  - ✓ Estimate the data-driven density function
  - ✓ If a new instance has a low probability according the trained density function, it will be identified as novel

Gaussian Density Estimation



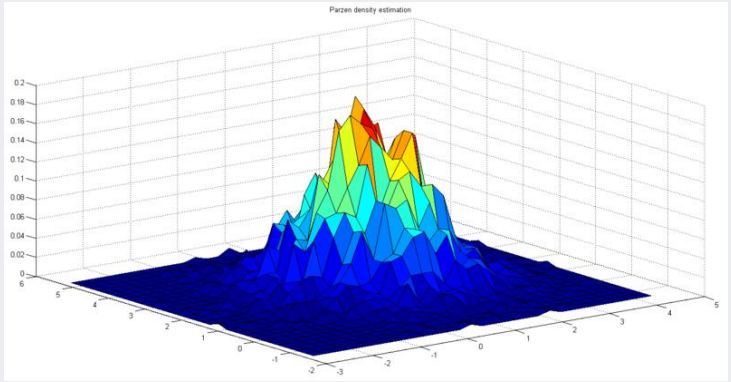
Number of modals = 1

Mixture of Gaussian Density Estimation



1 < Number of modals <= Number of instances

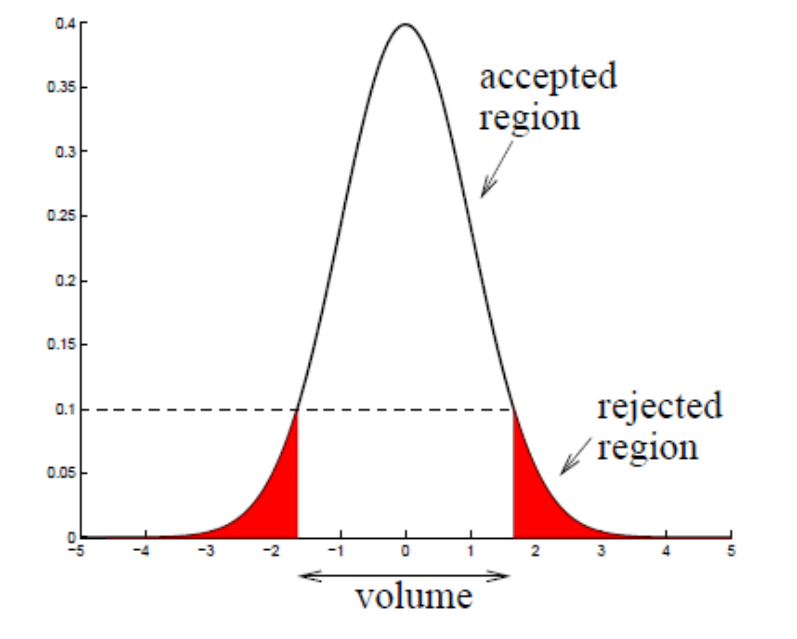
Kernel Density Estimation

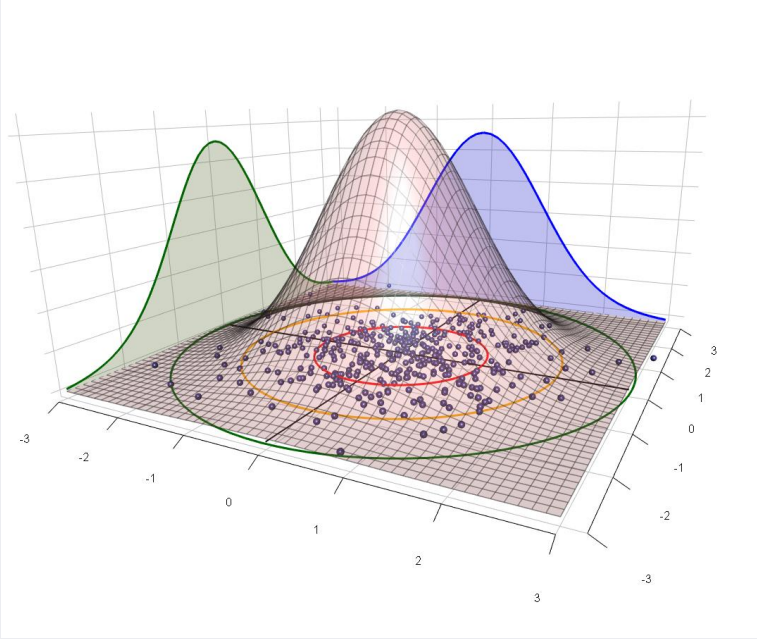


Number of modals = Number of instances

Gaussian Density Estimation

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





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

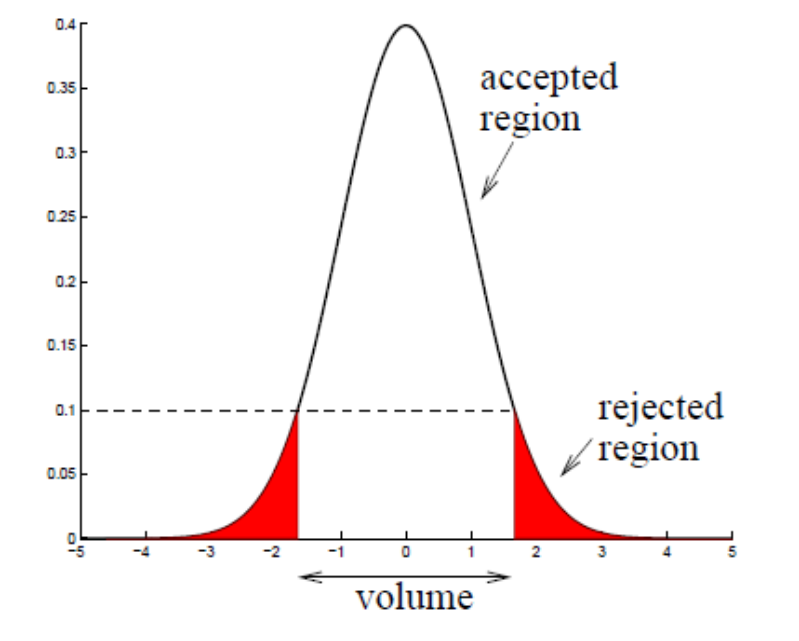
$$\boldsymbol{\mu} = \frac{1}{n}\sum_{\mathbf{x}_i \in \mathbf{X}^+} \mathbf{x}_i \text{ (mean vector)}, \quad \boldsymbol{\Sigma} = \frac{1}{n}\sum_{\mathbf{x}_i \in \mathbf{X}^+} (\mathbf{x}_i-\boldsymbol{\mu})(\mathbf{x}_i-\boldsymbol{\mu})^T \text{ (covariance matrix)}$$

Gaussian Density Estimation

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

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

    - 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 $\gamma = 1/\sigma^2$

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

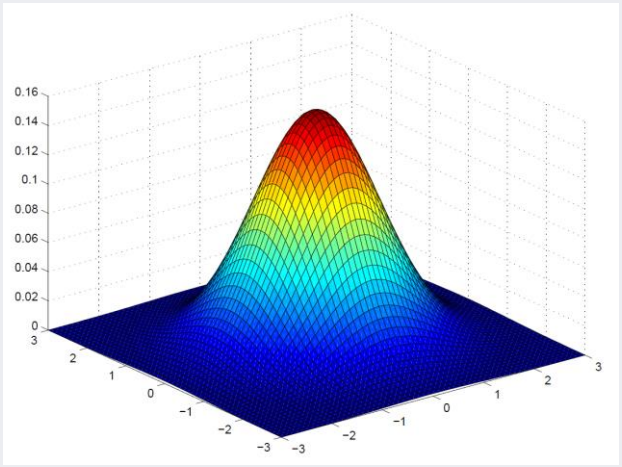
$$\frac{\partial Log\ L}{\partial \mu} = \gamma\sum_{i=1}^{N}(x_i-\mu) = 0 \rightarrow \mu = \frac{1}{N}\sum_{i=1}^{N}x_i$$

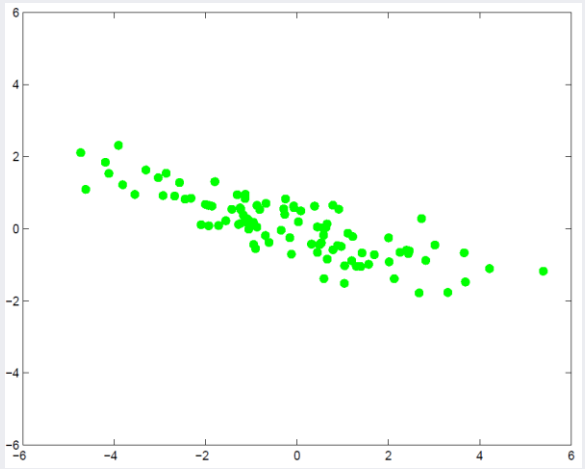
$$\frac{\partial Log\ L}{\partial \gamma} = -\frac{1}{2}\sum_{i=1}^{N}(x_i-\mu)^2 + \frac{N}{2\gamma} = 0 \rightarrow \sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i-\mu)^2$$

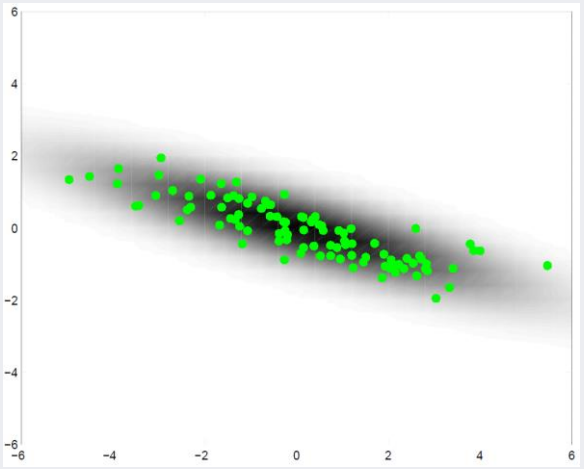
Gaussian Density Estimation

- Gaussian Density Estimation
  - ✓ In general,

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



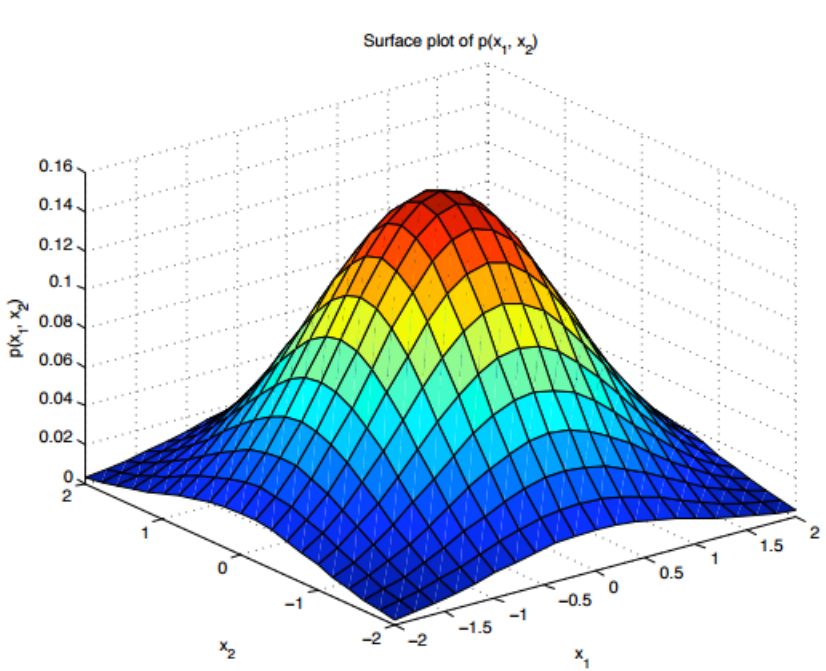


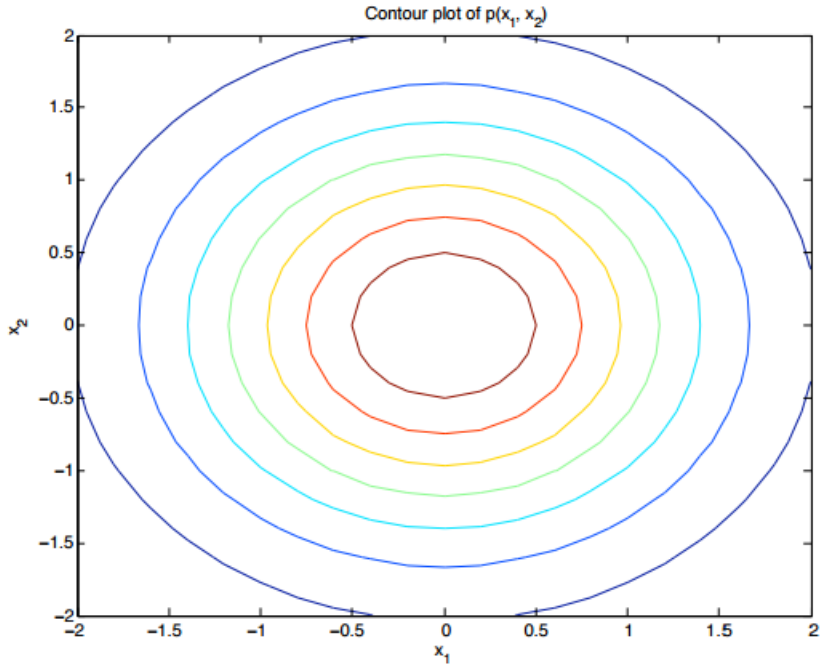


Gaussian Density Estimation

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

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



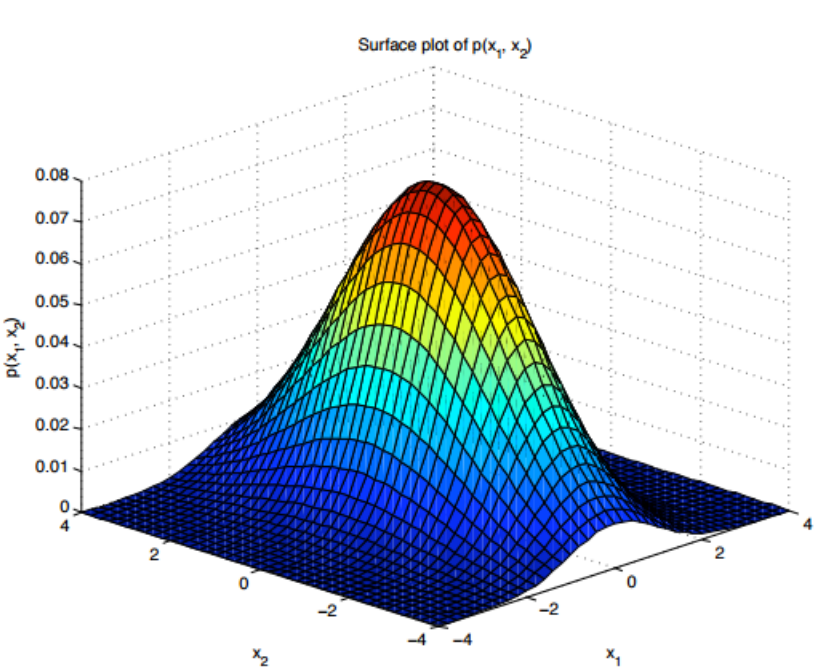


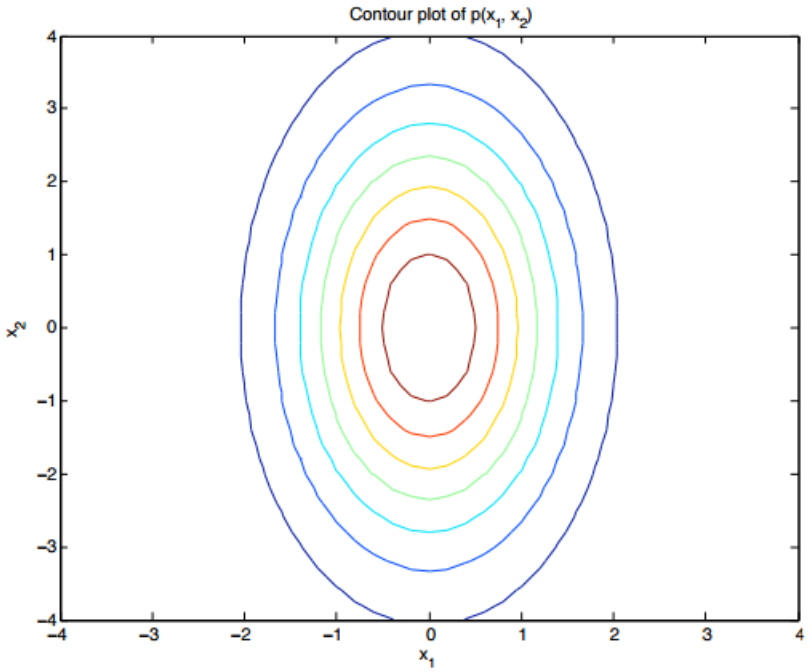
(a) Spherical Gaussian (diagonal covariance, equal variances)

Gaussian Density Estimation

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

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



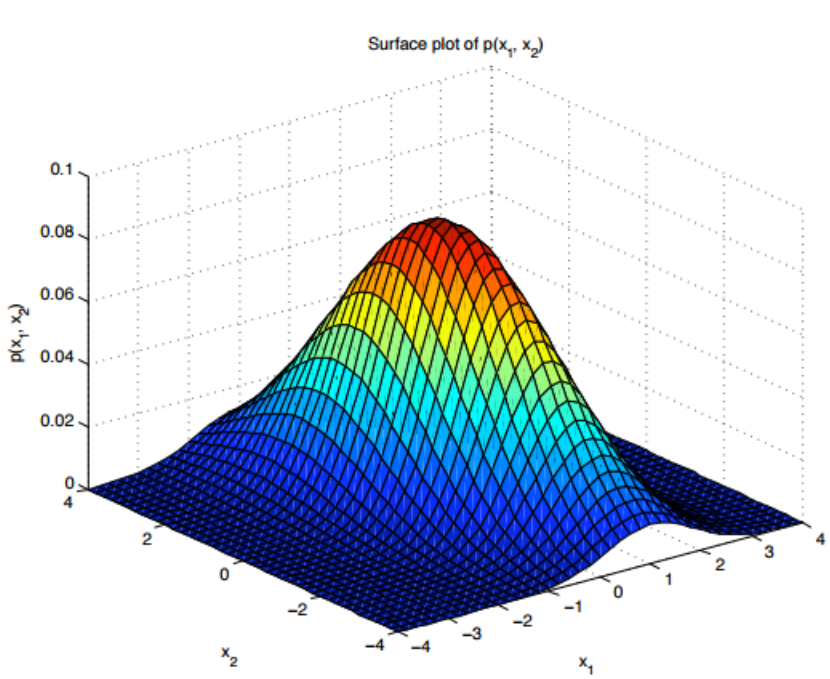


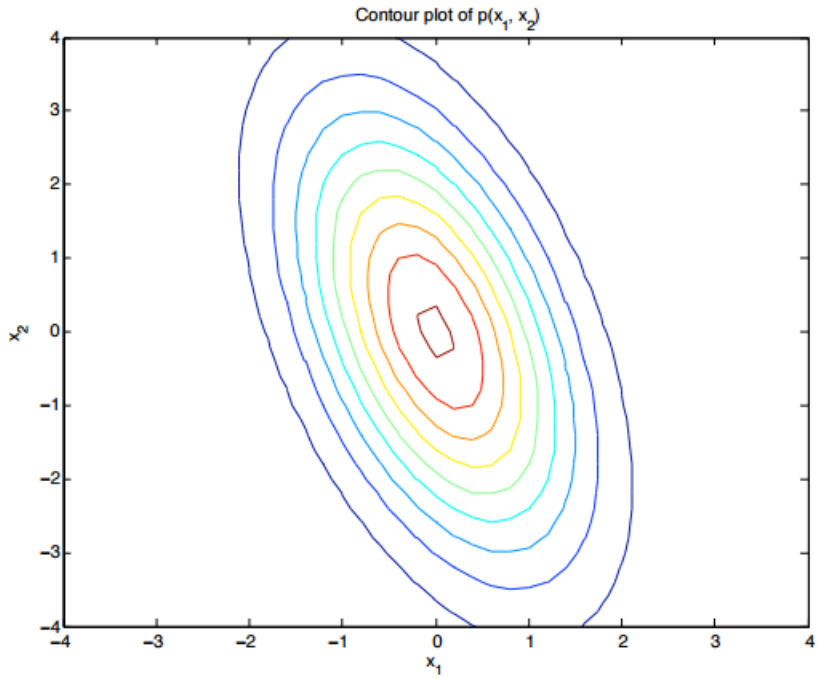
(b) Gaussian with diagonal covariance matrix

Gaussian Density Estimation

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

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

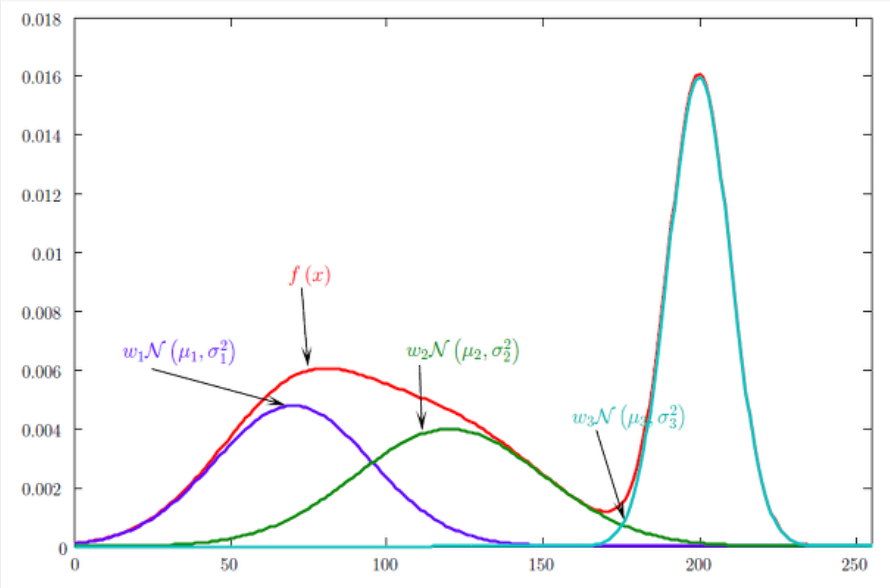




(c) Gaussian with full covariance matrix

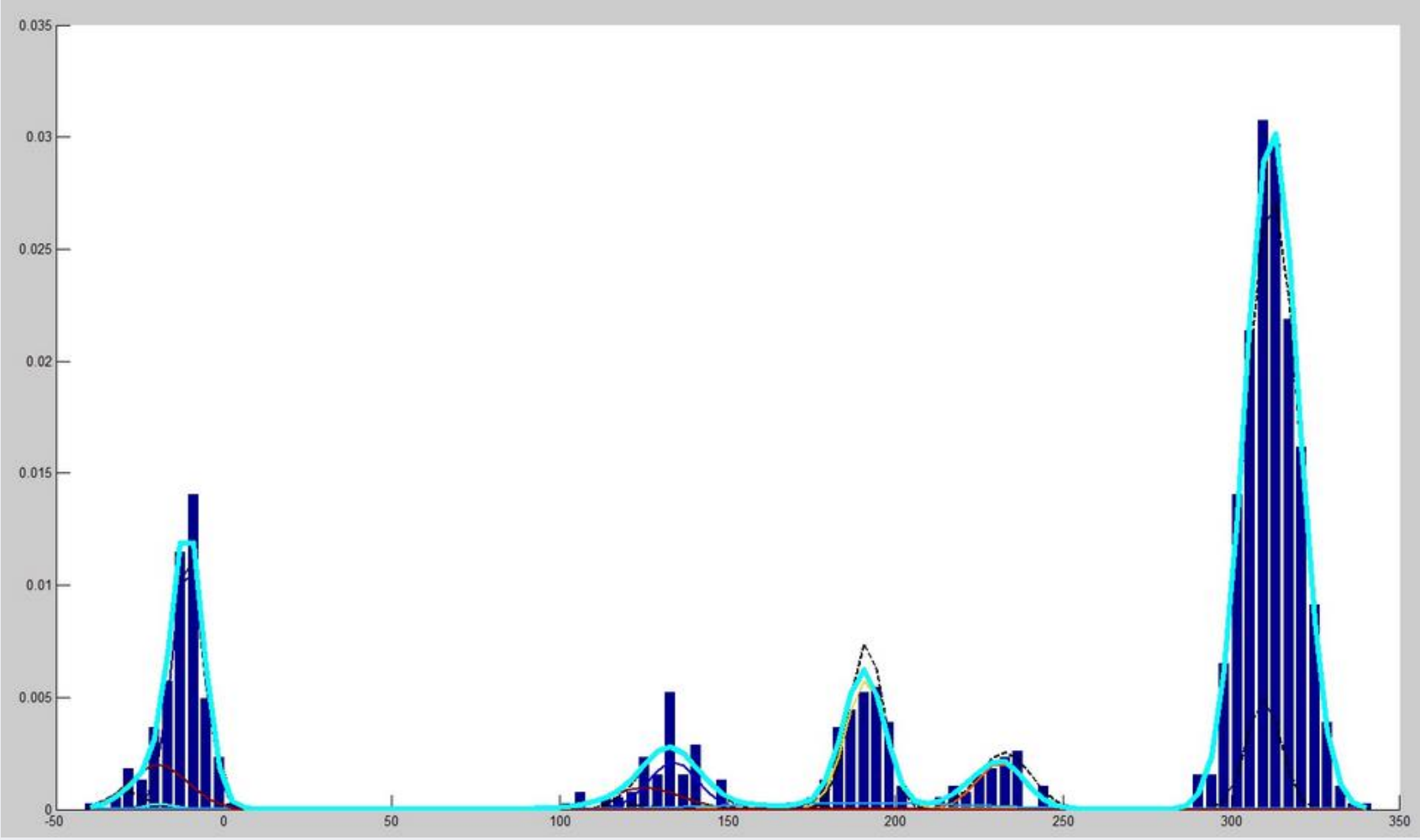
Mixture of Gaussian Density Estimation

- 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

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

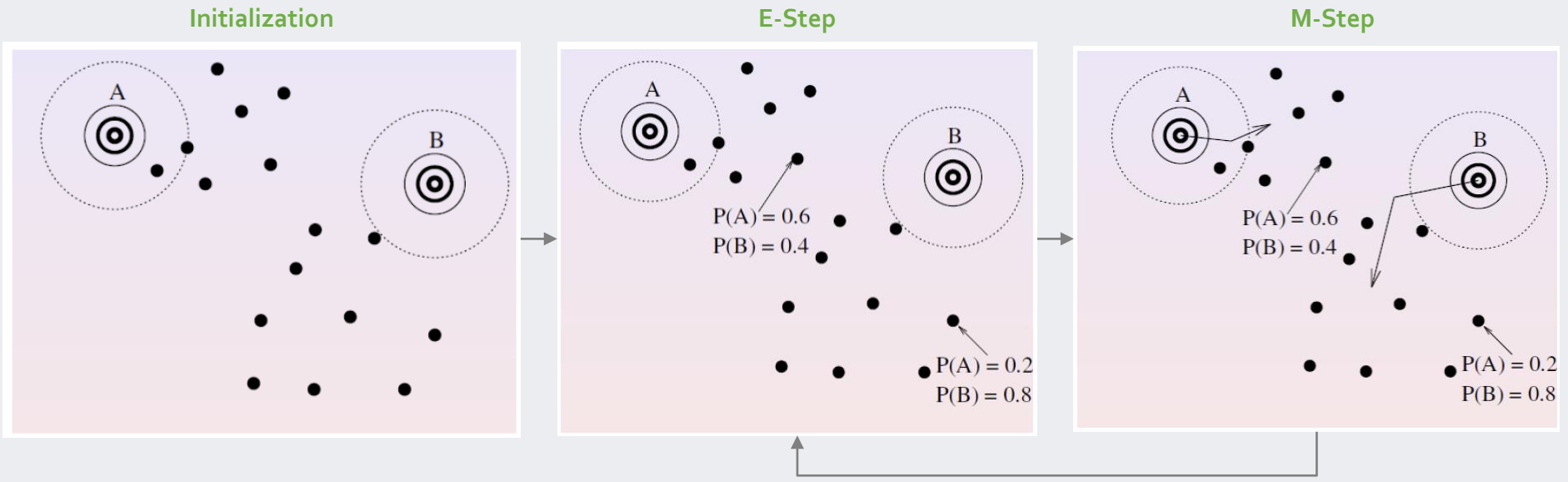
  - ✓ Distribution of each Gaussian model

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

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

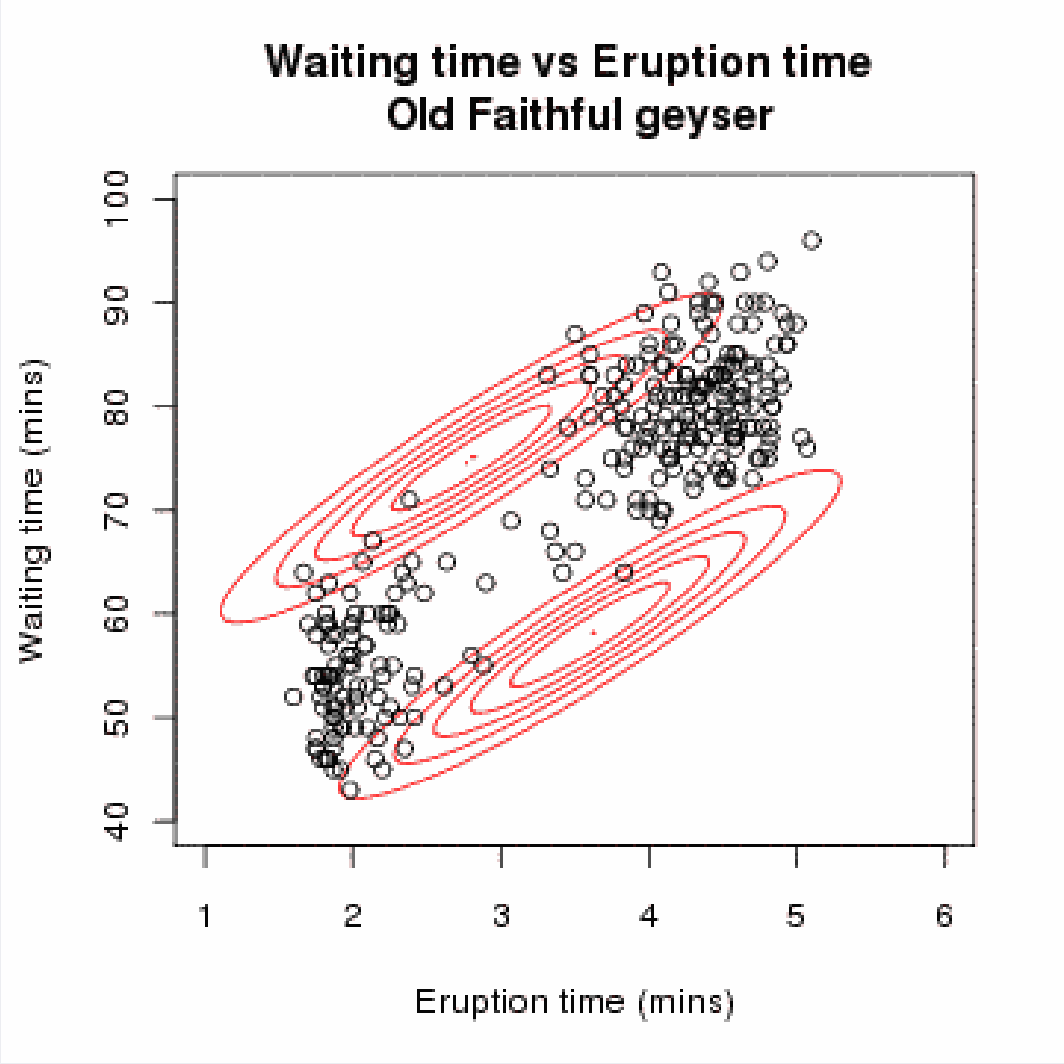
Mixture of Gaussian Density Estimation

- 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

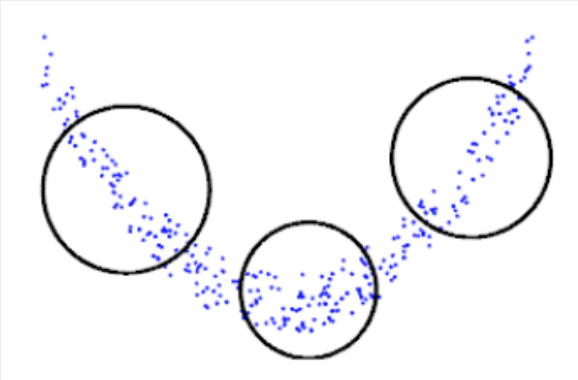
$$\boldsymbol{\mu}_m^{(new)} = \frac{\sum_{i=1}^{N} p(m|\mathbf{x}_i, \lambda)\mathbf{x}_i}{\sum_{i=1}^{N} p(m|\mathbf{x}_i, \lambda)}, \quad \sigma_m^{2(new)} = \frac{\sum_{i=1}^{N} p(m|\mathbf{x}_i, \lambda)\mathbf{x}_i^2}{\sum_{i=1}^{N} p(m|\mathbf{x}_i, \lambda)} - \boldsymbol{\mu}_m^{2(new)}$$

Mixture of Gaussian Density Estimation

- The shape of MoG according to the covariance matrix

Spherical

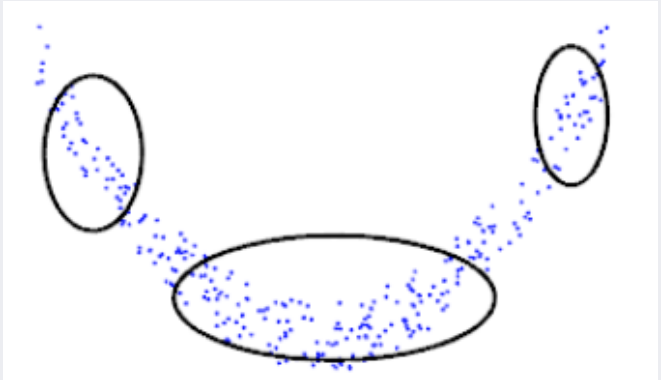
$$\Sigma = \sigma^2 \begin{bmatrix} 1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}$$



- Less precise
- Very efficient to compute

Diagonal

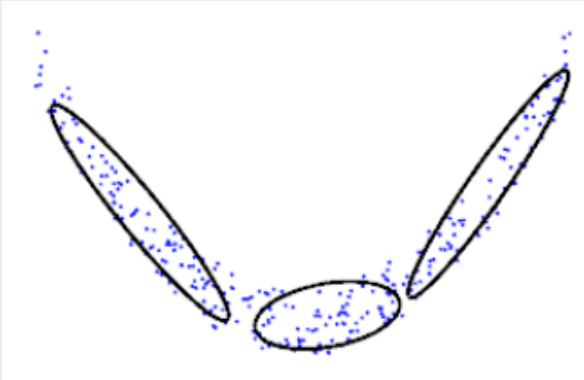
$$\Sigma = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_d^2 \end{bmatrix}$$



- More precise
- Efficient to compute

Full

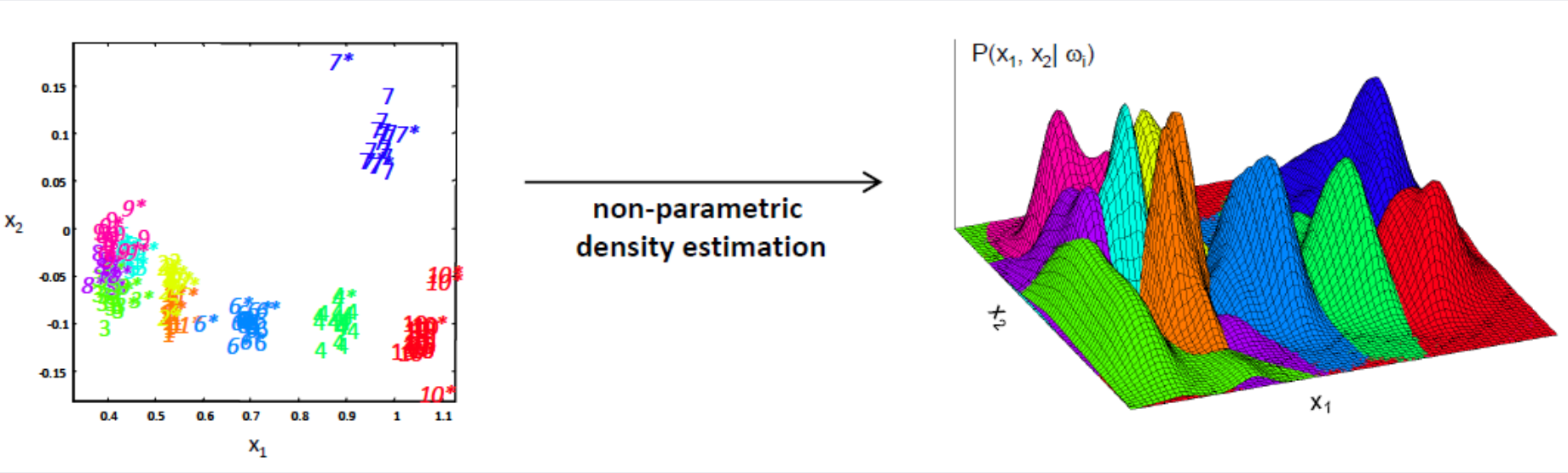
$$\Sigma = \begin{bmatrix} \sigma_{11} & \cdots & \sigma_{1d} \\ \vdots & \ddots & \vdots \\ \sigma_{d1} & \cdots & \sigma_{dd} \end{bmatrix}$$



- Very precise
- Less efficient to compute

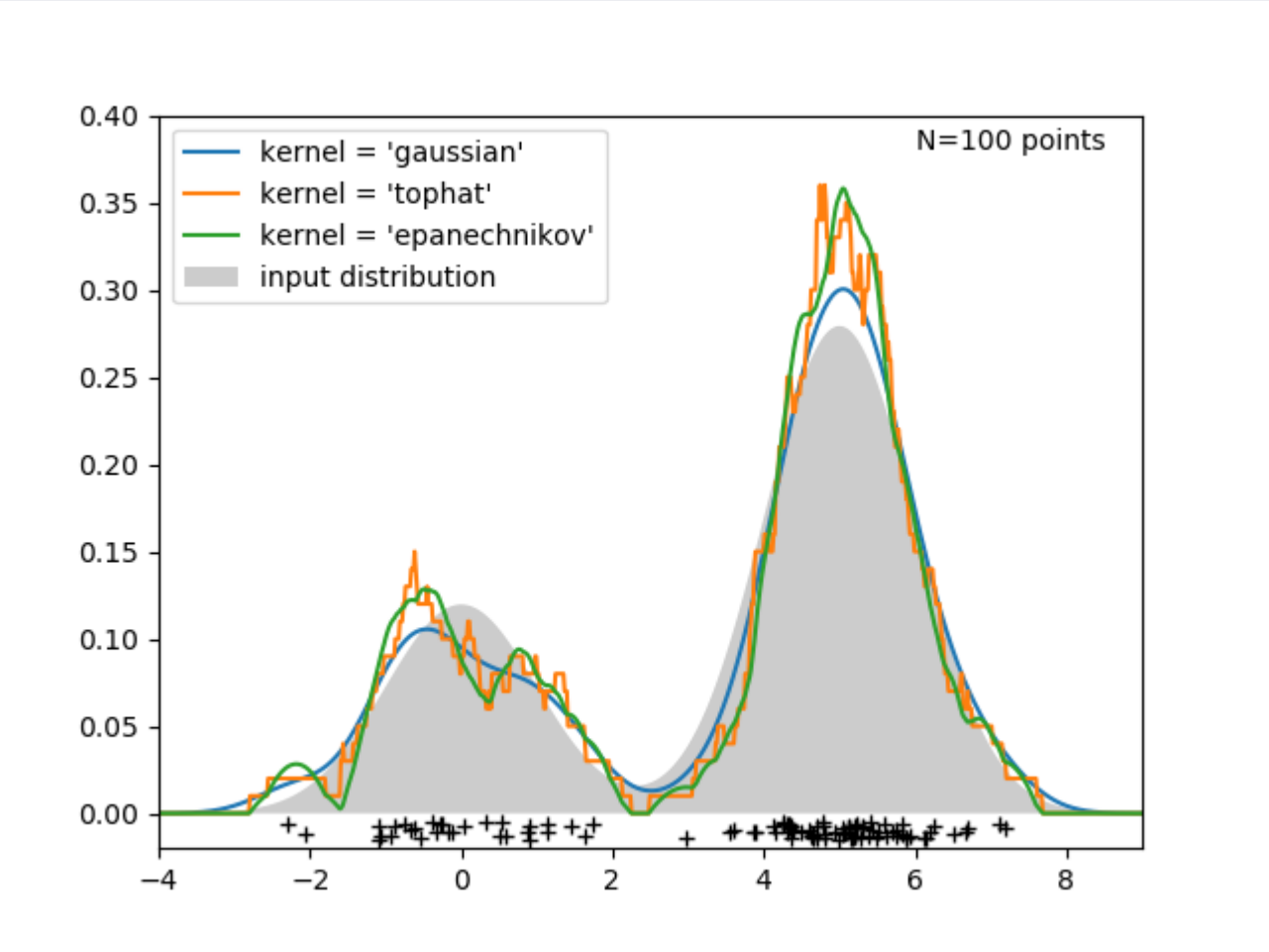
Kernel-density Estimation

- 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 → ∞, 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

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

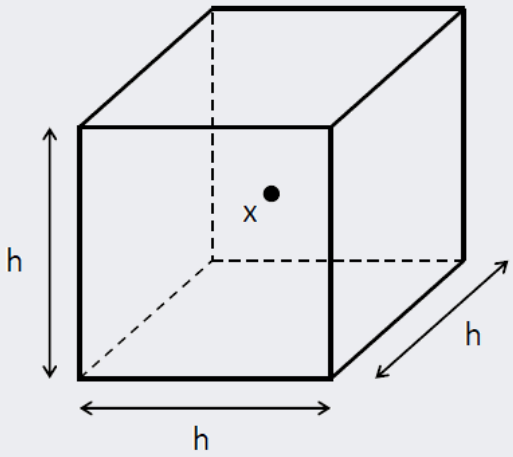
- ✓ Estimation becomes more accurate as we increase the number of sample points N and shrink the volume V
- ✓ In practice, the total number of examples is fixed so that we have to find a compromise for V
  - Large enough to include enough examples within R
  - Small enough to support the assumption that 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

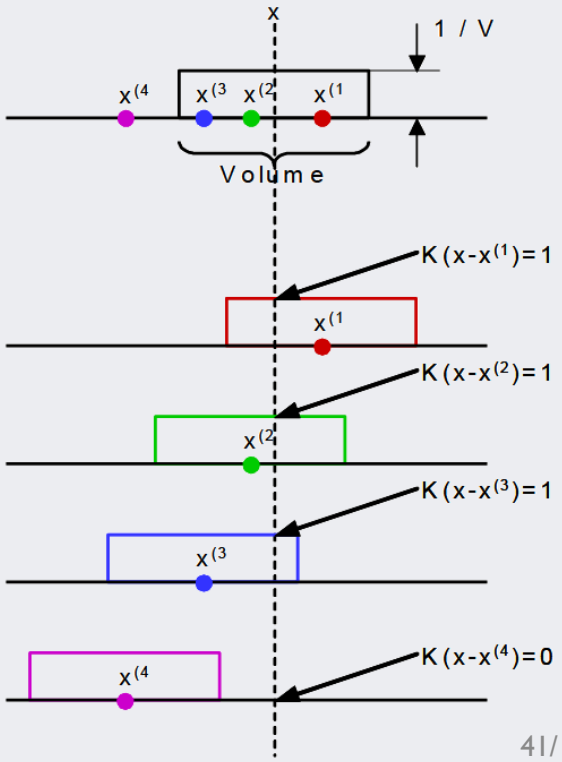
Parzen Window Density Estimation

- 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)

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

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



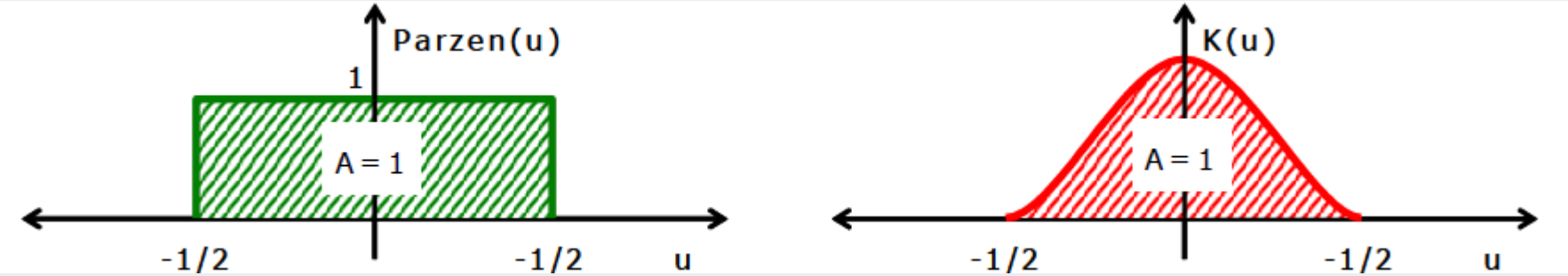


Parzen Window Density Estimation

- 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

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

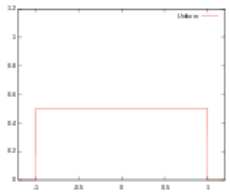
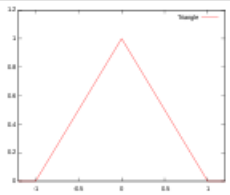
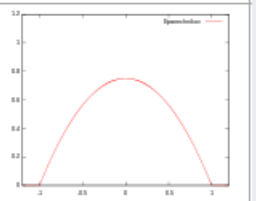
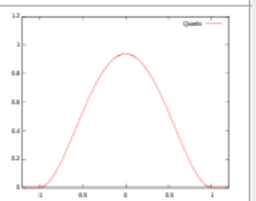
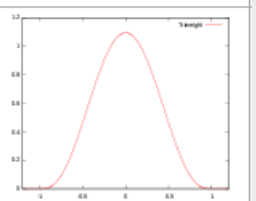
  - ✓ Commonly use a radially symmetric and unimodal pdf, such as Gaussian

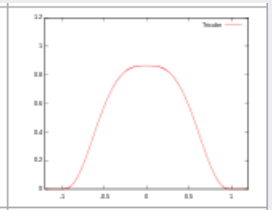
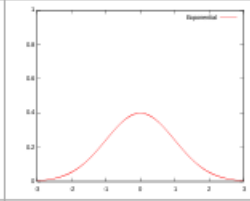
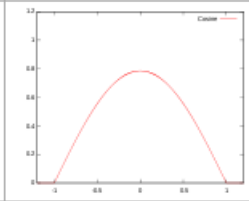


$$p(x) = \frac{1}{N}\sum_{i=1}^{N} K\left(\frac{\mathbf{x}^i - \mathbf{x}}{h}\right)$$

Parzen Window Density Estimation

- Example of smooth kernels

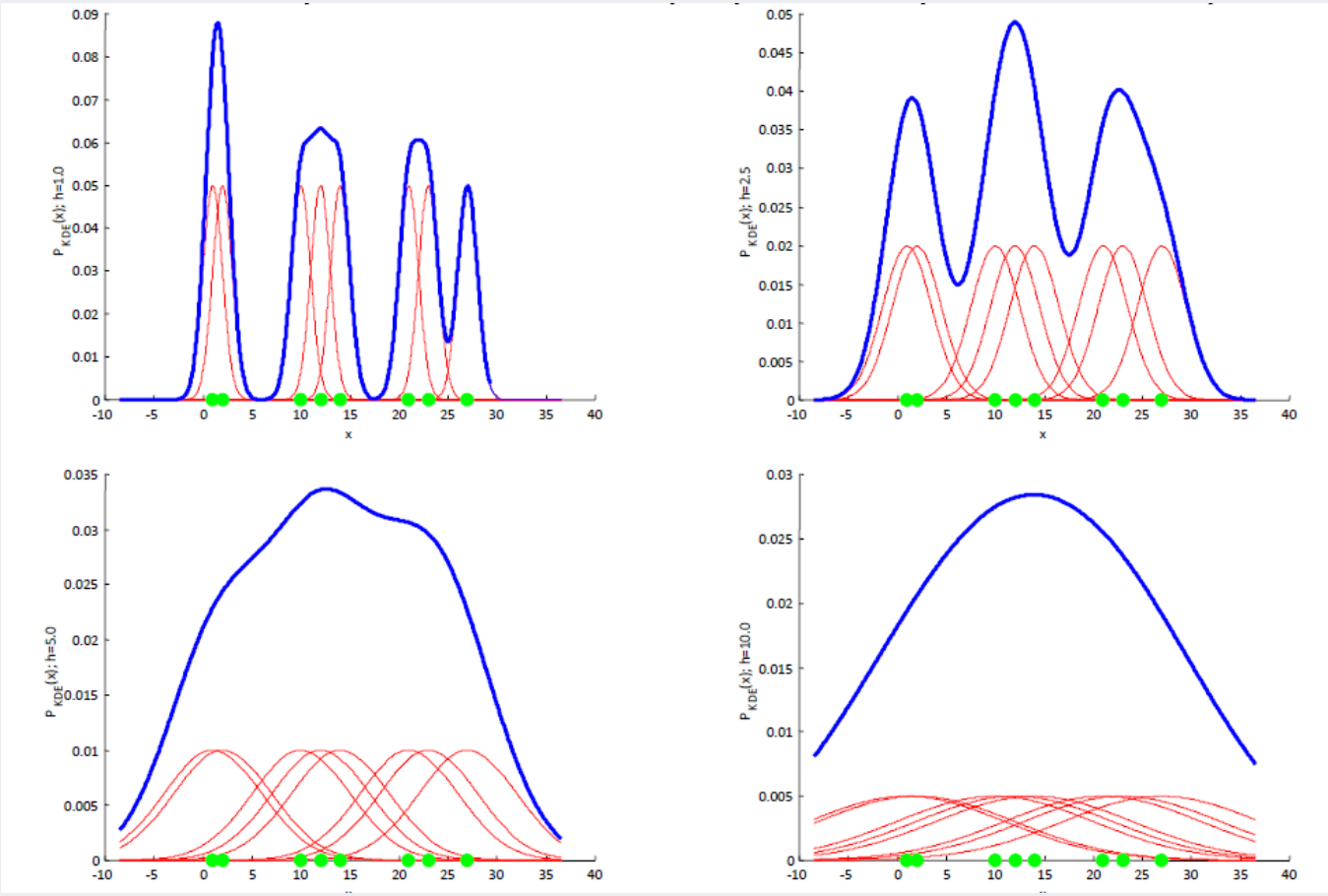
Uniform	$K(u) = \frac{1}{2}\,\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Triangular	$K(u) = (1 - \lvert u\rvert)\,\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Epanechnikov	$K(u) = \frac{3}{4}(1 - u^2)\,\mathbf{1}_{\{\lvert u\rvert \le 1\}}$	
Quartic (biweight)	$K(u) = \frac{15}{16}(1 - u^2)^2\,\mathbf{1}_{\{\lvert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

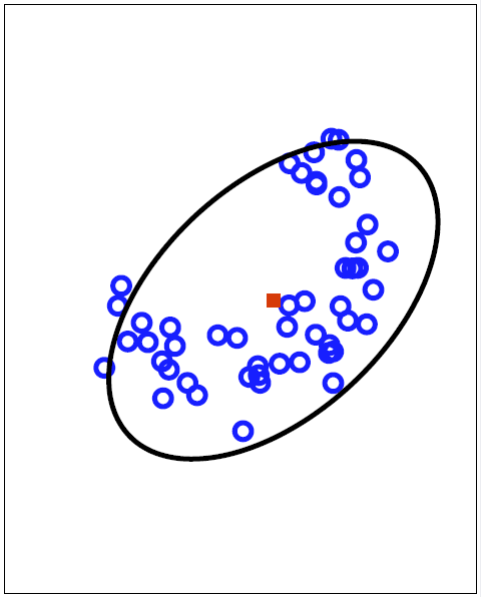
- Smoothing parameter (bandwidth) h
  - ✓ A large h will over-smooth the density distribution
  - ✓ A small h will result in a spiky density distribution



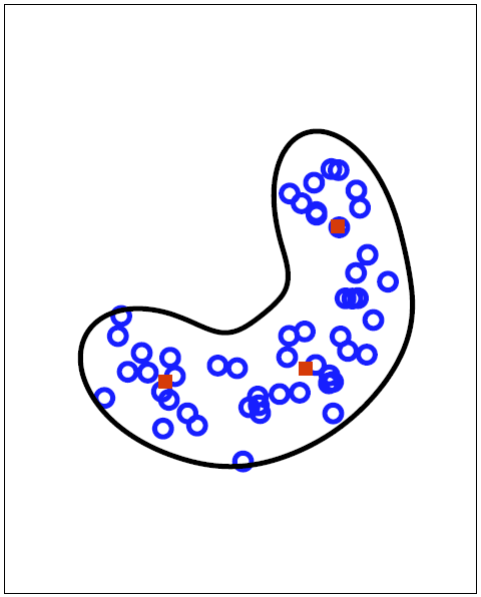
Parzen Window Density Estimation

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

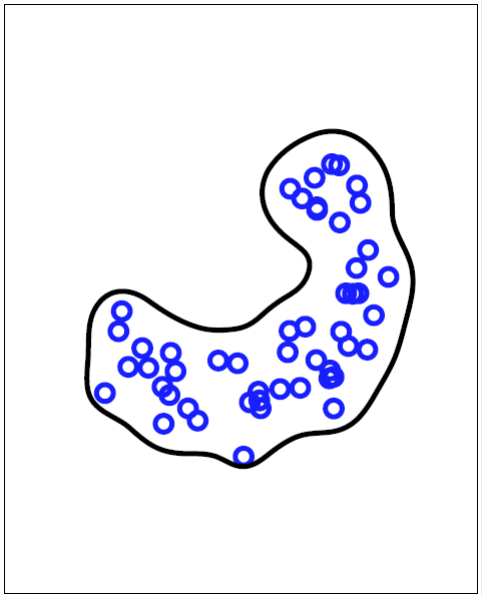
Gaussian density estimation



Mixture of Gaussian

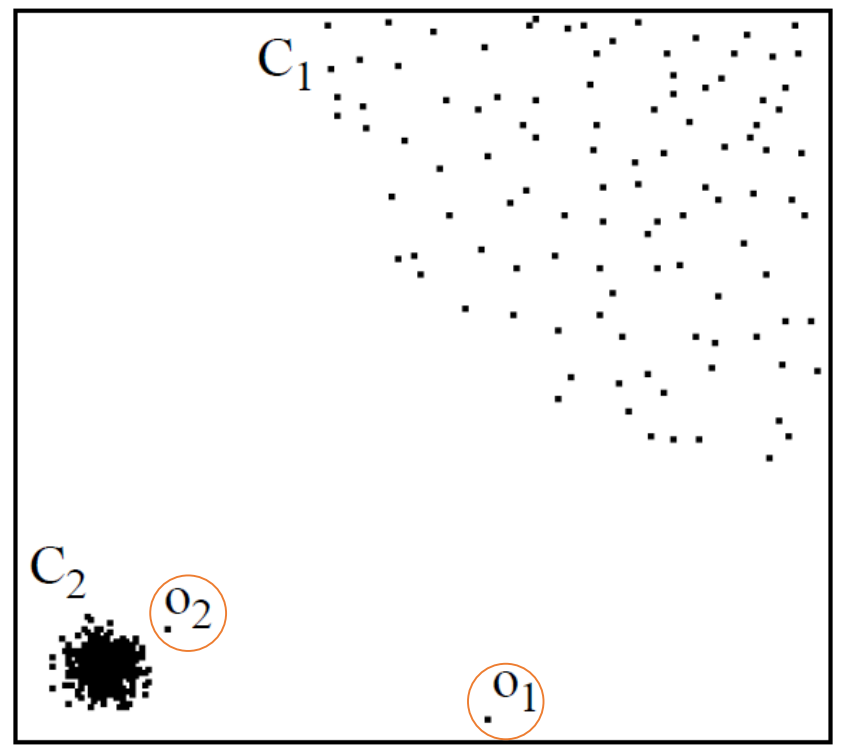


Parzen window with Gaussian Kernel



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

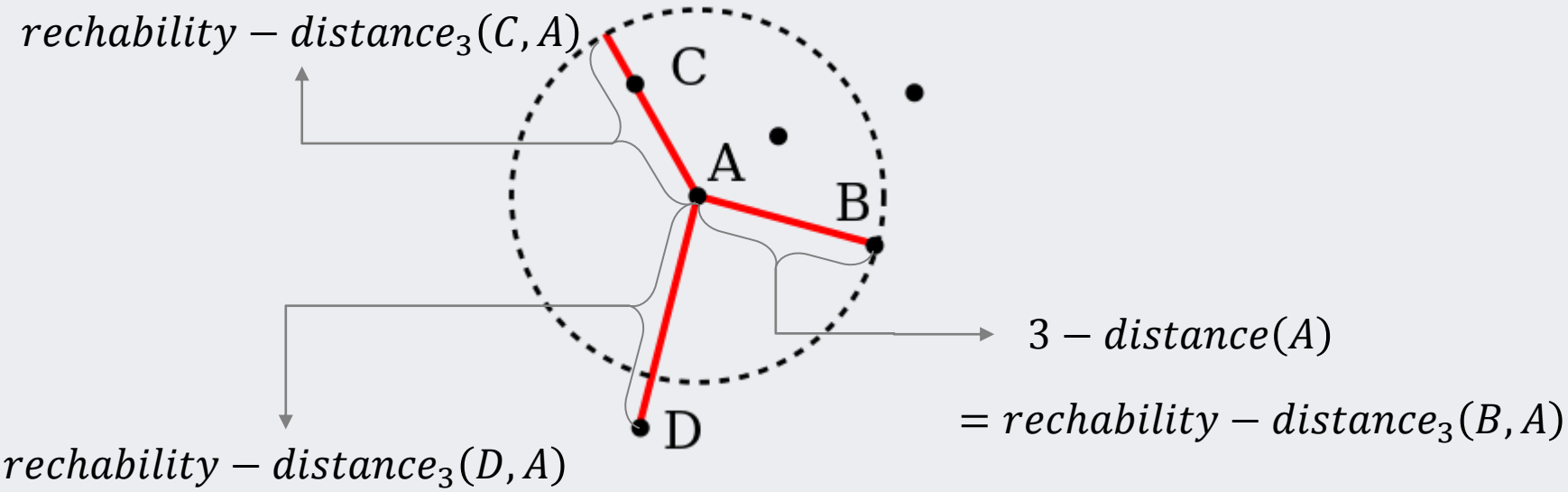
$$N_k(p) = \{q \in D \backslash \{p\} | \, d(p,q) \leq k - distance(p)\}$$

    - 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

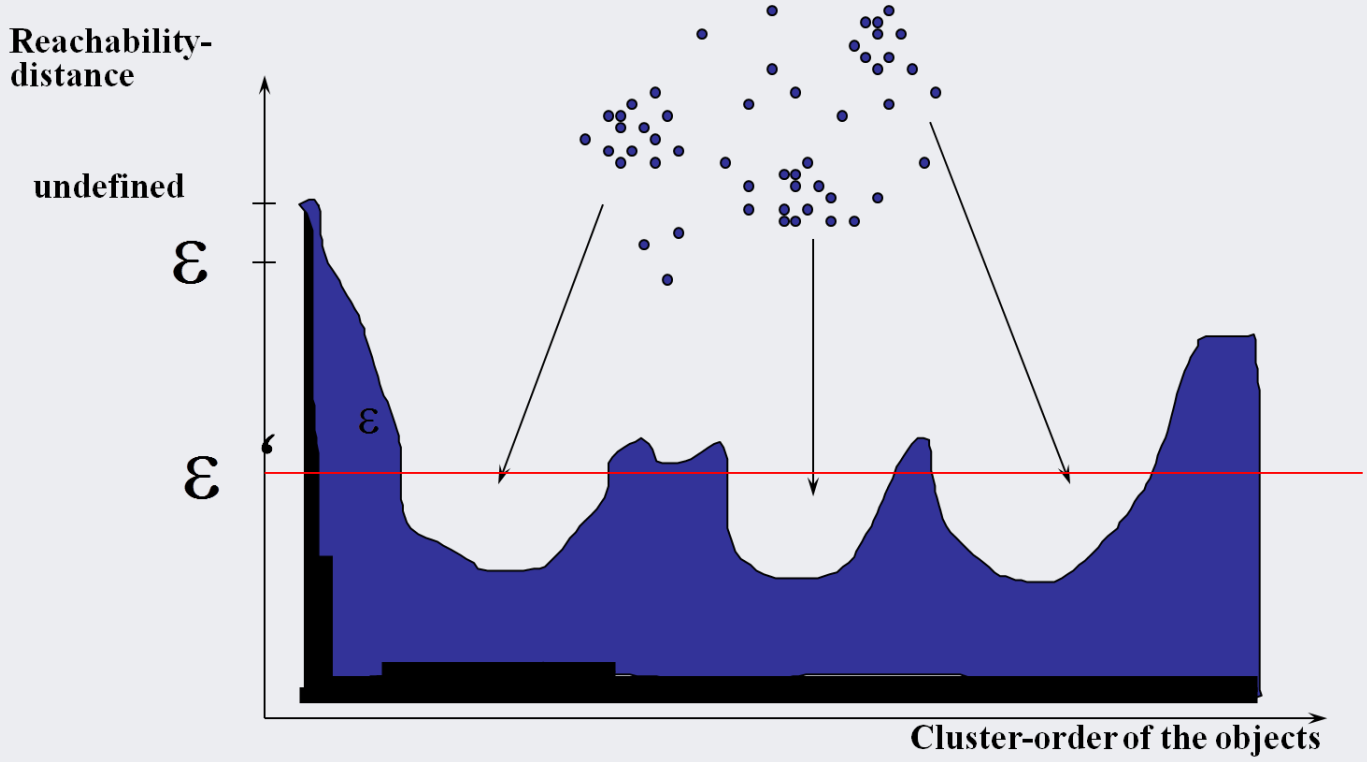
Local Outlier Factors (LOF)

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



Local Outlier Factors (LOF)

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



Local Outlier Factors (LOF)

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

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

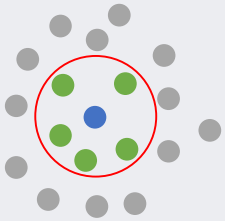
  - Case 1: p is located in the middle of a denser area: the denominator of $lrd_k(p)$ becomes small, which results in a large $lrd_k(p)$
  - Case 2: p is located in a spare are between two dense data clusters: the denominator of $lrd_k(p)$ becomes large, which results in a small $lrd_k(p)$

Local Outlier Factors (LOF)

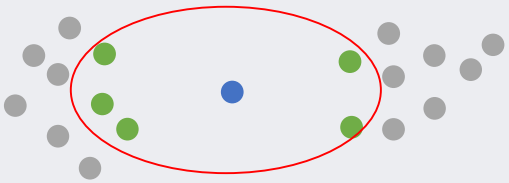
- Local Outlier Factors (LOF)
  - ✓ Definition 5: local outlier factor of an object p

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

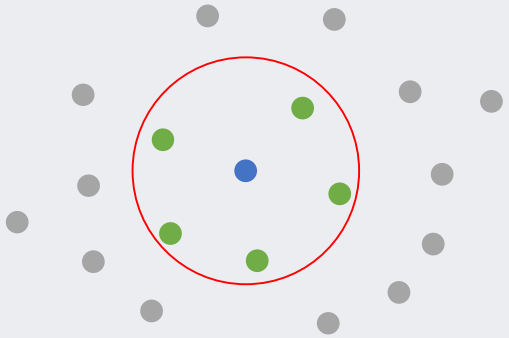
Case 1



Case 2



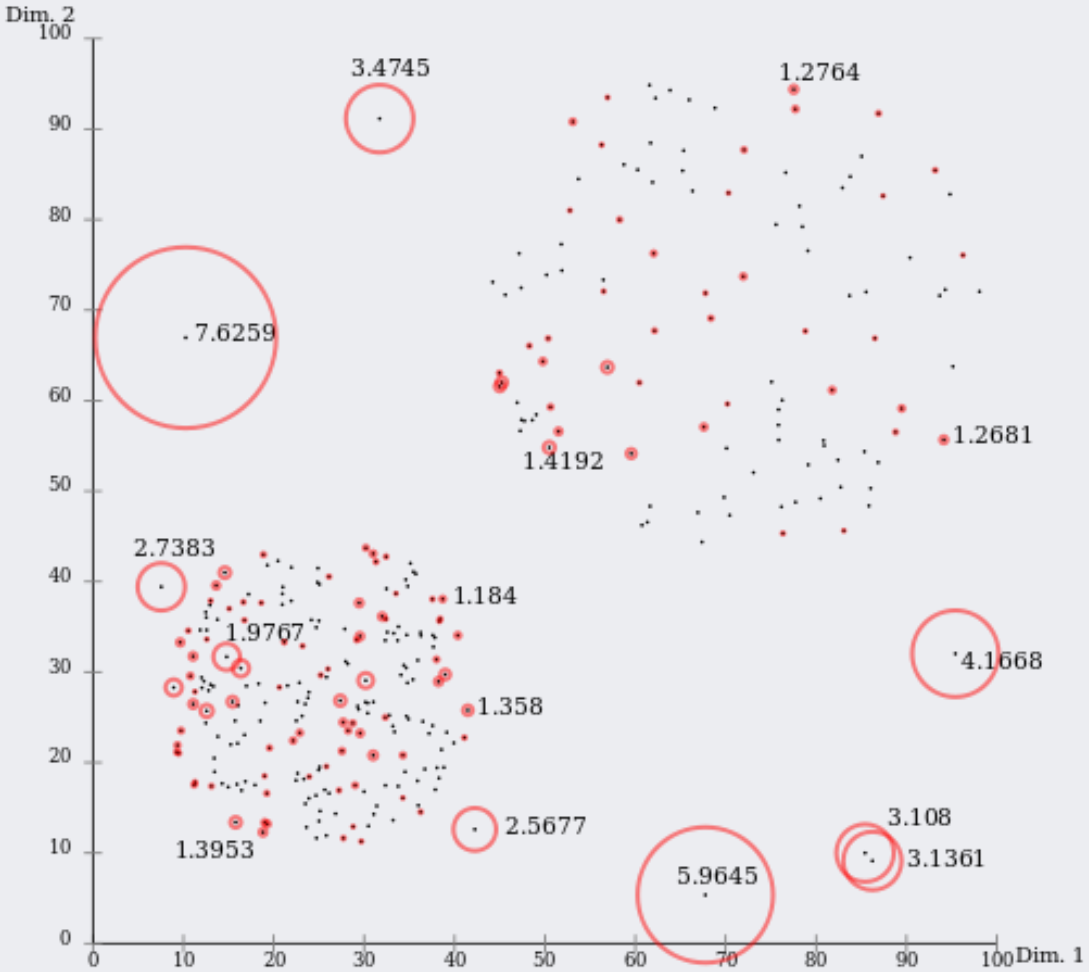
Case 3



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

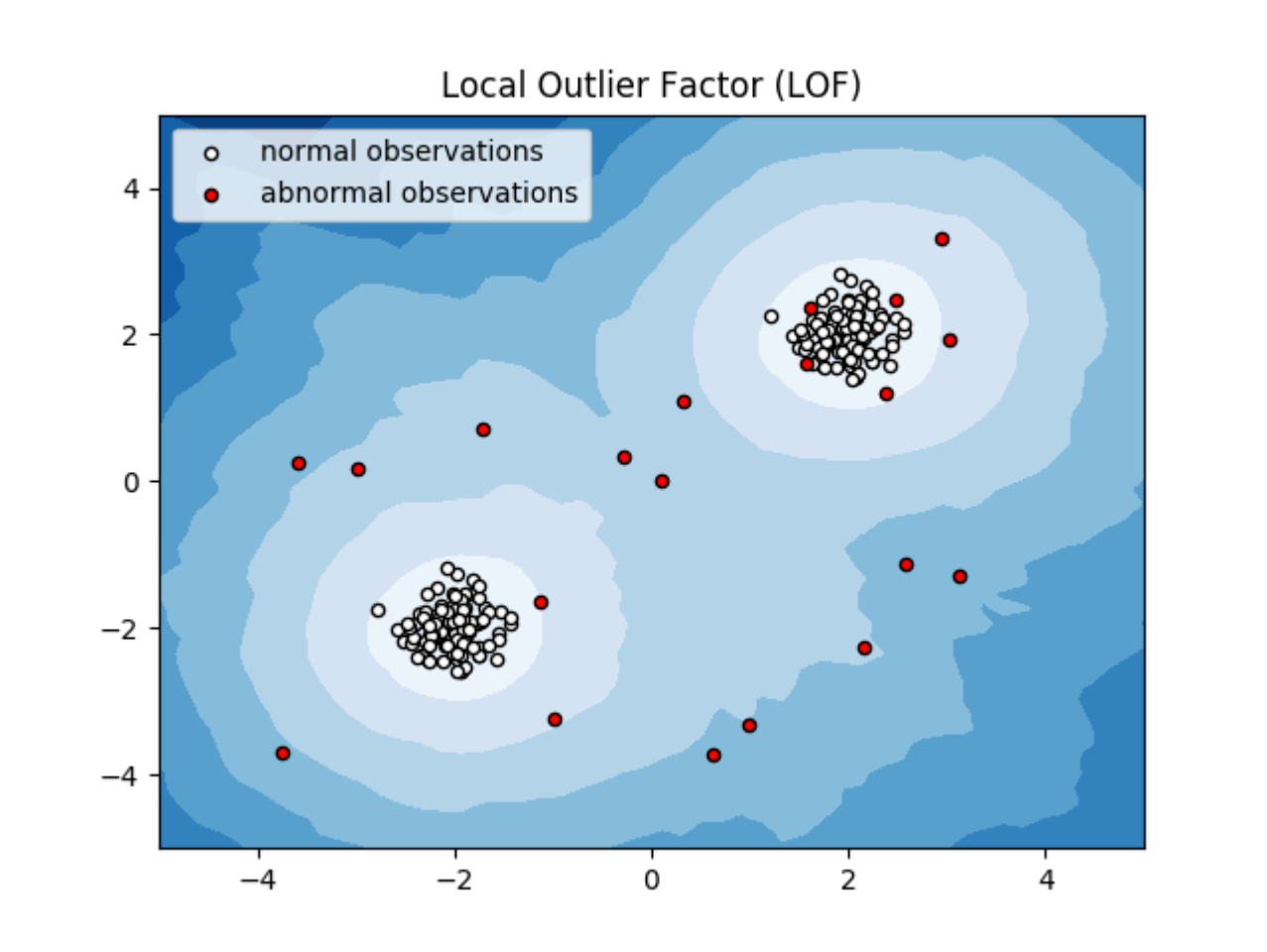
Local Outlier Factors (LOF)

- 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



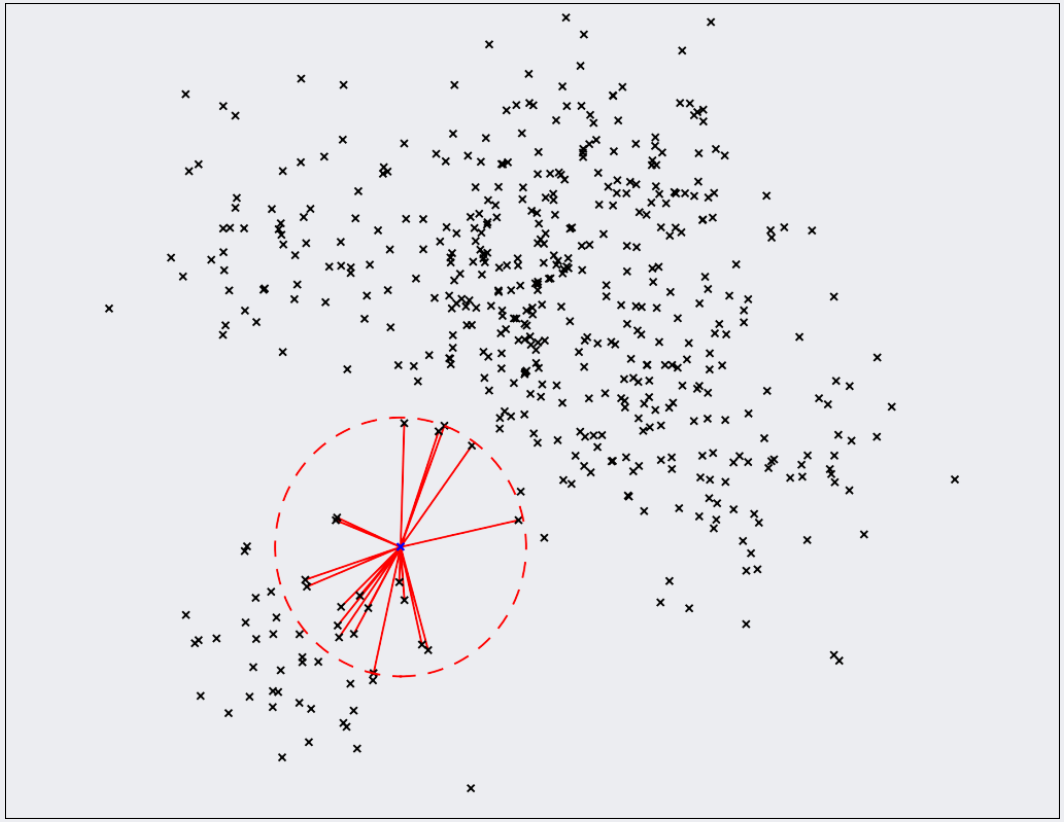
http://scikit-learn.org/stable/auto_examples/neighbors/plot_lof.html

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

$$d_{max}^{k} = \kappa(\mathbf{x}) = ||\mathbf{x} - z_k(\mathbf{x})||$$

  - ✓ Average distance to the k-nearest neighbors

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

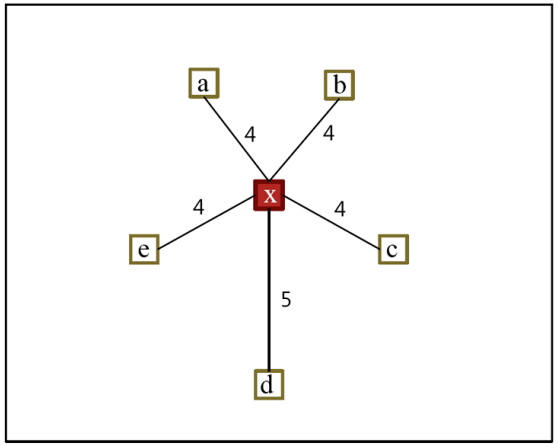
  - ✓ Distance to the mean of the k-nearest neighbors

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

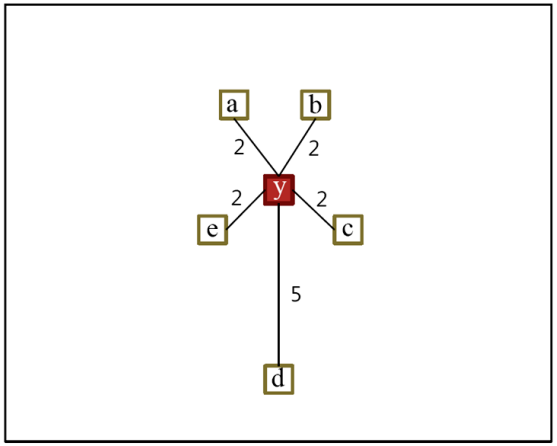
k-Nearest Neighbor-based Novelty Detection

Kang and Cho (2009)

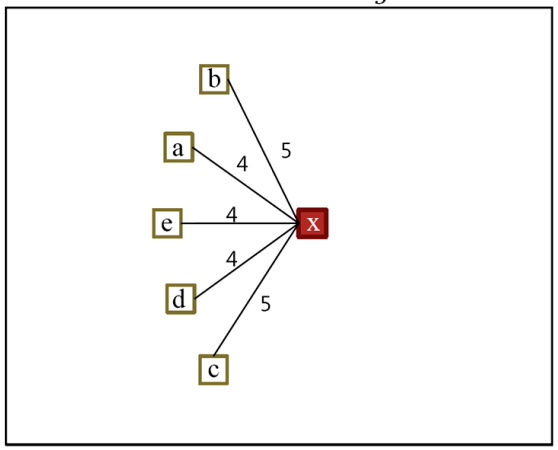
- Various distance information used for novelty score
  - ✓ Comparison among the maximum, average, and mean distance



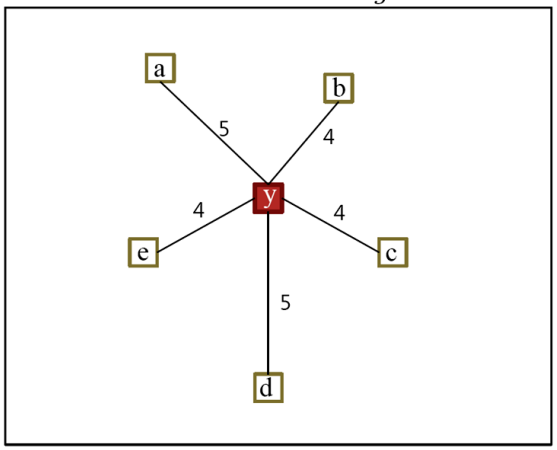
(a) $d^5_{max} = 5.0,\ d^5_{avg} = 4.2.$



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



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



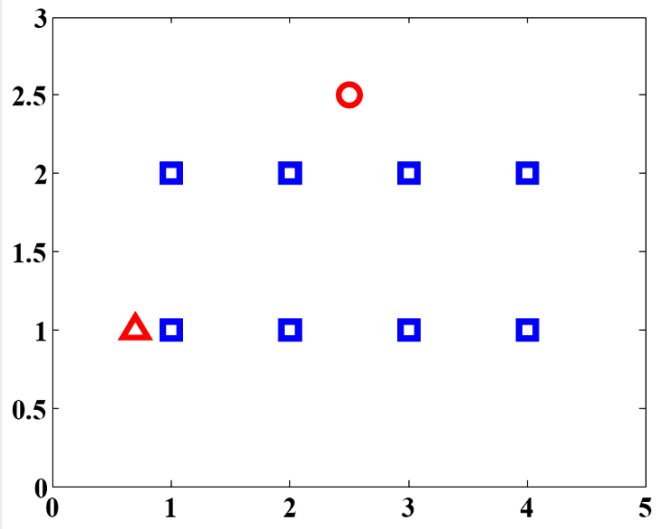
(d) $d^5_{avg} = 4.4,\ d^5_{mean} = 2.1.$

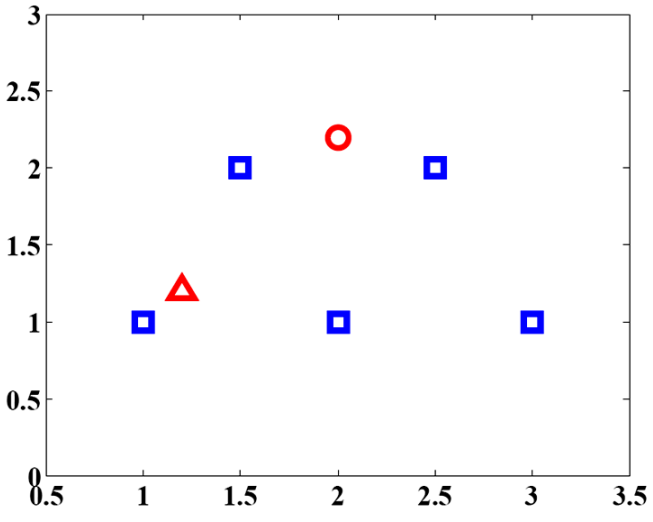
k-Nearest Neighbor-based Novelty Detection

Kang and Cho (2009)

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

A





B

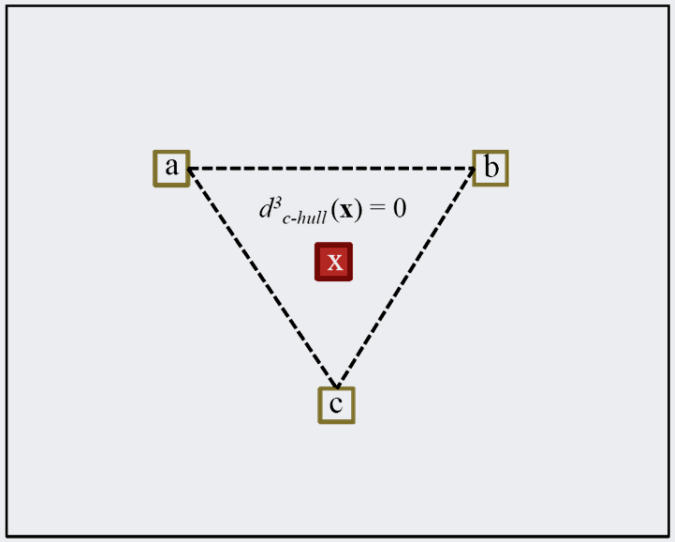
		d^k_{max}	d^k_{avg}	d^k_{mean}
A (k=4)	Circle	1.58	1.14	0.50
	Triangle	1.64	1.07	0.94
B (k=5)	Circle	1.56	1.08	0.80
	Triangle	1.86	1.09	0.88

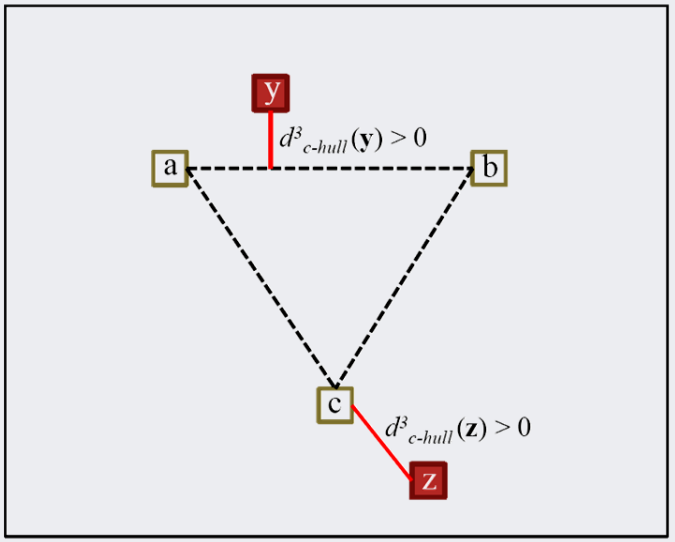
k-Nearest Neighbor-based Novelty Detection

- 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

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

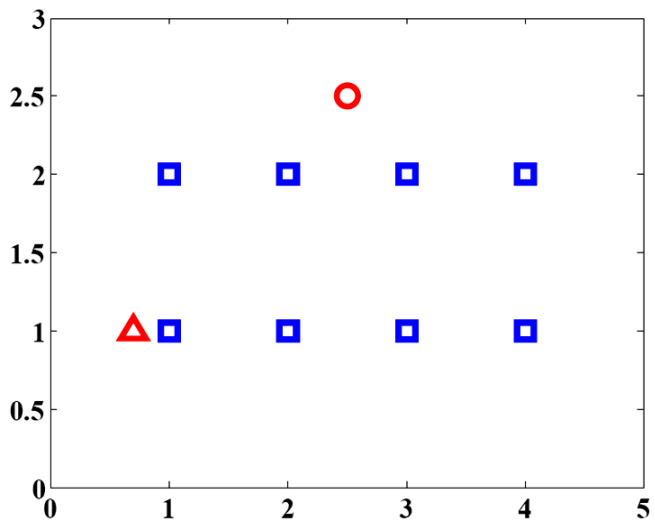
  - ✓ Put the penalty term using the convex distance for those instances located outside the convex hull of its k-nearest neighbors

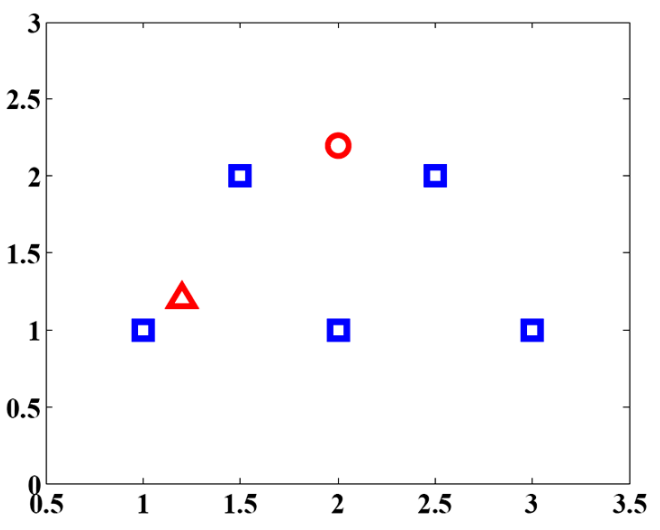
$$d_{hybrid}^{k} = d_{avg}^{k} \times \left(\frac{2}{1 + exp(-d_{c-hull}^{k})}\right)$$

k-Nearest Neighbor-based Novelty Detection

- Counter example revisited

A

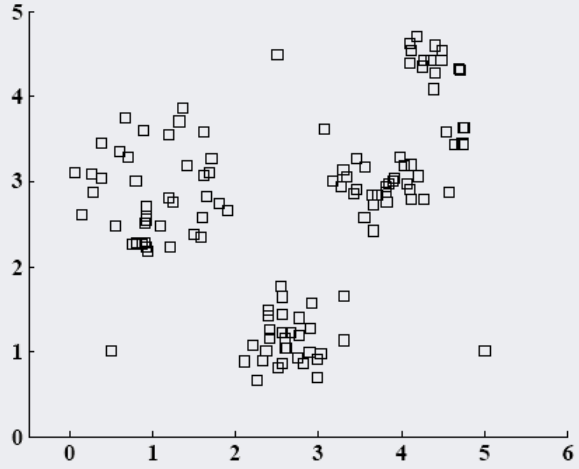




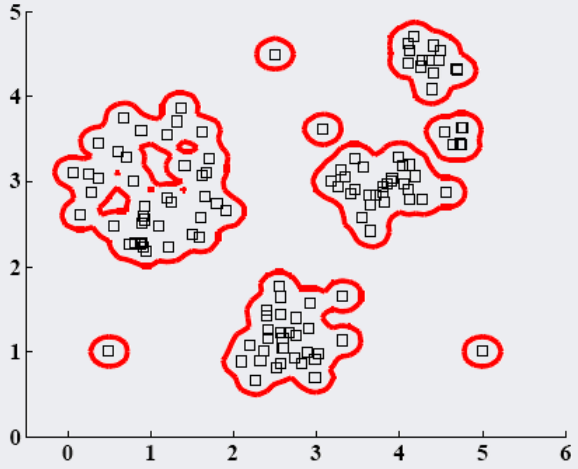
B

		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

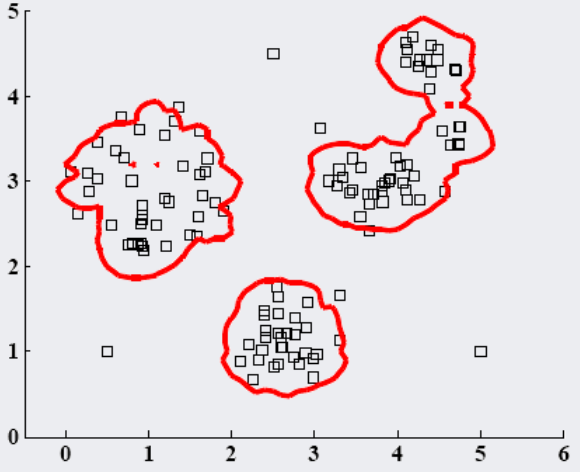
k-Nearest Neighbor-based Novelty Detection



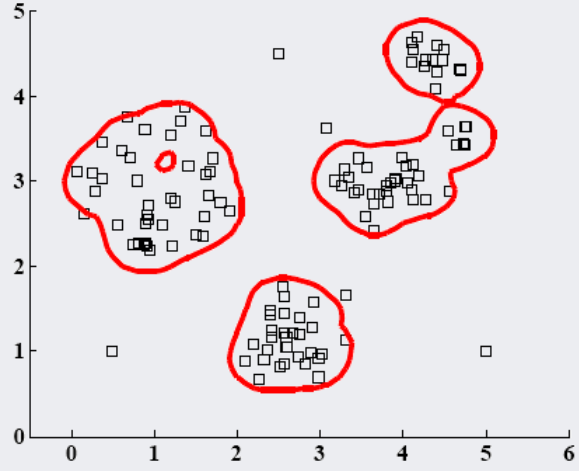
(a) Normal instances



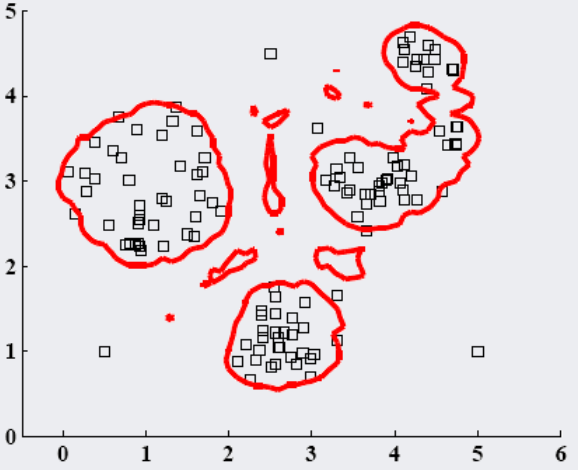
(b) 1-NN



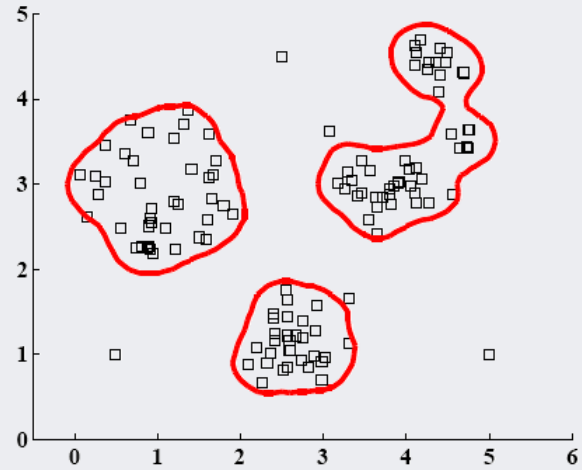
(c) d^5_{max}



(d) d^5_{avg}



(e) d^5_{mean}



(f) d^5_{hybrid}

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)

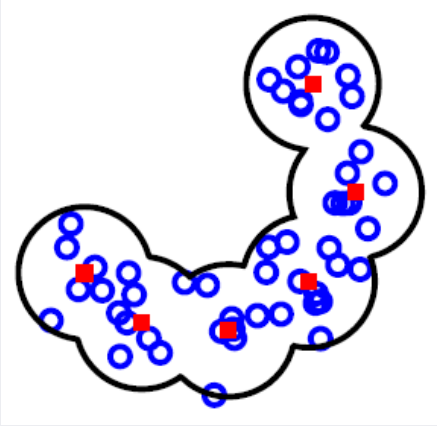
Data	Dim.	$\mathrm{Tr}N_n$	Gauss	MoG	Parzen	1-SVM	KMC	KCC	HC	PCA	d^k_{max}	d^k_{avg}	d^k_{mean}	1-NN	MST-CD	d^k_{hybrid}
Titanic	3	100	19.12	19.12	18.50	17.27	21.12	21.26	22.80	22.48	3.64	3.53	10.00	8.73	**1.33***	**1.33***
Liver	6	73	44.41	45.04	41.11	38.82	41.90	43.41	40.91	40.68	40.00	38.85	38.96	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

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

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

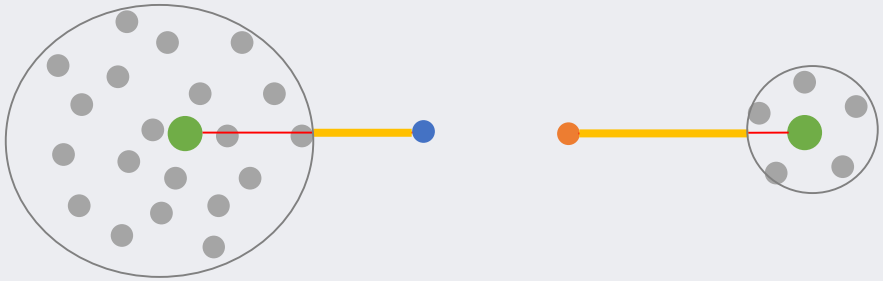


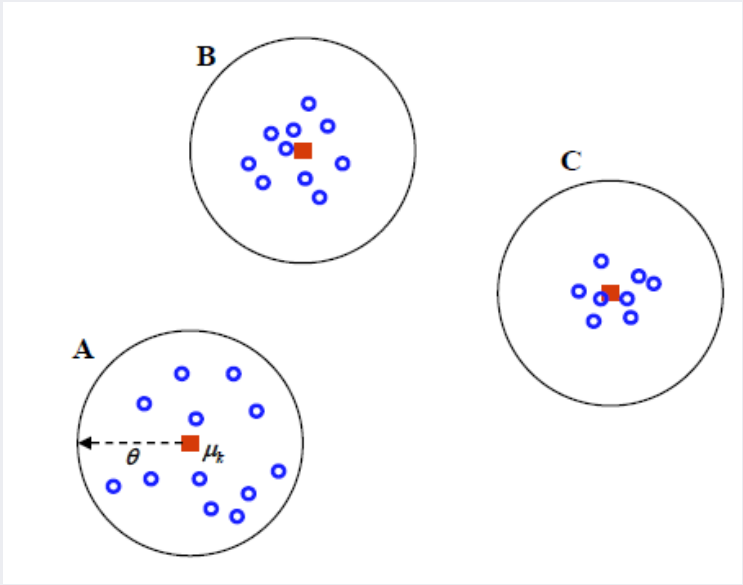
  - ✓ EM algorithm for K-Means clustering

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

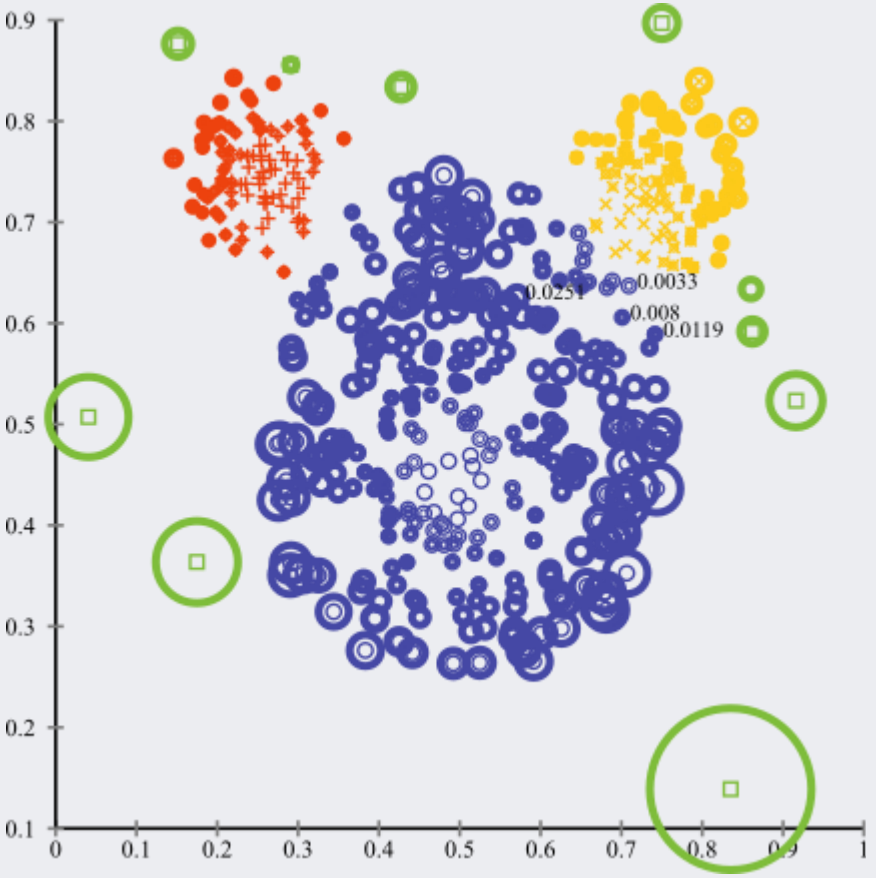
- Clustering-based Approach
  - ✓ Two novelty scores by KMC
    - Absolute distance to the nearest centroid
    - Relative distance to the nearest centroid





Clustering-based Approach

- KMC-based novelty score: Example



Principal Component Analysis-based Novelty Detection

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

$$\max \quad \mathbf{w}^T \mathbf{S} \mathbf{w}$$

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

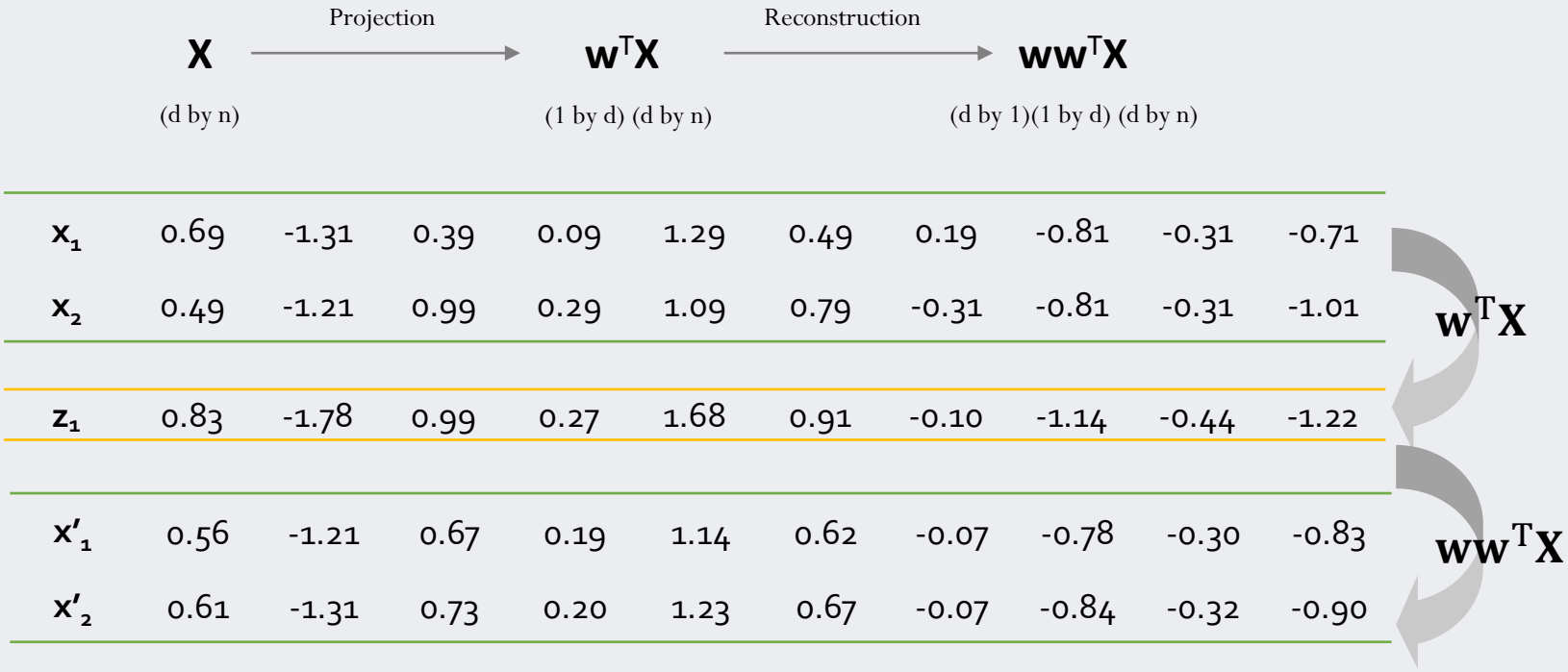
  - ✓ Solution

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

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

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



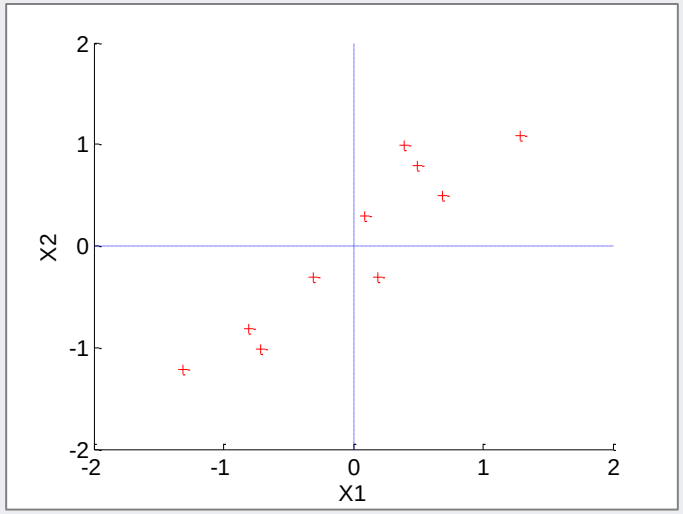
Principal Component Analysis-based Novelty Detection

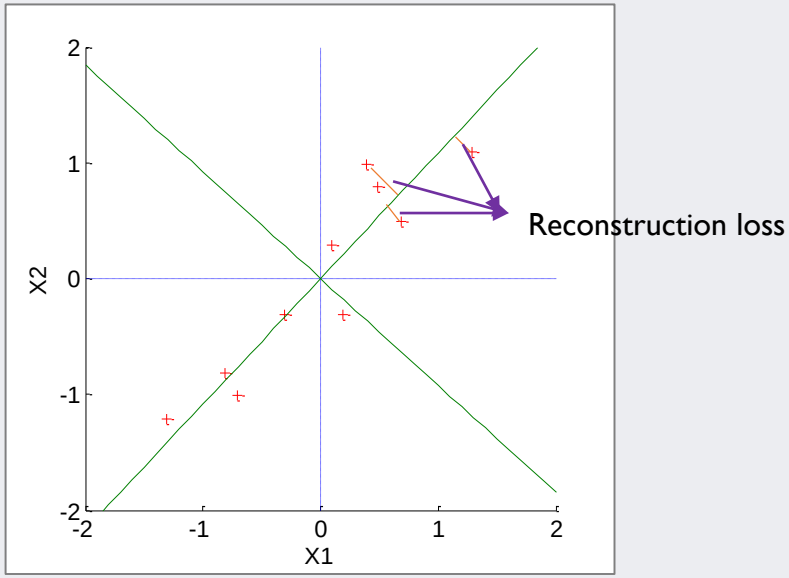
- PCA as a novelty detector
  - ✓ Compute the reconstruction loss

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

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

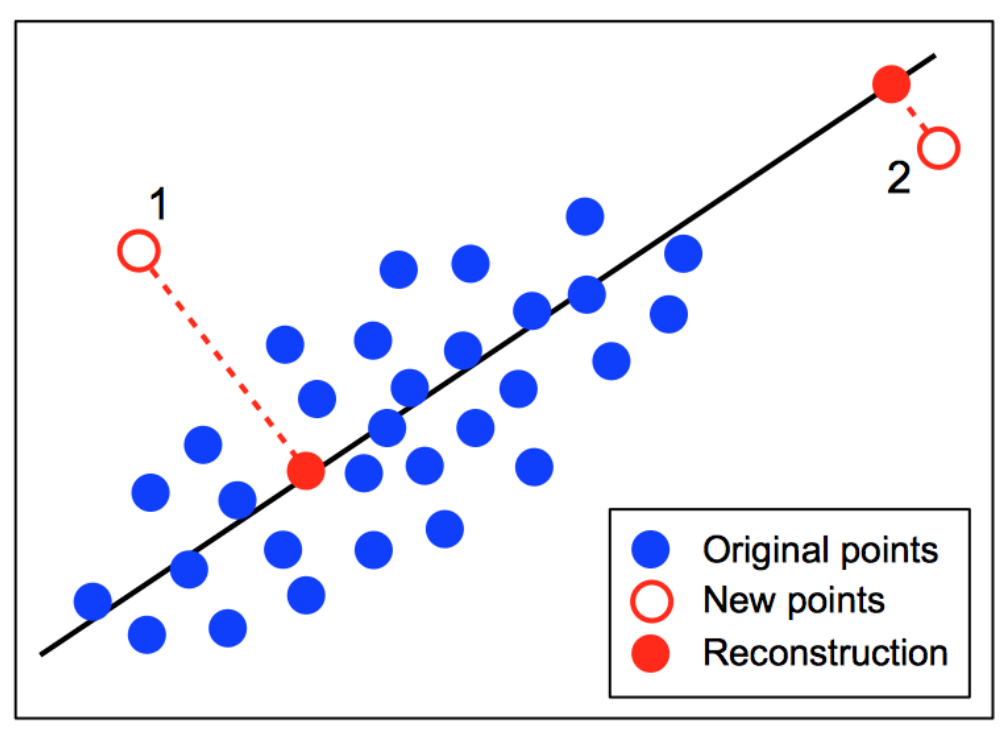
$$= \mathbf{x}^{\mathrm{T}}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{w}\mathbf{w}^{\mathrm{T}}\mathbf{x} = \|\mathbf{x}\|^2 - \left\|\mathbf{w}^{\mathrm{T}}\mathbf{x}\right\|^2$$

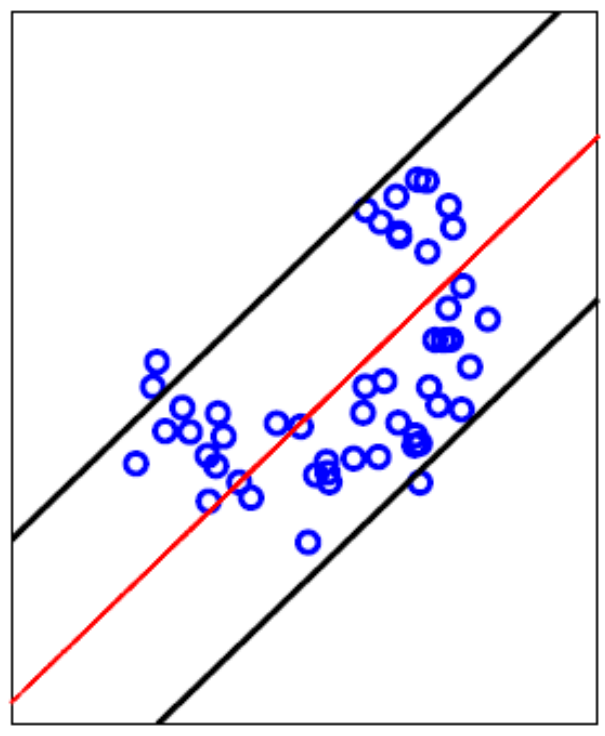




Principal Component Analysis-based Novelty Detection

- PCA as a novelty detector
  - ✓ Graphical interpretation



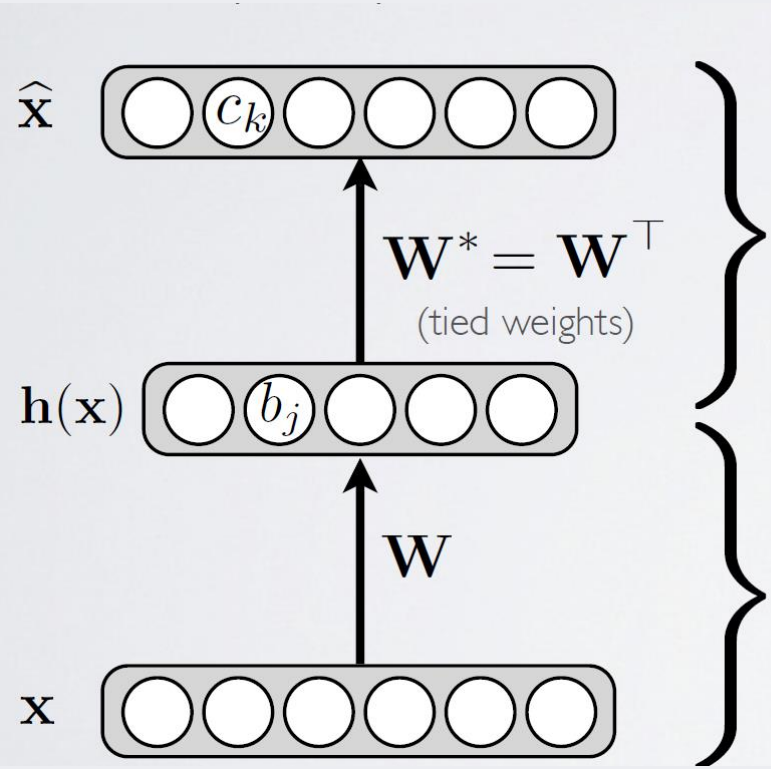


https://stats.stackexchange.com/questions/259806/anomaly-detection-using-pca-reconstruction-error

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: $l(f(\mathbf{x})) = \frac{1}{2}\sum_k (\hat{x}_k - x_k)^2$



Decoder

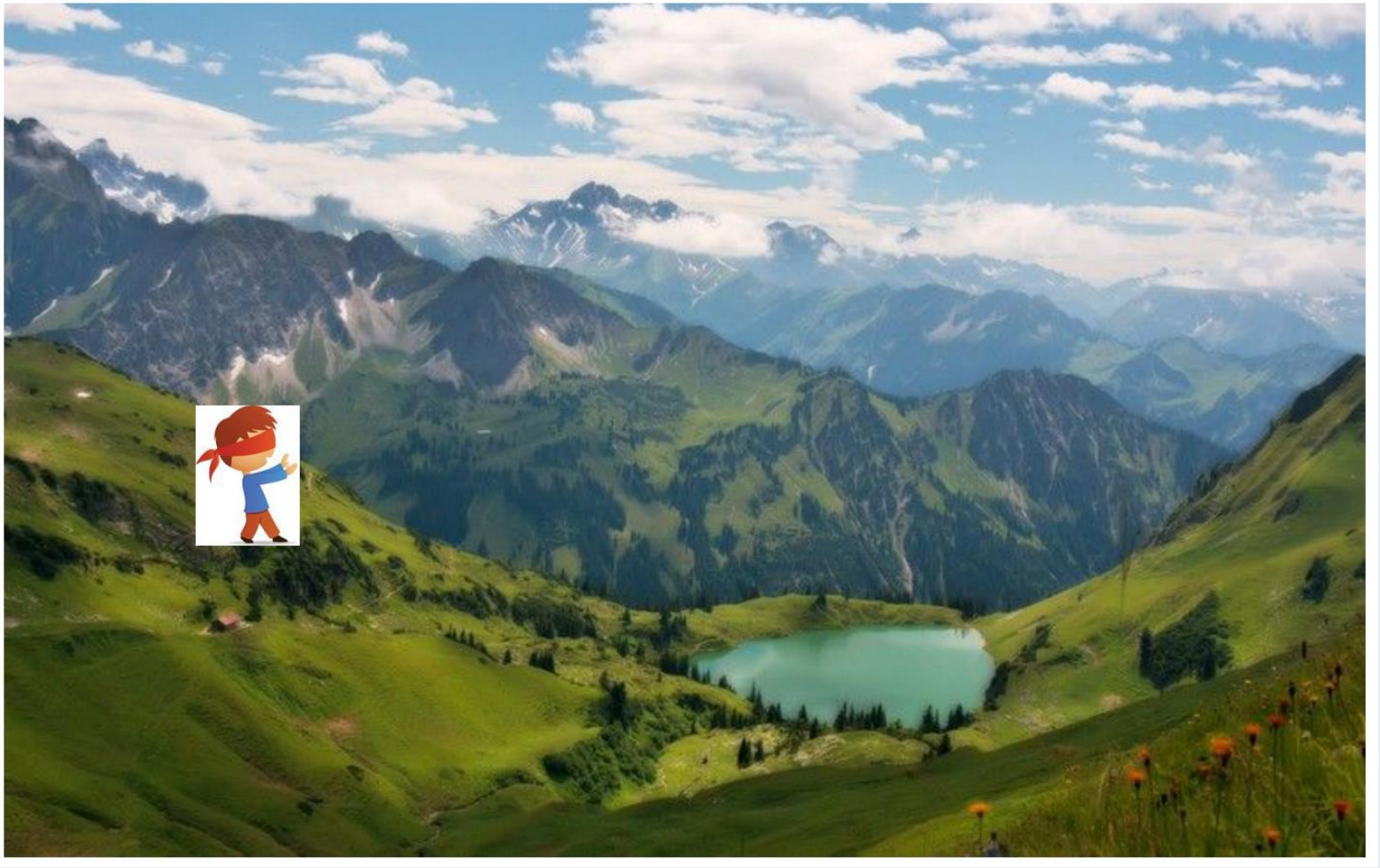
$$\hat{\mathbf{x}} = o(\hat{\mathbf{a}}(\mathbf{x})) = \underbrace{\text{sigm}}_{\text{for binary inputs}}(\mathbf{c} + \mathbf{W}^*\mathbf{h}(\mathbf{x}))$$

Encoder

$$\mathbf{h}(\mathbf{x}) = g(\mathbf{a}(\mathbf{x})) = \text{sigm}(\mathbf{b} + \mathbf{W}\mathbf{x})$$

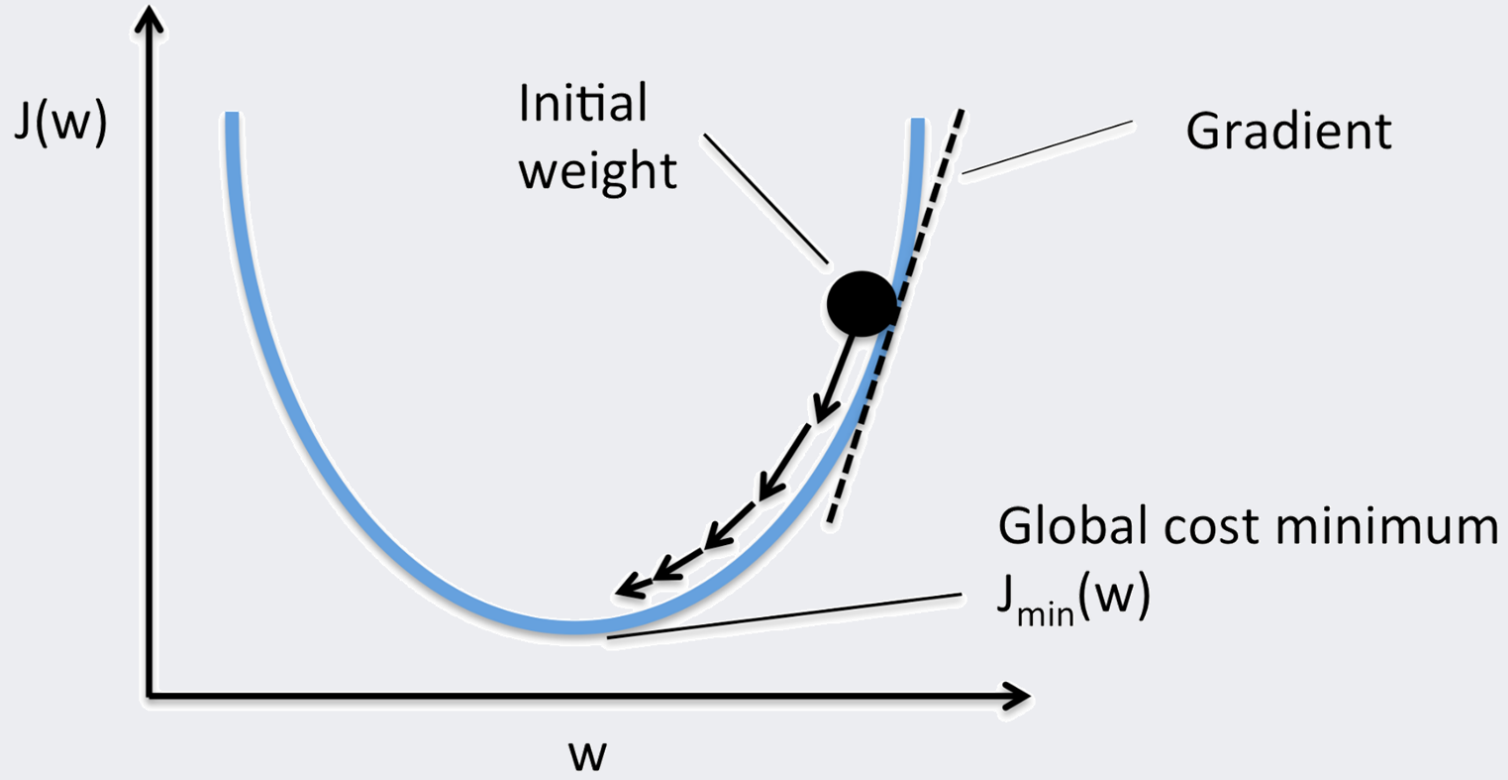
Auto-Encoder for Novelty Detection

- Auto-Encoder (Auto-Associative Neural Network)
  - ✓ Training: Gradient Descent



Auto-Encoder for Novelty Detection

- Auto-Encoder (Auto-Associative Neural Network)
  - ✓ Training: Gradient Descent
    - Blue line: the value of the objective function w.r.t. w
    - Black point: current position
    - Arrow: the direction that w should move toward to minimize the objective function



Auto-Encoder for Novelty Detection

- Gradient Descent
  - ✓ Taylor expansion of a function

$$f(x+\Delta x) = f(x) + \frac{f'(x)}{1!}\Delta x + \frac{f''(x)}{2!}(\Delta x)^2 + \cdots$$

  - ✓ For the minimization, the objective function decreases by moving the x toward the opposite direction of the first derivative if the value of first derivative is not zero.

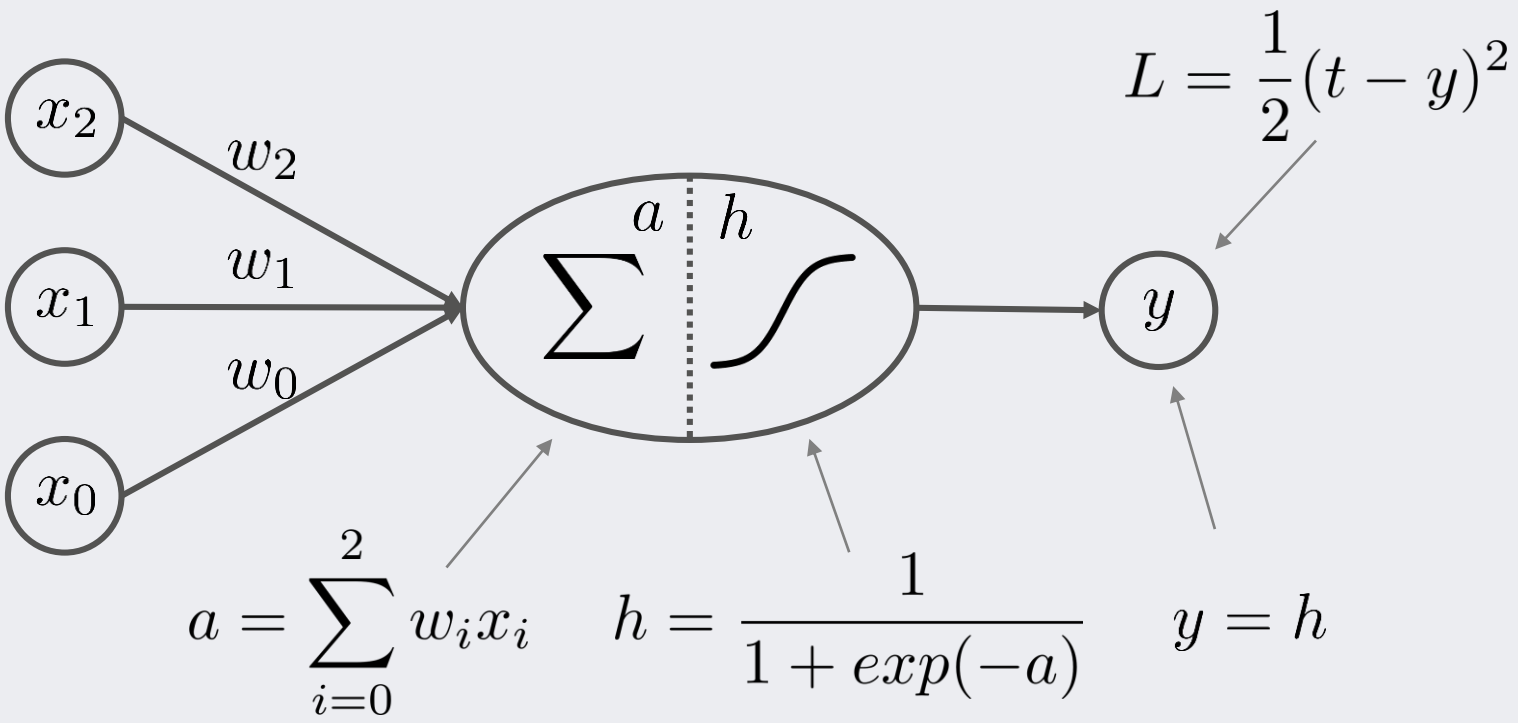
$$x_{new} = x_{old} - \eta f'(x), \quad \text{where } 0 < \eta < 1.$$

$$f(x_{new}) = f(x_{old} - \eta f'(x_{old})) \cong f(x_{old}) - \eta \left| f'(x) \right|^2 < f(x_{old})$$

Auto-Encoder for Novelty Detection

- Gradient Descent Example with Perceptron

원하는 값(t)과
예측값(y)의 차이를
손실함수로 정의



여러 변수들의 정보를
나름대로 취합해서

얼마만큼 다음 단계로
전달할지 결정한다
(활성화)

Auto-Encoder for Novelty Detection

- Gradient Descent Example with Perceptron
  - ✓ Chain rule

$$\frac{\partial L}{\partial y} = y - t \qquad \frac{\partial y}{\partial h} = 1$$

$$\frac{\partial h}{\partial a} = \frac{exp(-a)}{(1 + exp(-a))^2} = \frac{1}{1 + exp(-a)} \cdot \frac{exp(-a)}{1 + exp(-a)} = h(1 - h)$$

$$\frac{\partial a}{\partial w_i} = x_i$$

  - ✓ Gradient for w

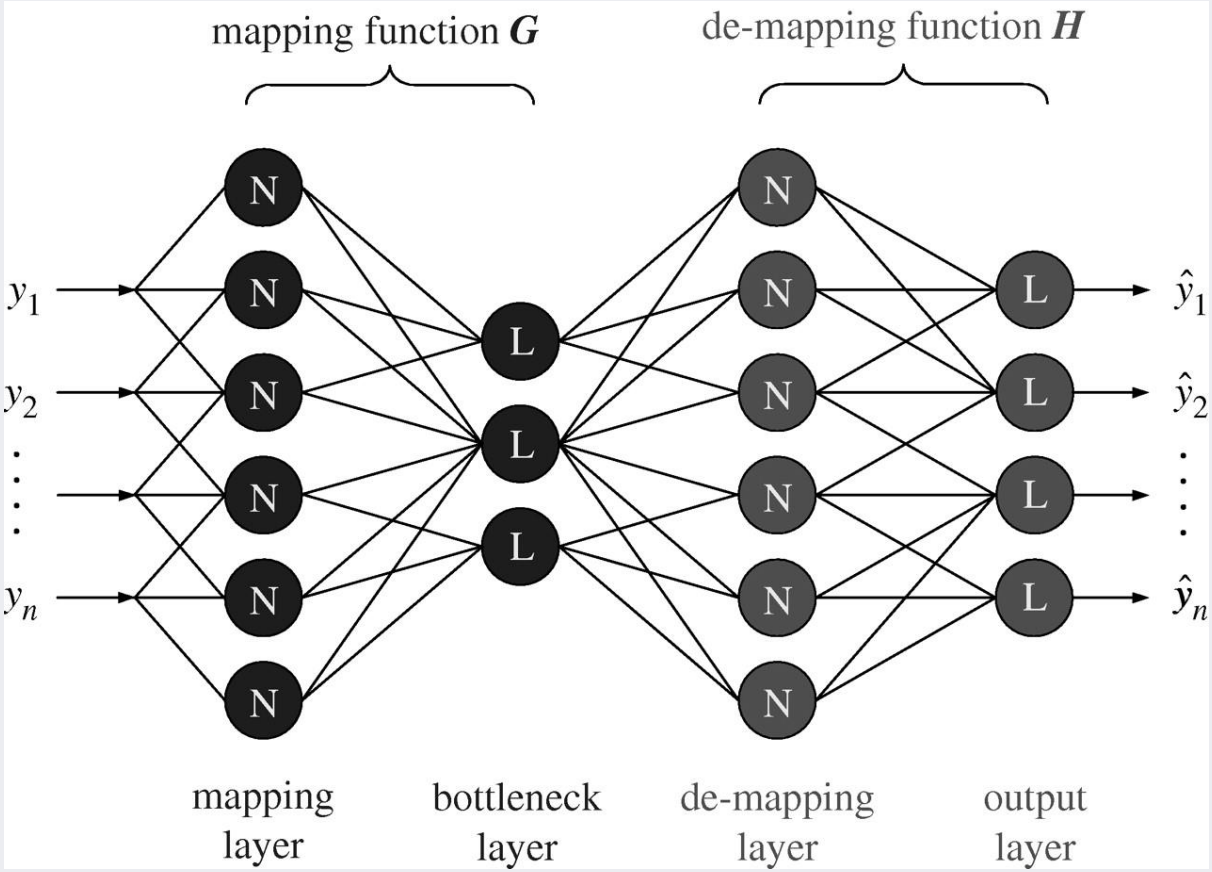
$$\frac{L}{\partial w_i} = \frac{L}{\partial y} \cdot \frac{\partial y}{\partial h} \cdot \frac{\partial h}{\partial a} \cdot \frac{\partial a}{\partial w_i} = (y - t) \cdot 1 \cdot h(1 - h) \cdot x_i$$

  - ✓ Update w

$$w_i^{new} = w_i^{old} - \eta \times \frac{L}{\partial w_i^{old}} = w_i^{old} - \eta \times (y - t) \cdot 1 \cdot h(1 - h) \cdot x_i$$

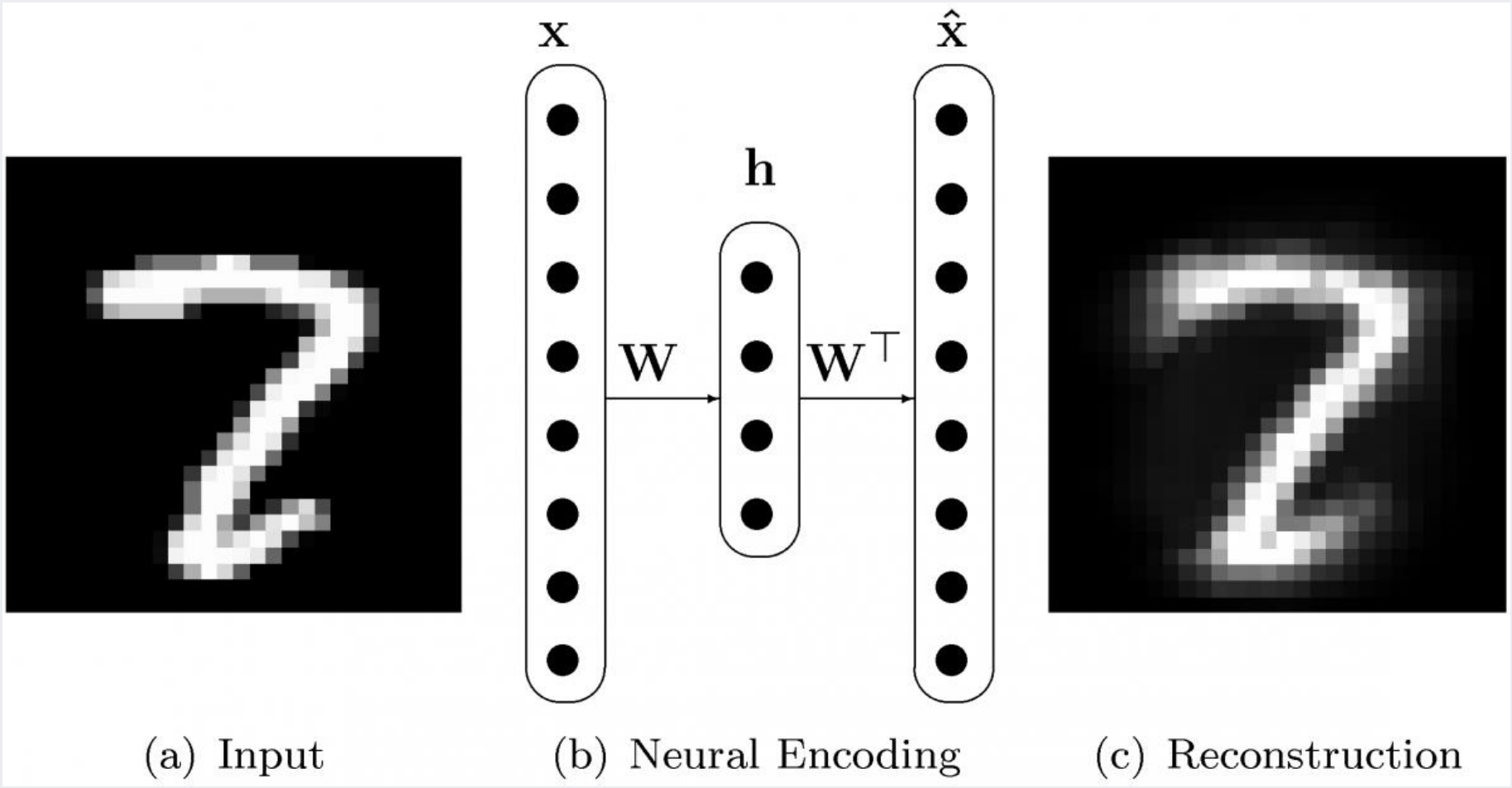
Auto-Encoder for Novelty Detection

- 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

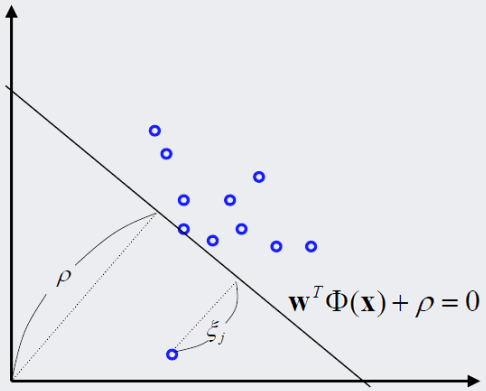
- Auto Encoder (Auto-Associative Neural Network)
  - ✓ Example



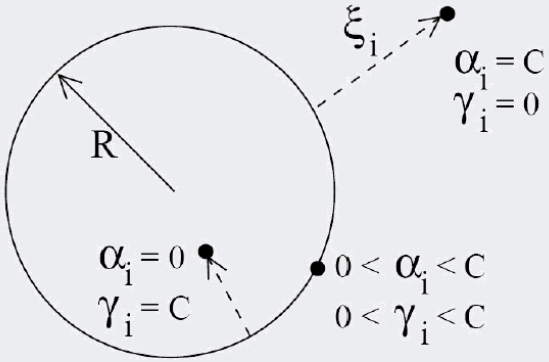
Support Vector-based Novelty Detection

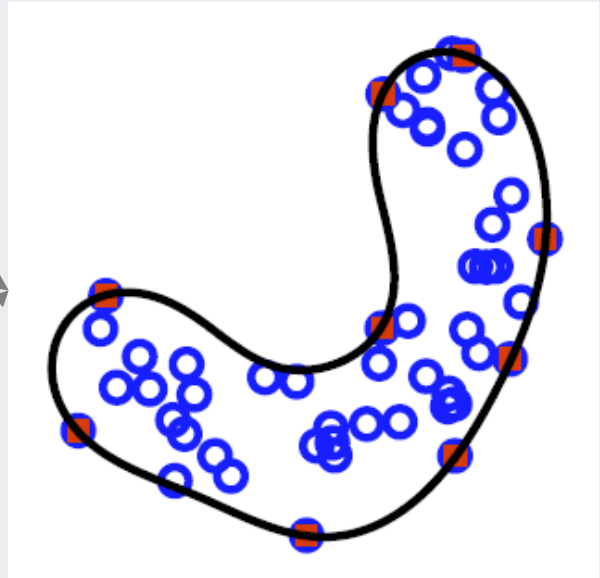
- Support vector-based novelty detection
  - ✓ Define boundaries of normal regions directly by finding function that separates the normal and abnormal observations

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

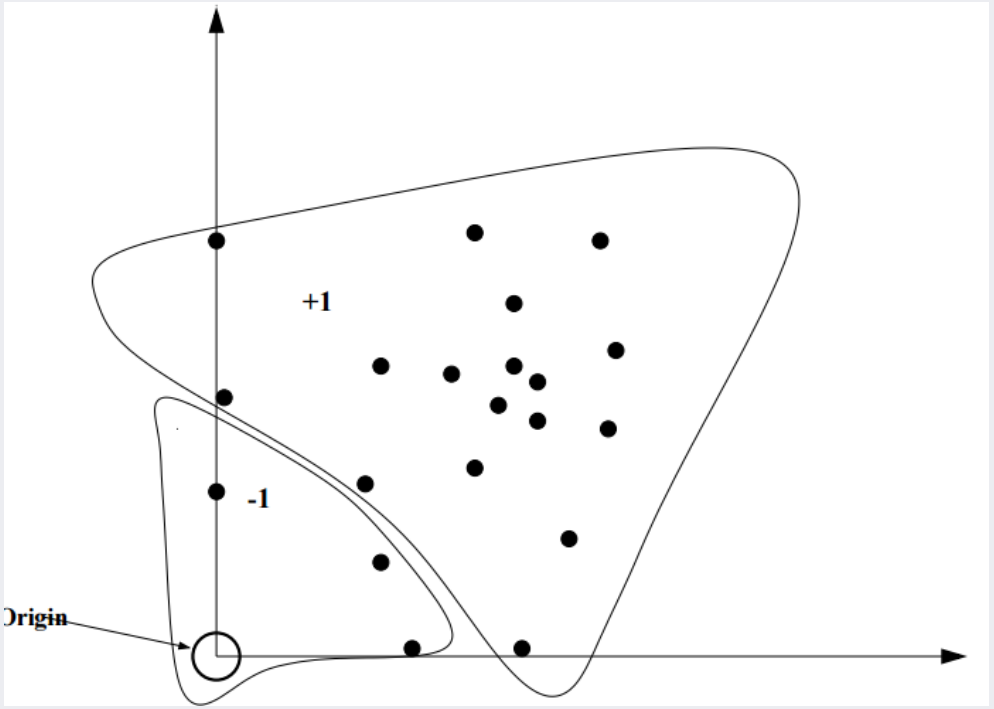
$$\min_{\mathbf{w}} \frac{1}{2}||\mathbf{w}||^2 + \frac{1}{\nu l}\sum_{i=1}^{l}\xi_i - \rho$$

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

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

    - Decision function

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



One-Class Support Vector Machine

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

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

  - ✓ KKT condition

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

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

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

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

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

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

One-Class Support Vector Machine

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

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

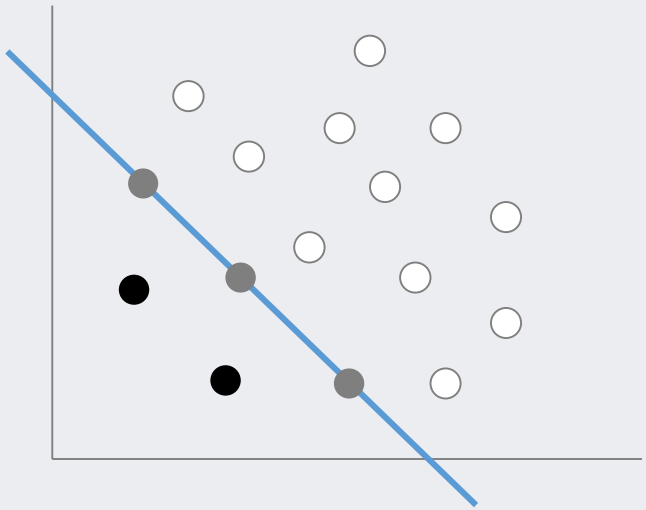
$$s.t. \quad \sum_{i=1}^{l}\alpha_i = 1, \quad 0 \le \alpha_i \le \frac{1}{\nu l} \qquad s.t. \quad \sum_{i=1}^{l}\alpha_i = 1, \quad 0 \le \alpha_i \le \frac{1}{\nu l}$$

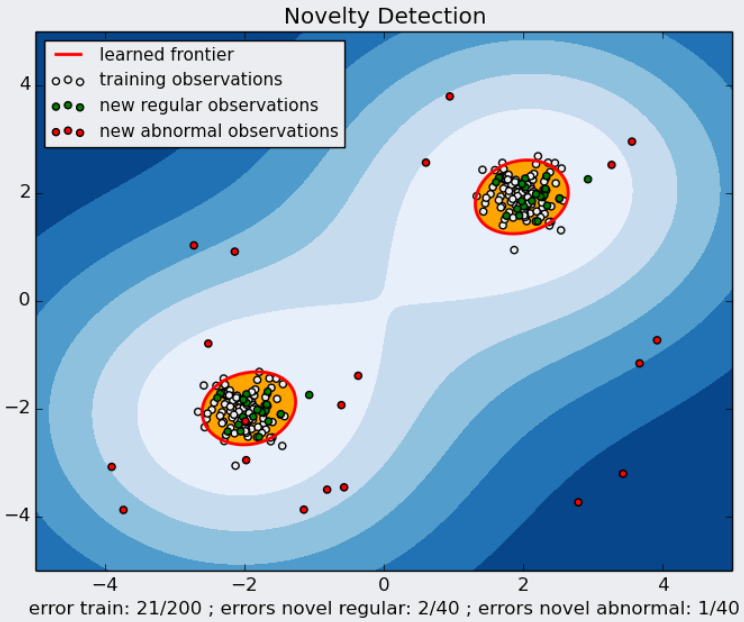
Some possible kernels $K(\cdot,\cdot)$:

$K(x, x_i) = x_i^T x$ (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

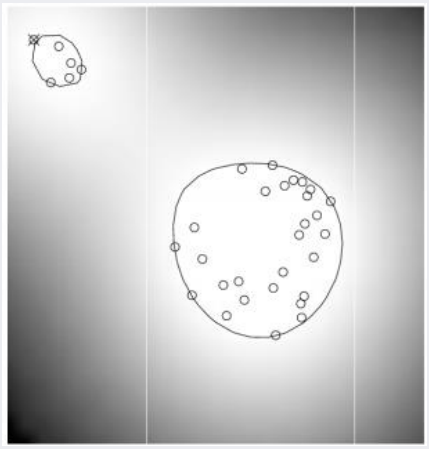
- One-class support vector machine (1-SVM)
  - ✓ Location of a point w.r.t. α_i
    - ○ ▪ Case 1: $\alpha_i = 0 \Rightarrow$ a non-support vector
    - ● ▪ Case 2: $\alpha_i = \frac{1}{\nu l} \Rightarrow \beta_i = 0 \Rightarrow \xi_i > 0 \Rightarrow$ Support vector (outsider the hyperplane)
    - ● ▪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

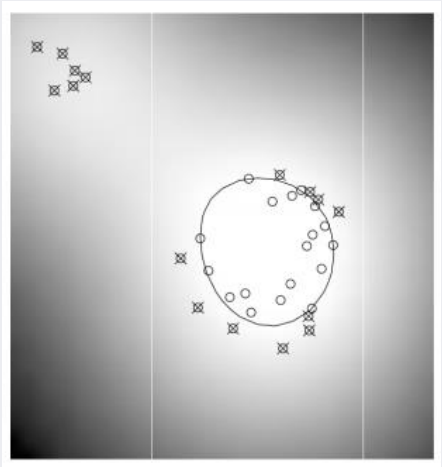




One-Class Support Vector Machine

- 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



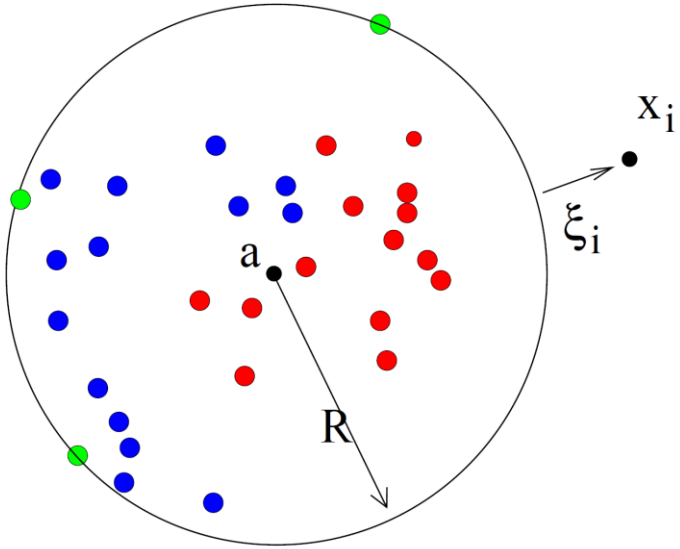


Support Vector Data Description

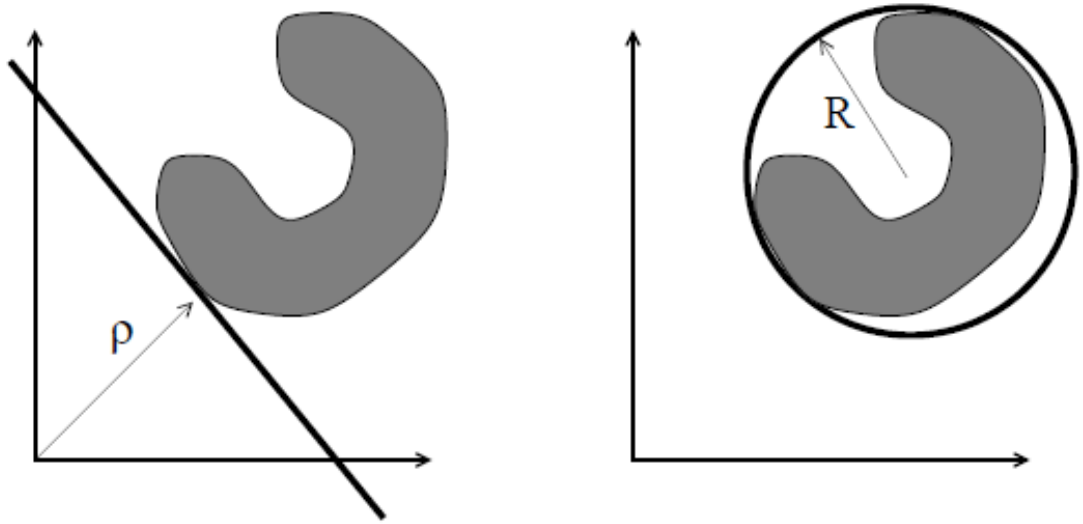
Tax and Duin (2004)

- 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

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

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

    - 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

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

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

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

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)

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

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

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

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

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)

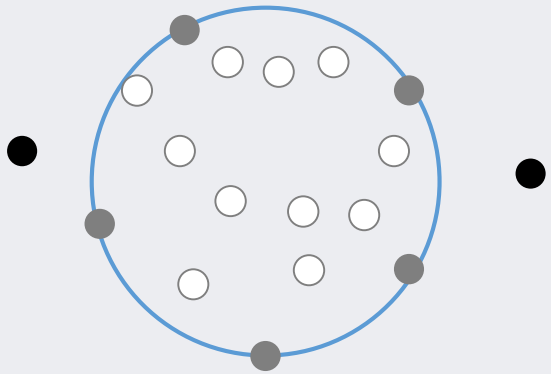
$$L = \sum_{i=1}^{l} \alpha_i \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_i) - \sum_{i=1}^{l} \sum_{j=1}^{l} \alpha_i \alpha_j \Phi(\mathbf{x}_i) \Phi(\mathbf{x}_j) \qquad (0 \leq \alpha_i \leq C)$$

    - Dual Lagrangian problem (Minimization)

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

Support Vector Data Description

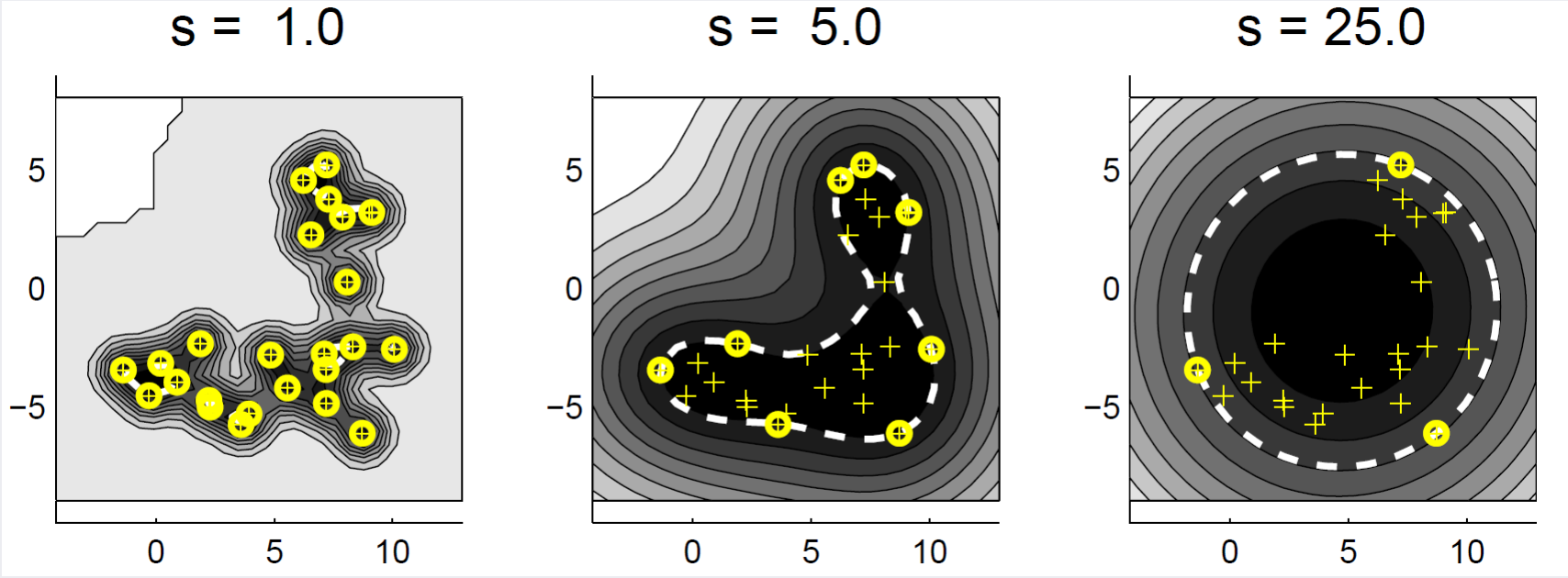
- Support Vector Data Description (SVDD)
  - ✓ Location of a point w.r.t. α_i
    - ○ ▪ Case 1: $\alpha_i = 0$ ⇒ a non-support vector
    - ● ▪ Case 2: $\alpha_i = C$ ⇒ $\beta_i = 0$ ⇒ $\xi_i > 0$ ⇒ Support vector (outsider the hypersphere)
    - ● ▪ Case 3: $0 < \alpha_i < C$ ⇒ $\beta_i > 0$ ⇒ $\xi_i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



Support Vector Data Description

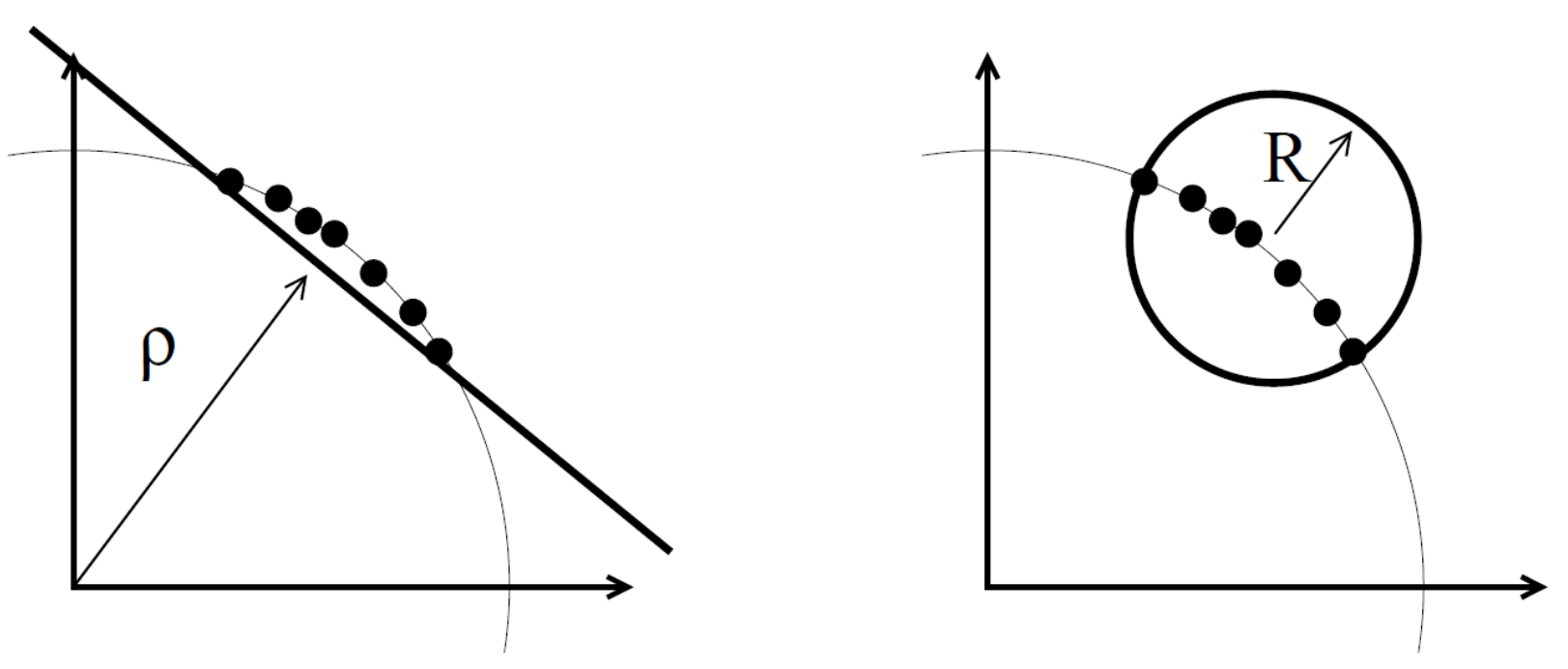
- Support Vector Data Description (SVDD)
  - ✓ SVDD with Gaussian (RBF) kernels

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



Support Vector Data Description

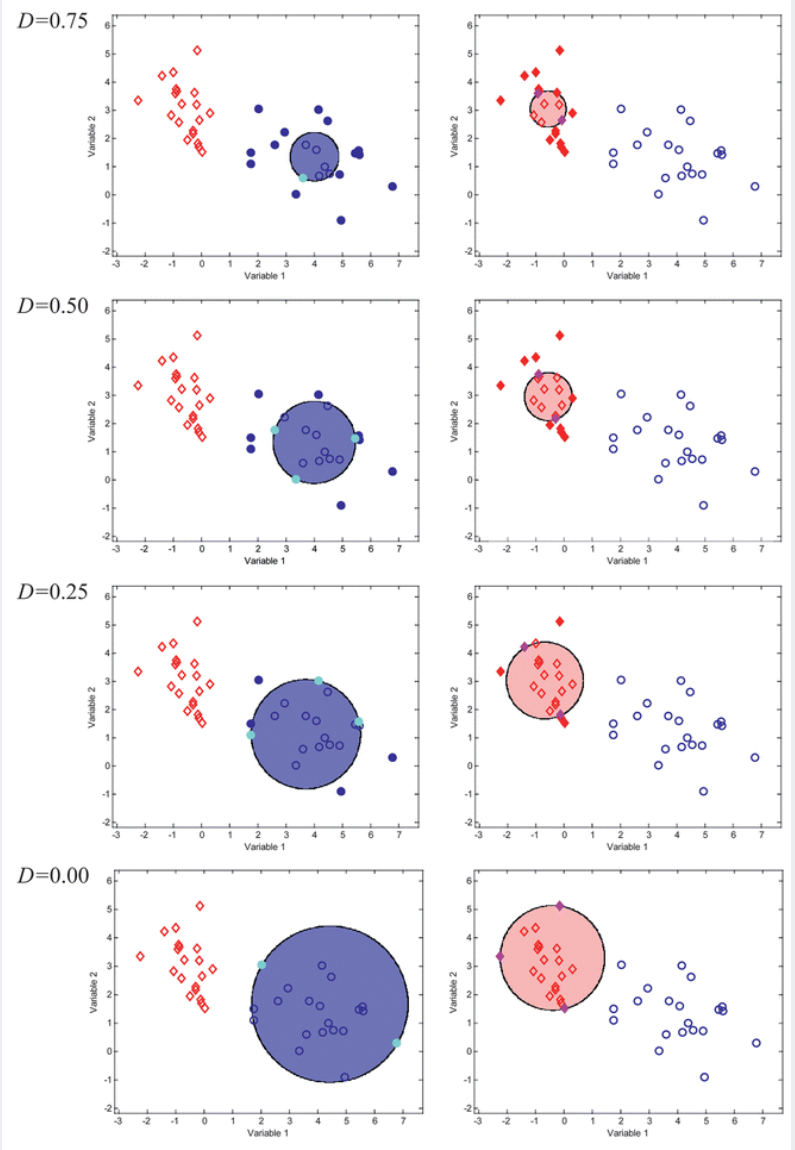
- Support Vector Data Description (SVDD)
  - ✓ When all data is normalized to unit norm vector, SVDD and 1-SVM are equivalent



  - 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

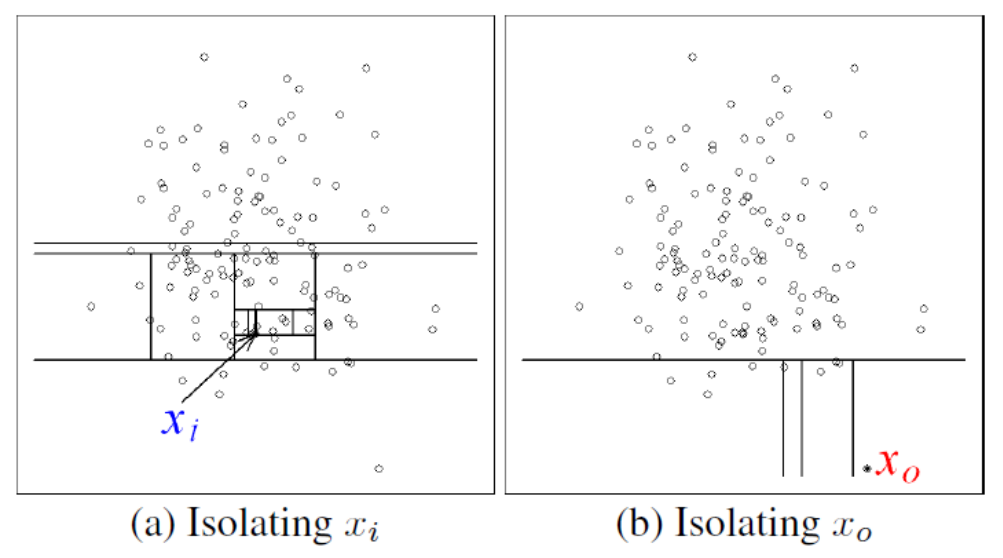


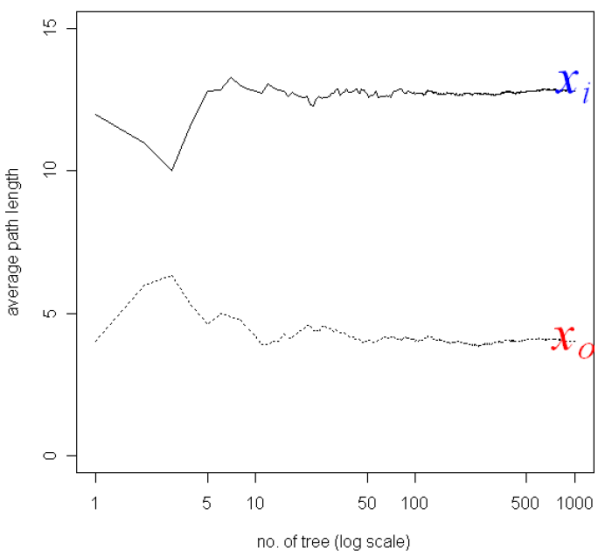
http://pubs.rsc.org/-/content/articlehtml/2010/an/b918972f

Isolation Forest

Liu et al. (2008, 2012)

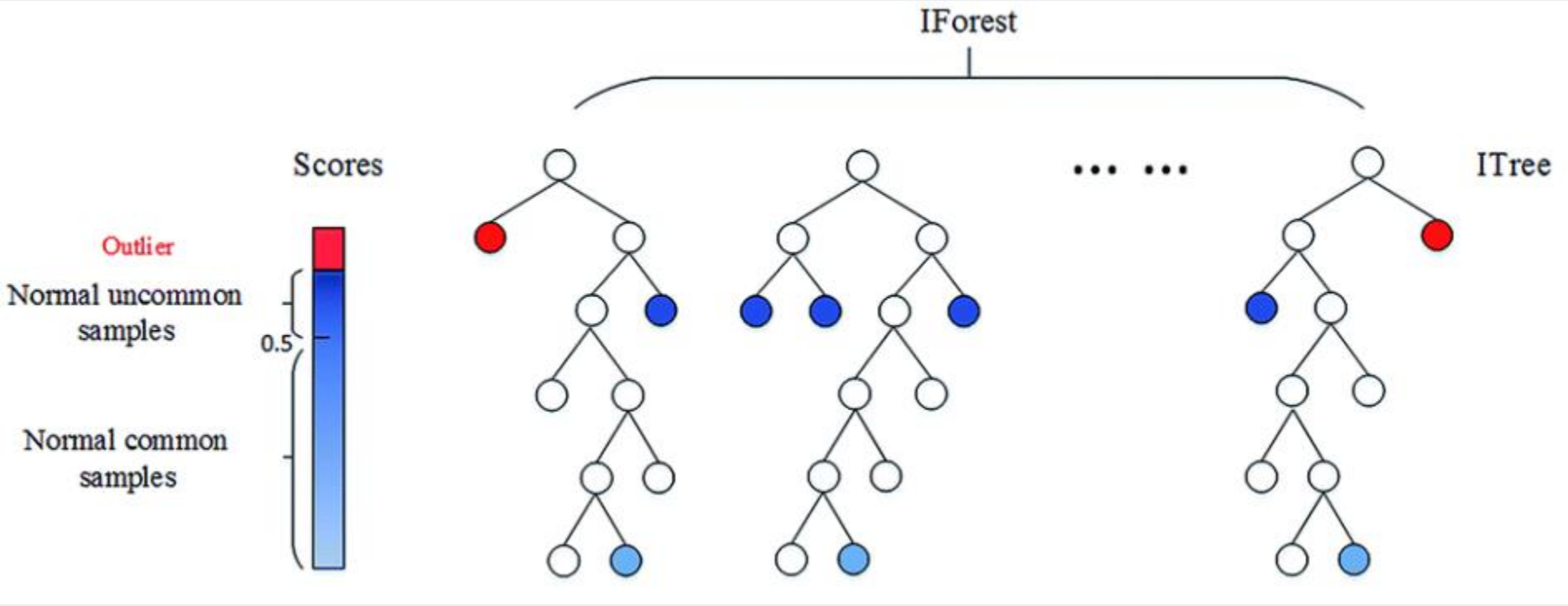
- Motivation: Few and Different
  - ✓ The minority consists of fewer instances
  - ✓ They have attribute-values, which are very different from those of normal instances
- A tree structure can be constructed effectively to isolate every single instances
  - ✓ Novel instances are isolated closer to the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





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

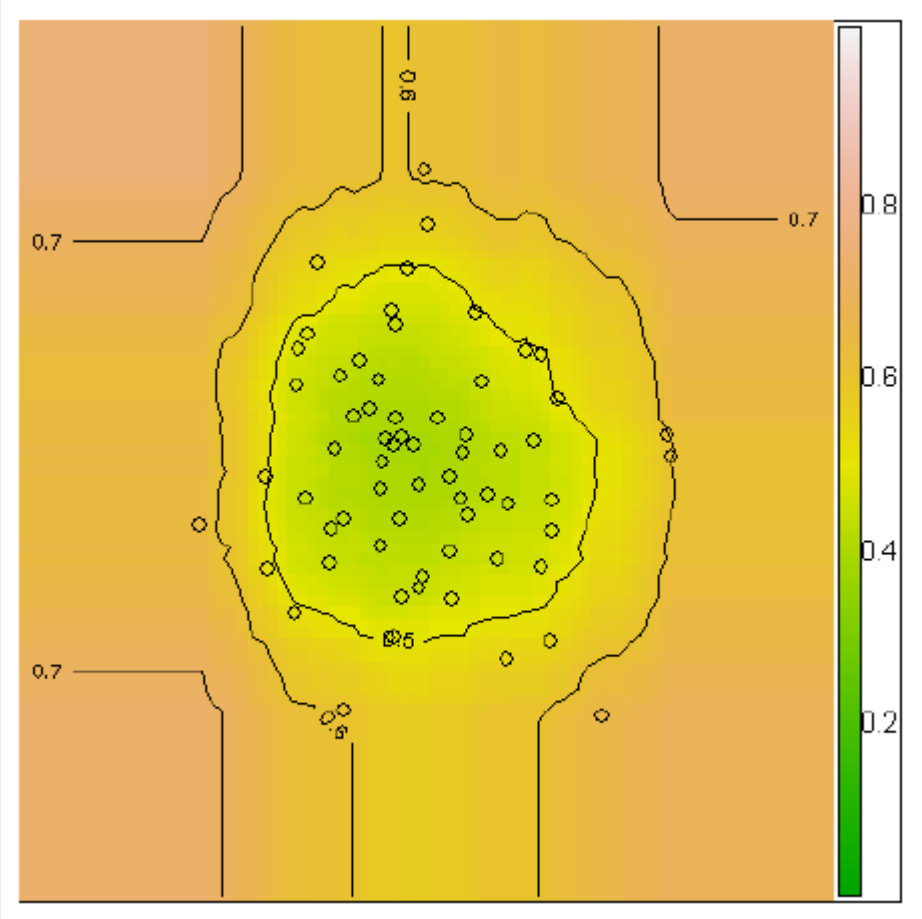
- Definition: Novelty score
  - ✓ The path length h(x) of an instance x is measured by the number of edges x traverses an iTree from the root node to the terminal node in which the instance x is located
  - ✓ h(x) is normalized by the average path length of h(x) given n
    - c(n) = 2H(n-1)-(2(n-1)/n)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

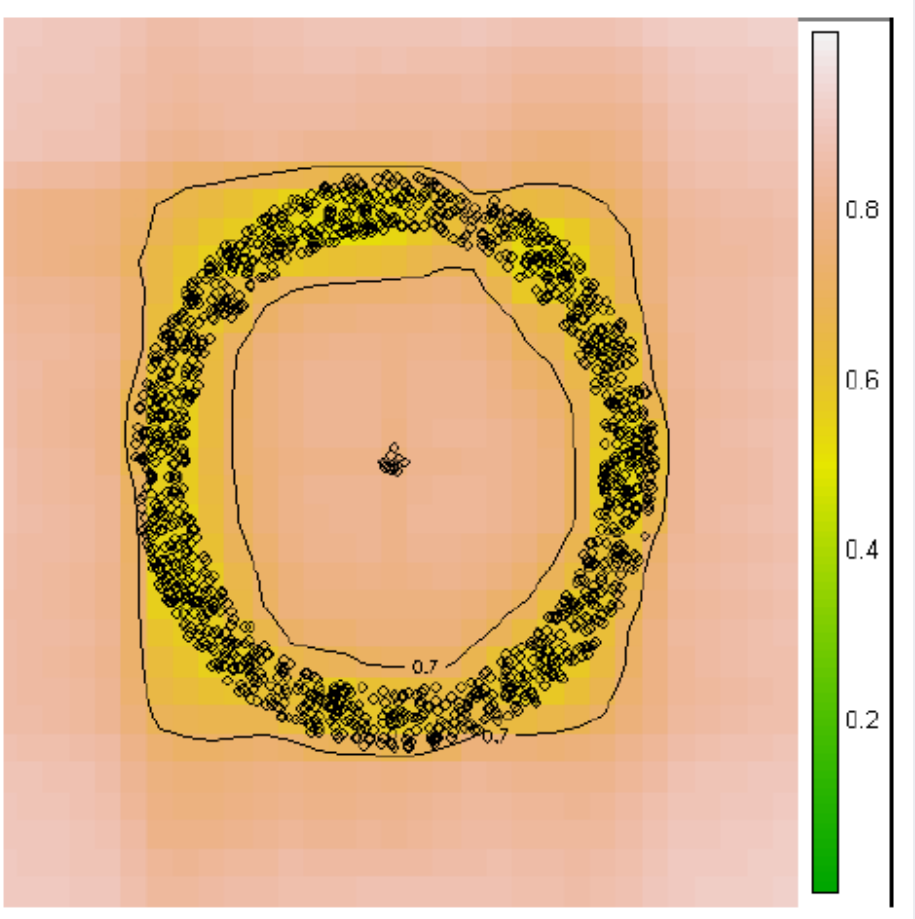
$$s(x, n) = s^{-\frac{E(h(x))}{c(n)}}$$

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

Isolation Forest

- Novelty score contour





Isolation Forest

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

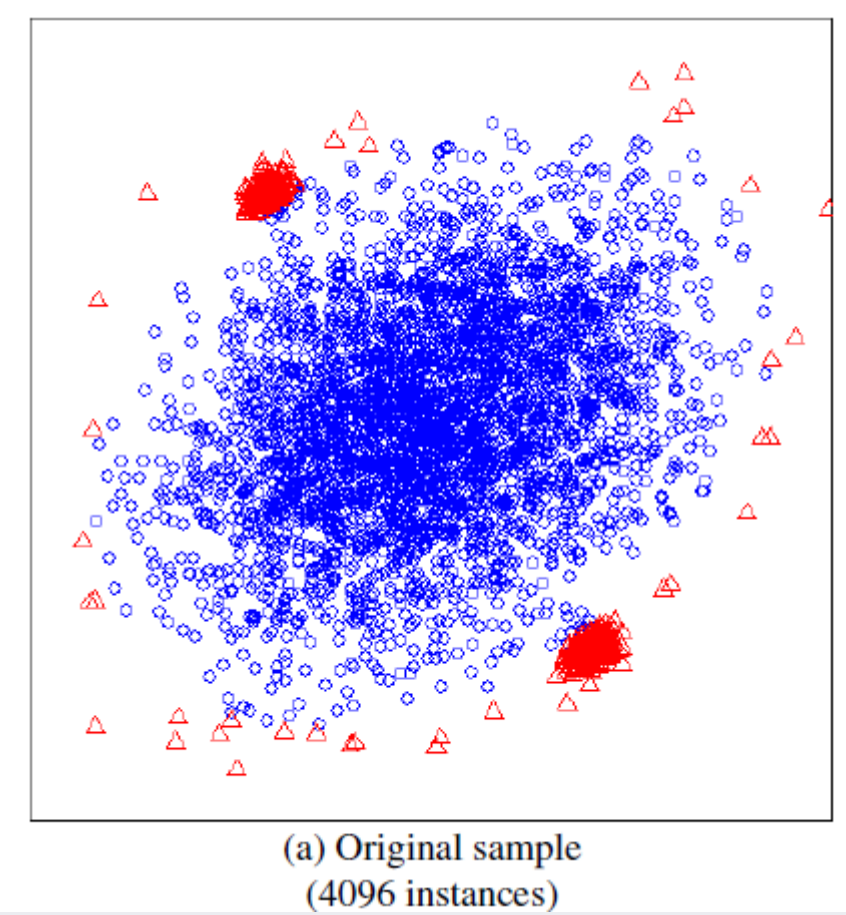
Algorithm 1 : $iForest(X, t, \psi)$

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

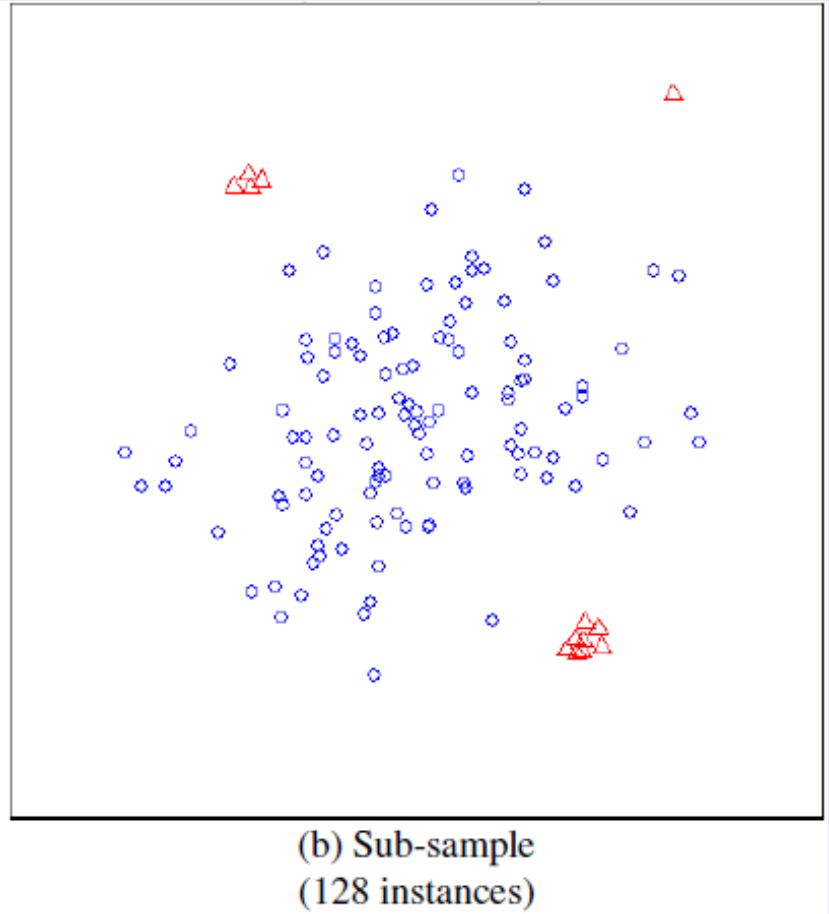
1: **Initialize** $Forest$
2: **for** $i = 1$ to t **do**
3: $\quad X' \leftarrow sample(X, \psi)$
4: $\quad Forest \leftarrow Forest \cup iTree(X')$
5: **end for**
6: **return** $Forest$

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

1: **if** X' cannot be divided **then**
2: return $exNode\{Size \leftarrow |X'|\}$
3: **else**
4: let Q be a list of attributes in X'
5: randomly select an attribute $q \in Q$
6: randomly select a split point p between the max and min values of attribute q in X'
7: $X_l \leftarrow filter(X', q < p)$
8: $X_r \leftarrow filter(X', q \geq p)$
9: return $inNode\{Left \leftarrow iTree(X_l),$
10: $Right \leftarrow iTree(X_r),$
11: $SplitAtt \leftarrow q,$
12: $SplitValue \leftarrow p\}$
13: **end if**

Isolation Forest

- Training Isolation Forest
  - ✓ Compute the path length

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

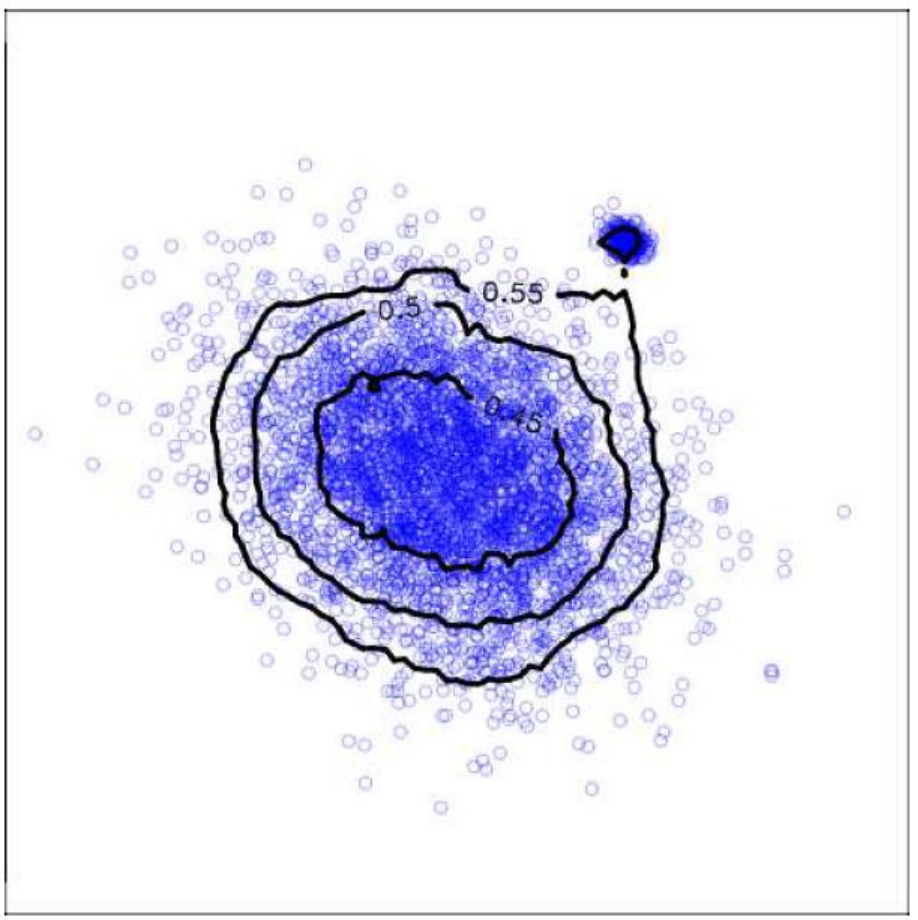
Inputs : x - an instance, T - an iTree, $hlim$ - height limit, e - current path length; to be initialized to zero when first called

Output: path length of x

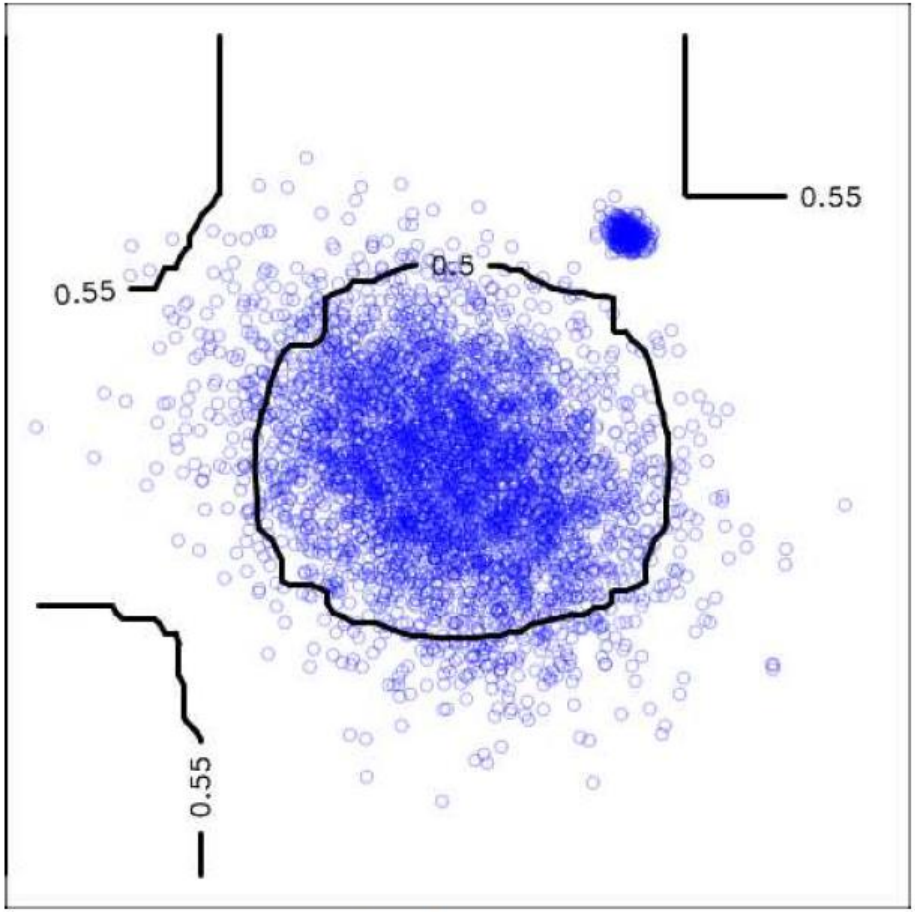
1: **if** T is an external node or $e \geq hlim$ **then**
2: return $e + c(T.size)$ {$c(.)$ is defined in Equation 1}
3: **end if**
4: $a \leftarrow T.splitAtt$
5: **if** $x_a < T.splitValue$ **then**
6: return $PathLength(x, T.left, hlim, e + 1)$
7: **else** $\{x_a \geq T.splitValue\}$
8: return $PathLength(x, T.right, hlim, e + 1)$
9: **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


Q & A

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References

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