

# Machine Learning for Time Series and Anomaly Detection

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# AD Lecture Outline (tentative)



- 1. Introduction
- 2. Overview over model families
- 3. Evaluation
- 4. Linear and kernel models
- 5. Distance- and density-based models
- 6. (Deep-Learning-based models)



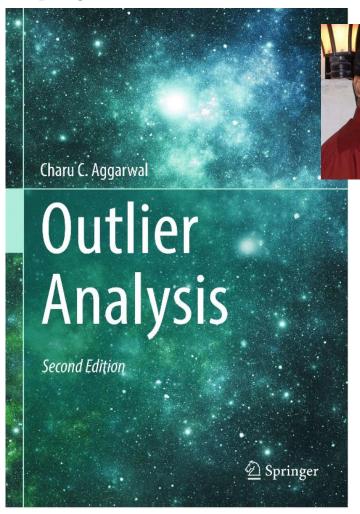
# Text book



https://link.springer.com/book/10.1007/978-3-319-47578-3

- Parts of the lecture are based on: Outlier Analysis by Aggarwal
- E-book can be accessed from the university for free!









# Lecture 1: Introduction to Anomaly Detection





• Terms anomaly and outlier are often used interchangeably



Douglas M. Hawkins

"The data come from some heavy tailed distribution such as Student's t. There is no question that any observation is in any way erroneous."





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Douglas M. Hawkins

"The data come from some heavy tailed distribution such as Student's t. There is no question that any observation is in any way erroneous."

"The data arise from two distributions. One of these, the 'basic distribution', generates 'good' observations, while another, the 'contaminating distribution', generates 'contaminants'."





• Terms anomaly and outlier are often used interchangeably

"...are patterns in data that do not conform to a well defined notion of normal behavior."



Varun Chandola





• Terms anomaly and outlier are often used interchangeably



Douglas M. Hawkins

"...are patterns in data that do not conform to a well defined notion of normal behavior."

"...are observation which deviates so much from the other observation as to arouse suspicions that it was generated by a different mechanism."



Varun Chandola





"Anomalies might be induced in the data for a variety of reasons, such as malicious activity, for example, credit card fraud, cyber-intrusion, terrorist activity or break-down of a system, but all of the reasons have the common characteristic that they are interesting to the analyst."

Chandola et al., Anomaly detection: A survey







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Chandola et al., Anomaly detection: A survey





# Application examples



- Intrusion detection
- Credit-card fraud
- Sensor events
- Medical diagnosis
- Law enforcement
- Earth science

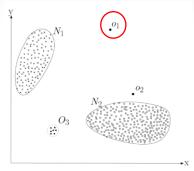


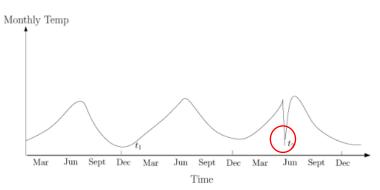


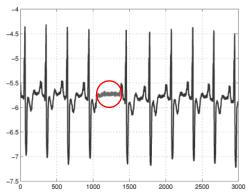
# Types of Anomalies



- Point anomalies: present or absent with respect to all other data points
- Contextual anomalies: not conspicuous in isolation but in context
  - Temporal context
  - Spatial context
  - Other dependencies
- Collective anomalies: a group or sequence of data points is anomalous





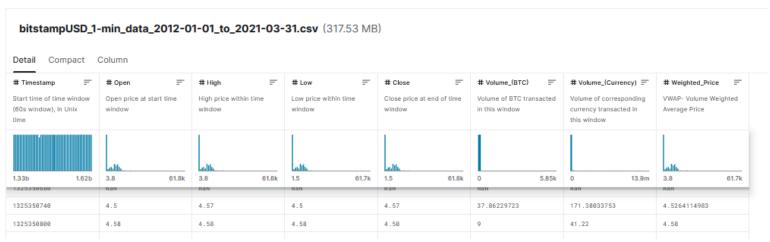


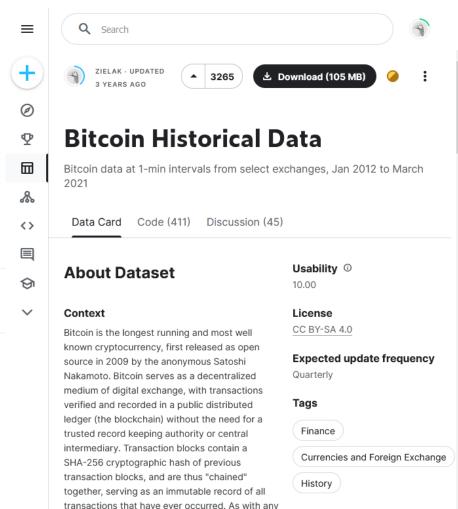


# **Example: Types of Anomalies**



- Kaggle: Bitcoin Historical Data
- https://www.kaggle.com/datasets/ mczielinski/bitcoin-historical-data/









```
# download the bitcoin history file if needed
import os
from urllib.request import urlretrieve

url = ("https://www.dropbox.com/scl/fi/ufra7gag7g1l5ktbtk43w/bitstampUSD_1-min_data_2012-01-
01_to_2021-03-31.csv?rlkey=bcj9imqn8muw29urg8gt1tda9&dl=1")
filename = "bitstampUSD_1-min_data_2012-01-01_to_2021-03-31.csv"

if not os.path.exists("bitstampUSD_1-min_data_2012-01-01_to_2021-03-31.csv"):
    urlretrieve(url, filename)
```





```
import pandas as pd
import matplotlib.pyplot as plt
from matplotlib.dates import date2num
from datetime import datetime, timedelta
# Load the Data
df = pd.read csv('bitstampUSD 1-min data 2012-01-01 to 2021-03-31.csv')
df['Timestamp'] = pd.to datetime(df['Timestamp'], unit='s')
df.set_index(df['Timestamp'], inplace=True)
df.drop('Timestamp', axis=1, inplace=True)
# We look at a specific time frame
data slice = df[(df.index > '2012-01-01 00:00') & (df.index < '2017-01-28 23:59')]
# Plot data of the "Low" column
ax = data slice['Low'].plot()
plt.show()
```



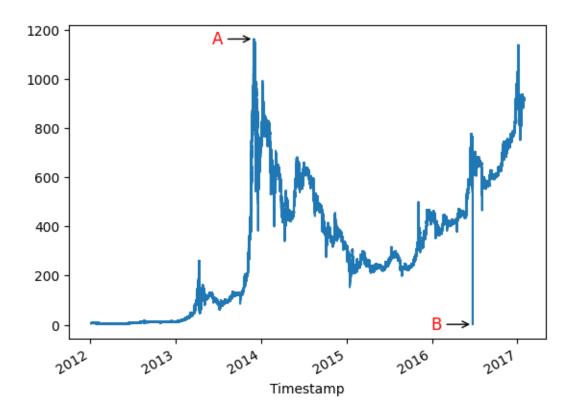






#### **Question:**

What type of anomalies are A and B?







```
# Point A:
# Get the maximum 'Low' value and the corresponding date
print("Point A:")
max low row = data slice.loc[data slice['Low'].idxmax()]
max low value = max low row['Low']
max_low_date = max_low_row.name
print(f"The maximum 'Low' value is {max low value} on {max low date}")
display(df[(df.index > '2013-11-30 03:34:00') & (df.index < '2013-11-30 03:42:00')]['Low'])</pre>
Point A:
The maximum 'Low' value is 1162.99 on 2013-11-30 03:38:00
Timestamp
2013-11-30 03:35:00
                     1162.00
2013-11-30 03:36:00
                     1162.00
2013-11-30 03:37:00
                     1162.97
2013-11-30 03:38:00
                    1162.99
                    1162.99
2013-11-30 03:39:00
2013-11-30 03:40:00
                    1162.67
2013-11-30 03:41:00
                      1162.67
Name: Low, dtype: float64
```





```
# Point B:
print("Point B:")
min low row = data slice.loc[data slice['Low'].idxmin()]
# Get the minimum 'Low' value and the corresponding date
min low value = min low row['Low']
min_low_date = min_low_row.name
print(f"The minimum 'Low' value is {min low value} on {min low date}")
display(df[(df.index > '2016-06-23 12:32') & (df.index < '2016-06-23 12:40')]['Low'])
Point B:
The minimum 'Low' value is 1.5 on 2016-06-23 12:36:00
Timestamp
2016-06-23 12:33:00
                    590.54
2016-06-23 12:34:00
                    590.40
2016-06-23 12:35:00
                    586.71
2016-06-23 12:36:00
                     1.50
2016-06-23 12:37:00
                    584.06
2016-06-23 12:38:00
                    587.15
2016-06-23 12:39:00
                    586.43
Name: Low, dtype: float64
```

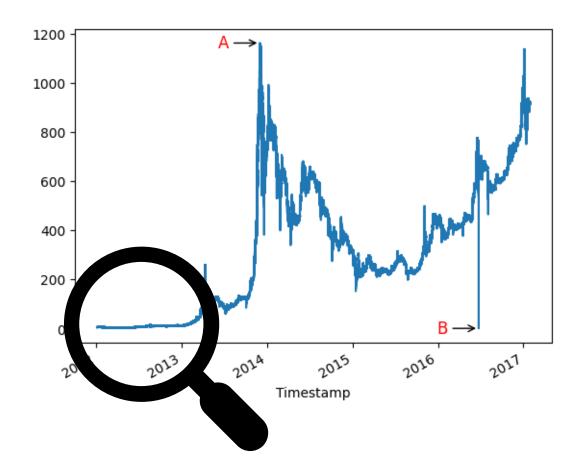




#### **Question:**

What type of anomalies are A and B?

- A seems to be a collective anomaly (anomalous group of points)
- B might be a point or contextual anomaly

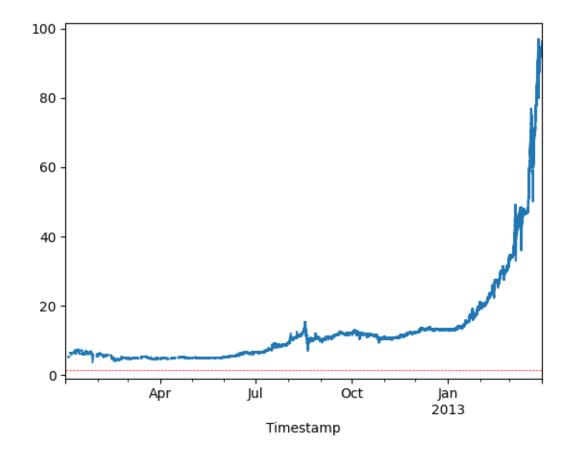






```
Point B:
The minimum 'Low' value is 1.5 on 2016-06-23
12:36:00
Timestamp
2016-06-23 12:33:00
                       590.54
2016-06-23 12:34:00
                       590.40
2016-06-23 12:35:00
                       586.71
2016-06-23 12:36:00
                      1.50
                       584.06
2016-06-23 12:37:00
2016-06-23 12:38:00
                       587.15
2016-06-23 12:39:00
                       586.43
Name: Low, dtype: float64
```

```
data_slice = df[(df.index > '2012-01-01 00:00')
& (df.index < '2013-03-31 23:59')]
ax = data_slice['Low'].plot()
ax.axhline(y=1.5, color='red', linestyle='--', linewidth=0.5)
plt.show()</pre>
```



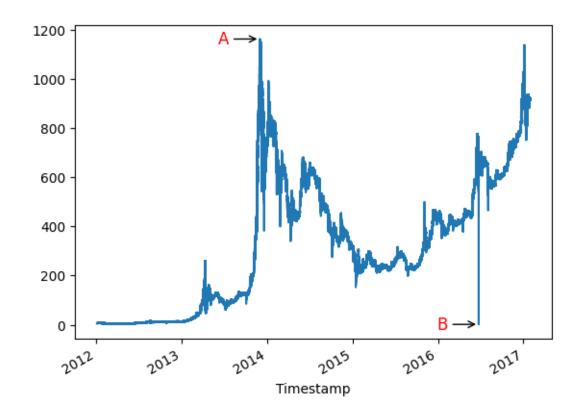




#### Question:

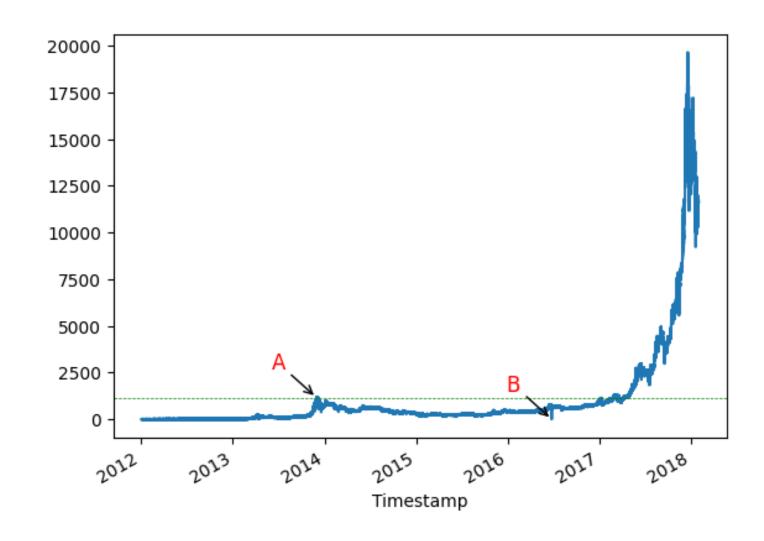
What type of anomalies are A and B?

- A seems to be a collective anomaly (anomalous group of points)
- B is a point anomaly





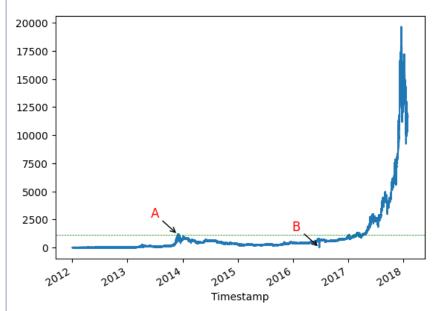








```
data slice = df[(df.index > '2012-01-01 00:00') & (df.index < '2018-01-28 23:59')]
ax = data slice['Low'].plot()
for name, annotate time in annotate times.items():
    annotate value = data slice.loc[annotate time, 'Low']
    annotate time dt = datetime.strptime(annotate time, '%Y-%m-%d %H:%M:%S')
    annotate time dt -= timedelta(days=180)
    ax.annotate(name, xy=(annotate_time, annotate_value),
                xytext=(date2num(annotate time dt), annotate value + 1500),
                arrowprops=dict(facecolor='black', arrowstyle='->'),
                fontsize=12, color='red')
ax.axhline(y=1162.99, color='green', linestyle='--', linewidth=0.5)
plt.show()
```



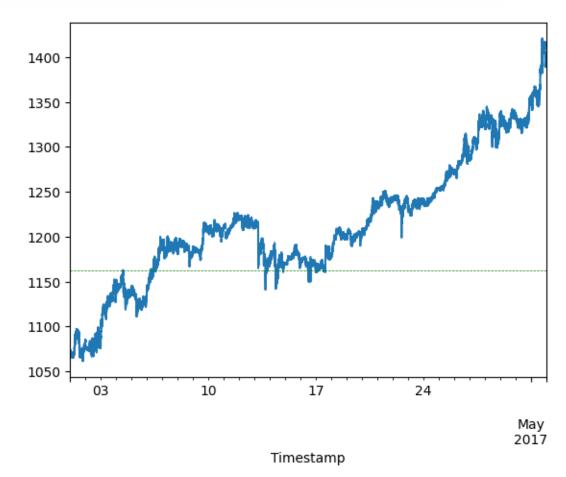




#### **Question:**

What type of anomalies are A and B?

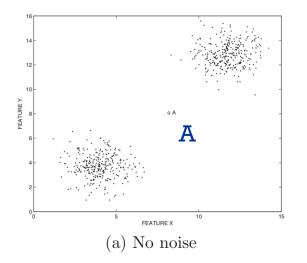
- A is a contextual and collective anomaly (anomalous group of points in their context)
- B is a point anomaly







- In real applications: Noise in data
- Noise typically also "generated by a different mechanism"
- Noise may not be of interest to the analyst

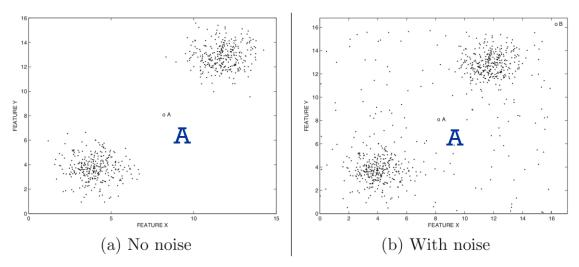


- Main patterns are identical (two clusters)
- (a): Point A is anomaly





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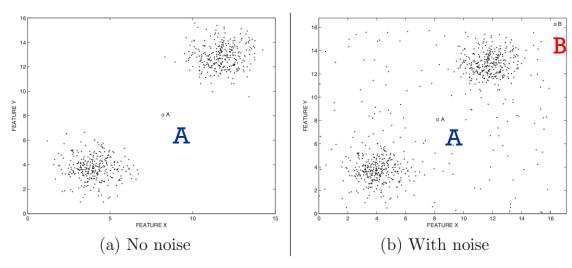


- Main patterns are identical (two clusters)
- (a): Point A is anomaly
- (b): Point A is quite likely noise (fits pattern of random noise)





- In real applications: Noise in data
- Noise typically also "generated by a different mechanism"
- Noise may not be of interest to the analyst



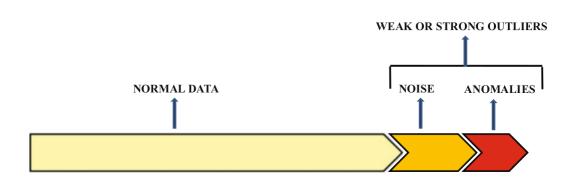
- Main patterns are identical (two clusters)
- (a): Point A is anomaly
- (b): Point A is quite likely noise (fits pattern of random noise)
- Anomaly vs. outlier: is it of interest to an analyst (A vs. B)?
- Noise: semantic boundary between normal data and true anomalies

from https://link.springer.com/book/10.1007/978-3-319-47578-3





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- Noise typically also "generated by a different mechanism"
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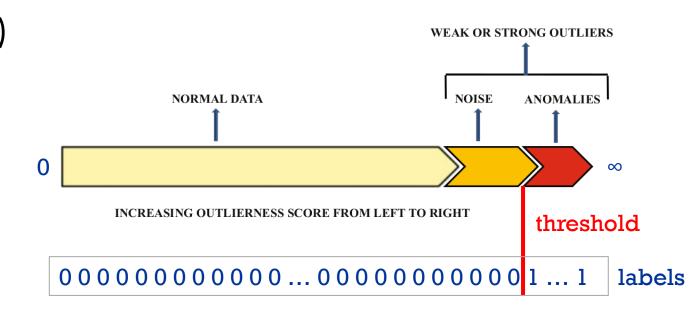
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- Anomaly vs. outlier: is it of interest to an analyst (A vs. B)?
- Noise: semantic boundary between normal data and true anomalies



# **Outlier Detection Output**



- Binary labels (is an outlier or not)
- Outlier scores (level of outlierness)
- Outlier score can be converted to binary
  - By threshold
  - By extreme value analysis
  - As a machine learning task
- Often important: Are known anomalies available / is training data available
- => supervision vs. unsupervised



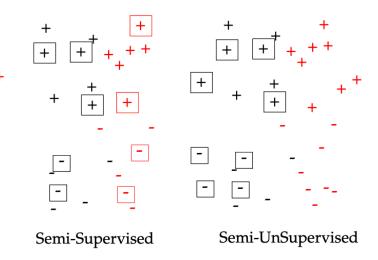


#### Supervised vs. Unsupervised Outlier Detection



- Unsupervised methods
  - Either for noise removal or anomaly detection
  - Often used in an exploratory setting
- Supervised methods: applicationspecific anomaly detection

- Different levels of supervision:
  - Fully supervised: normal and abnormal data available
  - PU learning / contaminated supervised: examples of outliers given, normal data may contain outliers
  - Semi-supervised: only normal / only outliers available
  - Semi-unsupervised: some but not all classes are known





# The Data Model is Everything



- Outlier detection algorithms:
   learn a model of **normal** data
- Outlier score of a data: deviations from this model
- Models make different assumptions about the data



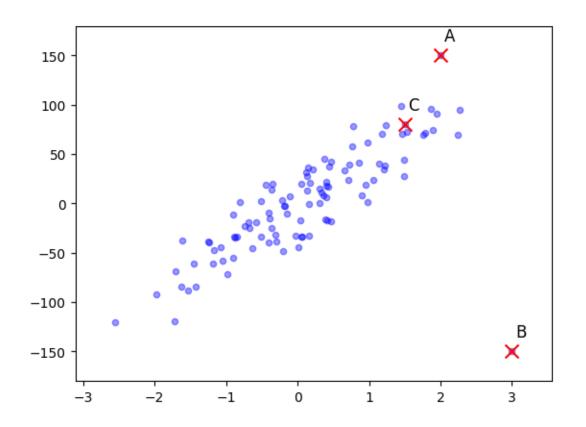




#### Example 1

#### Question:

How would you model the following examples, and can you make up a criterion on the "outlierness"?





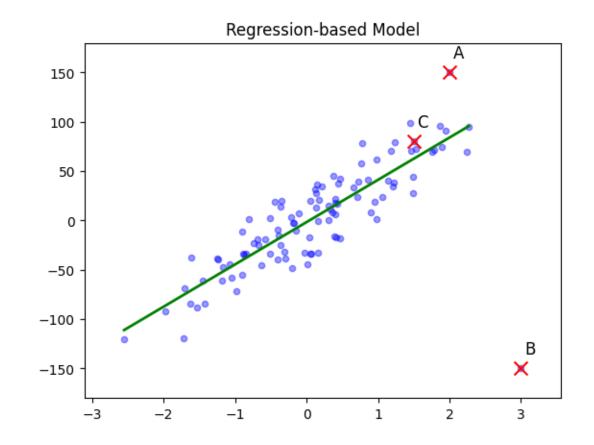


#### Example 1

#### Question:

How would you model the following examples, and can you make up a criterion on the "outlierness"?

Linear model, distance to the line



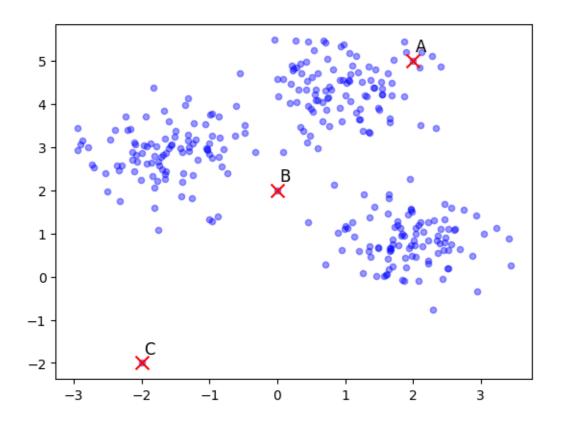




#### Example 2

#### Question:

How would you model the following examples, and can you make up a criterion on the "outlierness"?





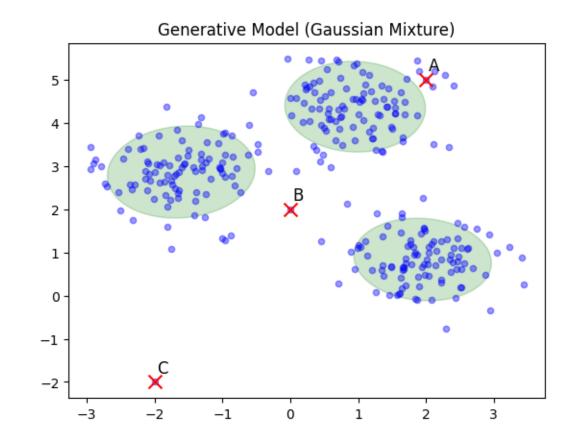


#### Example 2

#### Question:

How would you model the following examples, and can you make up a criterion on the "outlierness"?

Clustering based model, distance to cluster centroid



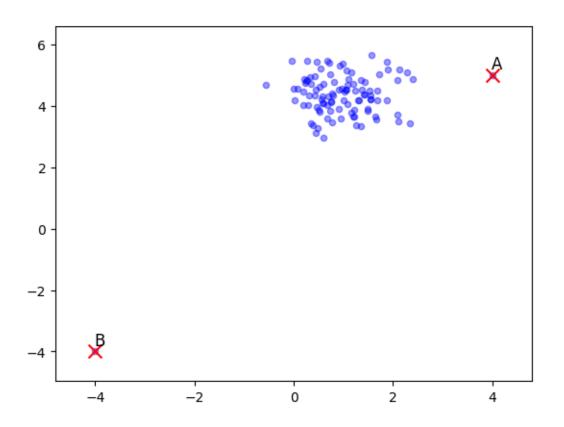




#### Example 3

#### Question:

How would you model the following examples, and can you make up a criterion on the "outlierness"?





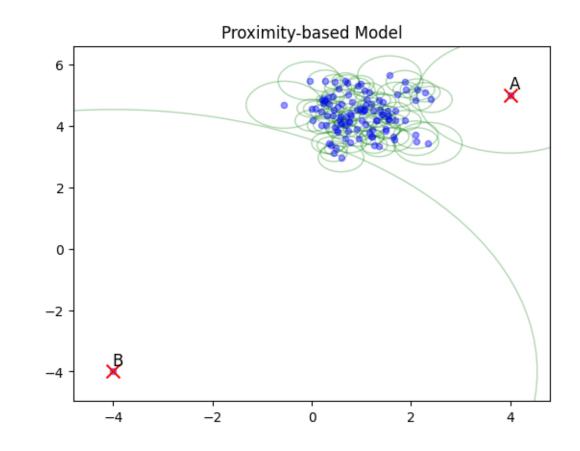


#### Example 3

#### Question:

How would you model the following examples, and can you make up a criterion on the "outlierness"?

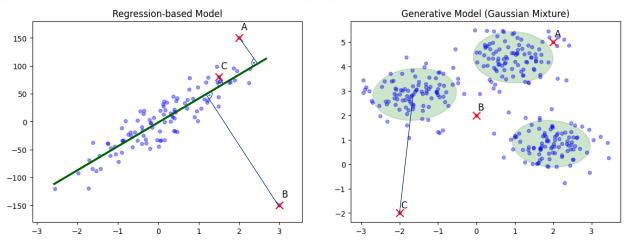
Density- / proximity-based models, distance to n neighbors

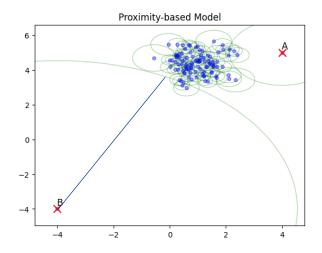






- Outlier score corresponds to the fit between data point and model
- Choice of data model is crucial
- Anomaly detection is typically an unsupervised problem
  - Examples of outliers are not given to learn the best model
  - Understanding of data and data deviations important









# Overview of Anomaly Detection Methods



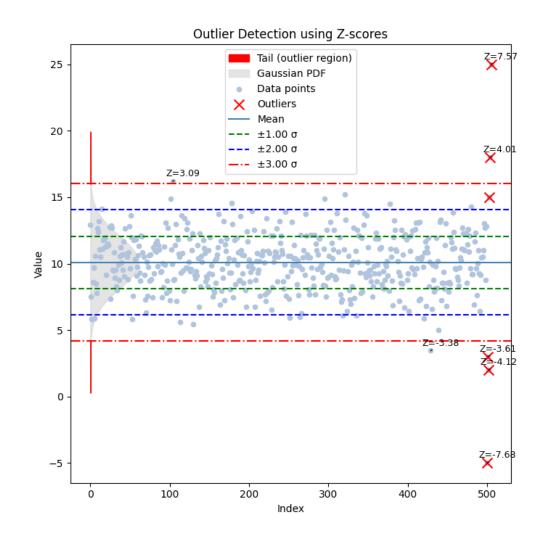
### **Z-value Test for Outlier Detection**



- Simple model for outlier detection
- One-dimensional data  $X_i, \dots, X_N$  with mean  $\mu$  and standard deviation  $\sigma$
- Z-value for a data point  $X_i$ :

$$z_i = \frac{|x_i - \mu|}{\sigma}$$

- Z-value denotes the number of standard deviations to mean
- Implicit assumption: data follows normal distribution





## **Z-value Test for Outlier Detection**



• " $3\sigma$  rule-of-thumb":  $z_i \geq 3$  as decision criterion for anomalies:

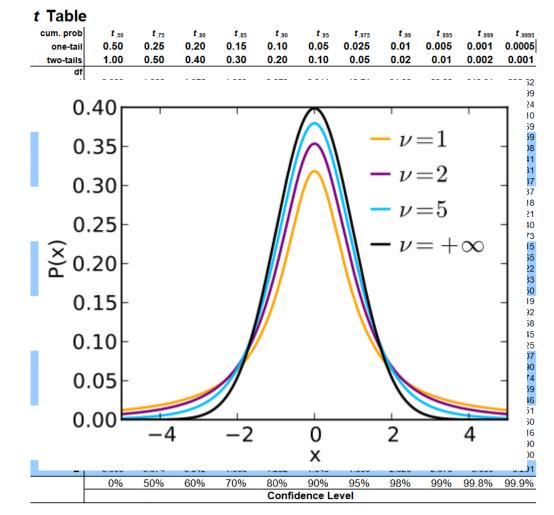
$$P(z < 3) = 0.9973$$

- Typically:  $\mu$  and  $\sigma$  not explicitly known
  - For enough data (n > 30) assumption of normality
  - For few data interpretation by Student's tdistribution and the (absolute of the) tvalue

$$t_i = \left| \frac{x_i - \mu}{\sigma / \sqrt{n}} \right|$$

for sample size n

unbiased 
$$\sigma = \sqrt{\frac{\sum_{i}(x_{i}-\mu)^{2}}{n-1}}$$



https://www.sjsu.edu/faculty/gerstman/StatPrimer/t-table.pdf





Given 100 samples S with estimated

mean: 7.13

std.dev: 1.86

including  $x = \{1, 2, 13, 14\} \subset S$ .

- 1. Calculate the Z-values for these points.
- 2. Decide, which will be labeled as outliers according to the " $3\sigma$  rule-of-thumb".

```
Calculate: z = |x-\mu|/\sigma
Data point (1):
        z-score = 6.13 / 1.86 =
       = 3.2957
Data point (2):
        z-score = 5.13 / 1.86
       = 2.7581
Data point (13):
       z-score = 5.87 / 1.86
       = 3.1559
Data point (14):
        z-score = 6.87 / 1.86
       = 3.6935
Outliers: 1, 13, 14 =>=3
```





Given 100 samples S with estimated

mean: 7.13

std.dev: 1.86

including  $x = \{1, 2, 13, 14\} \subset S$ .

- 1. Calculate the Z-values for these points.
- 2. Decide, which will be labeled as outliers according to the " $3\sigma$  rule-of-thumb".

```
mean = 7.13
std = 1.86
p = [1, 2, 13, 14]

z_val = [abs(x - mean) / std for x in p]
print("z-values", z_val)

# > z-values [3.2956989247311825, 2.758064516129032,
3.1559139784946235, 3.693548387096774]

out = [p[i] for i, z in enumerate(z_val) if abs(z) > 3]
print("Outliers:", out)

# > Outliers: [1, 13, 14]
```





Given the following data points:

3, 8, 6, 15, 13, 7

- 1. Calculate the mean and sample standard deviation.
- 2. Compute the t-values for each data point.
- 3. Identify if any points are outliers for a tail probability mass of 0.05.

t Table	<b>!</b>										
cum. prob	t .50	t.75	t .80	t .85	t.90	t .95	t .975	t .99	t .995	t .999	t .9995
one-tail	0.50	0.25	0.20	0.15	0.10	0.05	0.025	0.01	0.005	0.001	0.0005
two-tails	1.00	0.50	0.40	0.30	0.20	0.10	0.05	0.02	0.01	0.002	0.001
df											
1	0.000	1.000	1.376	1.963	3.078	6.314	12.71	31.82	63.66	318.31	636.62
2	0.000	0.816	1.061	1.386	1.886	2.920	4.303	6.965	9.925	22.327	31.599
3	0.000	0.765	0.978	1.250	1.638	2.353	3.182	4.541	5.841	10.215	12.924
4	0.000	0.741	0.941	1.190	1.533	2.132	2.776	3.747	4.604	7.173	8.610
5	0.000	0.727	0.920	1.156	1.476	2.015	2.571	3.365	4.032	5.893	6.869
6	0.000	0.718	0.906	1.134	1.440	1.943	2.447	3.143	3.707	5.208	5.959
7	0.000	0.711	0.896	1.119	1.415	1.895	2.365	2.998	3.499	4.785	5.408
8	0.000	0.706	0.889	1.108	1.397	1.860	2.306	2.896	3.355	4.501	5.041
9	0.000	0.703	0.883	1.100	1.383	1.833	2.262	2.821	3.250	4.297	4.781
10	0.000	0.700	0.879	1.093	1.372	1.812	2.228	2.764	3.169	4.144	4.587





Given the following data points:

3, 8, 6, 15, 13, 7

- 1. Calculate the mean and sample standard deviation.
- 2. Compute the t-values for each data point.
- 3. Identify if any points are outliers for a tail probability mass of 0.05.

```
import numpy as np
data = [3, 8, 6, 15, 13, 7]
mean = np.mean(data)
print("Mean:", mean)
std = np.std(data, ddof=1)
print("Sample Standard Deviation:", std)
# > Sample Standard Deviation: 4.501851470969102
n = len(data)
t val = [(x - mean) / (std / np.sqrt(n)) for x in data]
print("t-values:", t val)
# > t-values: [-3.083274062967549, -
0.36273812505500547, -1.4509525002200228,
3.4460121880225554, 2.357797812857538, -
0.9068453126375141
t critical = 2.571 \# df = 5 and alpha = 0.05
outliers = [data[i] for i, t in enumerate(t val) if
abs(t) > t_critical]
print("Outliers:", outliers)
# > Outliers: [3, 15]
```



### Z-value Test for Outlier Detection (cont.)

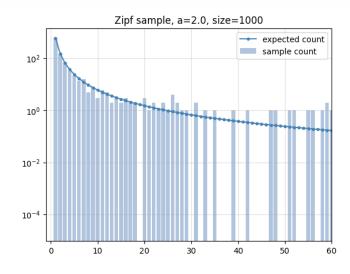


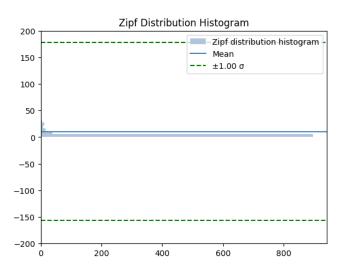
- What if data is not normal distributed?
- E.g. zipf with  $k \ge 1$ , a > 1

$$zipf(k;a) = \frac{k^{-a}}{\zeta(a)}$$

with the Riemann Zeta function

$$\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s}$$





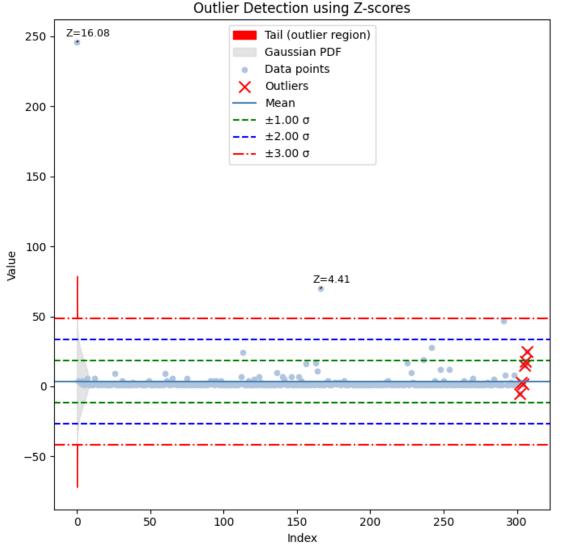


### Z-value Test for Outlier Detection (cont.)



 What if data is not normal distributed?

Standard deviation and mean (and thus Z-value) are not meaningful







- Mistakes made at the modeling stage can result in incorrect understanding of the data
- Best choice of a model is often data-specific
- Core principle based on assumptions about the structure of normal patterns
- Choice of the "normal" model: understanding of data patterns in that particular domain



## Connection with Supervised Models



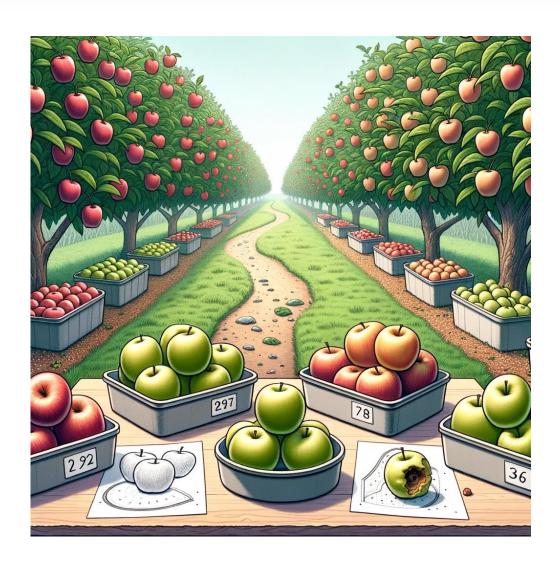
- Anomaly detection: classification problem for which (one) class label is unobserved
- As #normal samples >> #anomalies
  - Treat whole unlabeled (contaminated) data as normal and create a (noisy) model
  - Deviation from normal model treated as outliers
- => Theory and methods from classification can generalize to anomaly detection



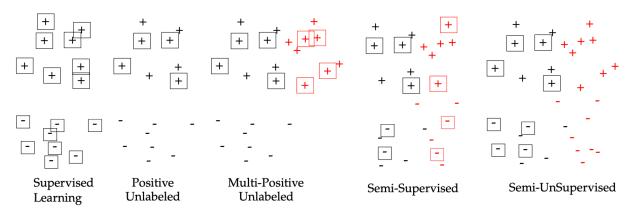


### Connection with Supervised Models (cont.)





- One-class analog of multi-class classification
- Unobserved nature of labels (or outlier scores) typically "unsupervised" perspective
- If labels are given, anomaly detection simplifies to imbalanced classification





## Connection with Supervised Models (cont.)



- Differentiation between instancebased and explicit generalization to model normal behavior
- Instance-based: No model constructed up front, most relevant instance from training used to make predictions
- Explicit Generalization:
   (Summarizing) model created up front, outlierness scored based on this model of normal behavior

Type	<b>Unsupervised Analog</b>	<b>Supervised Model</b>	
Instance-based	<u>k-NN distance, LOF,</u> <u>LOCI</u>	k-nearest neighbor	
Explicit Generalization	Principal component Analysis	Linear Regression	
Explicit Generalization	Expectation- maximization	Naive Bayes	
<b>Explicit Generalization</b>	Mahalanobis method	Rocchio	
<b>Explicit Generalization</b>	<u>Isolation Trees</u>	<b>Decision Trees</b>	
<b>Explicit Generalization</b>	<b>Isolation Forest</b>	Random Forest	
<b>Explicit Generalization</b>	FP-Outlier	Rule-based	
Explicit Generalization	One-class Support Vector Machines	Support Vector Machines	
Explicit Generalization	Replicator Neural Networks (Auto- Encoder)	Neural Networks	
Explicit Generalization	Principle Component Analysis, Matrix Factorization	Matrix Factorization	

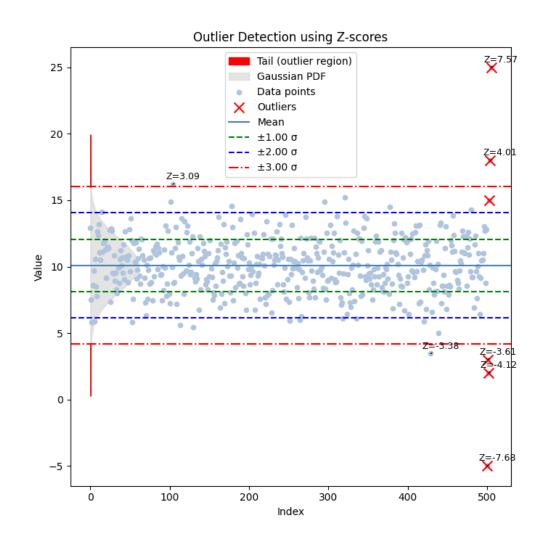


## Connection with Supervised Models (cont.)



#### Question:

 Is z-value test for outlier detection instance-based or explicit generalization?







# Overview of Anomaly Detection Methods



## **Anomaly Detection Methods**



- Extreme-Value Analysis
- Probabilistic and Statistical Models
- Linear Models
- Proximity-Based Models
- Information-Theoretic Models
- Outlier Ensembles
- High-Dimensional Outlier Detection



## Extreme-Value Analysis



- Most basic form of outlier detection
- Assumption: Values that are too large or too small are outliers
- Determining the statistical tails of the underlying distribution
- z-value Test:
  - Normal distributed data: statistical interpretation
  - Arbitrary distributions: rather "heuristic idea of the outlier score"
- Extreme-value statistics is different from the general definition of outliers
- generative probabilities vs. extremity in value

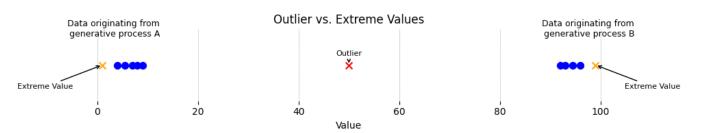




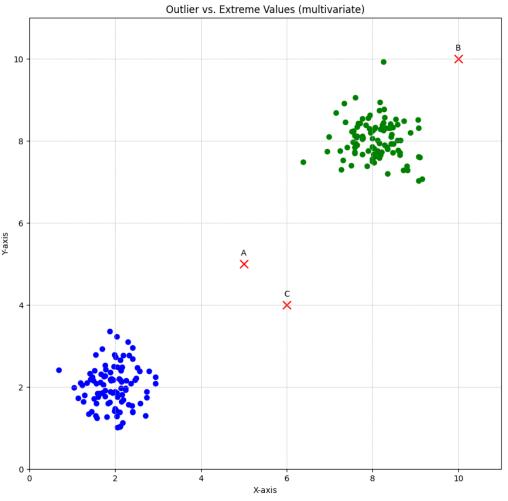
## Extreme-Value Analysis (cont.)



• [1, 4, 5.5, 7, 8, 9, <del>50</del>, 92, 93, 94.5, 96, 99]



- Probabilistic and density-based models: Outlier is 50 (in line with outlier definition)
- Extreme-Value Analysis: 1 and 99 are outliers from an extreme-value perspective
- Special kinds of outliers even in the multivariate case

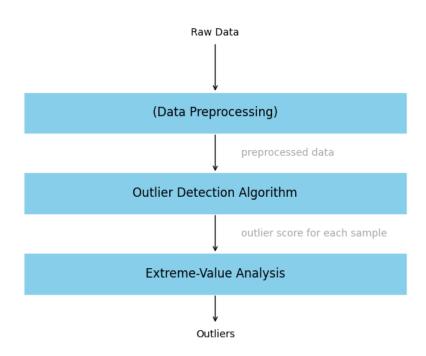




## Extreme-Value Analysis (cont.)



- Extreme-value analysis for outlier detection algorithms as final step
- Algorithms quantify deviations of data from normal patterns as (univariate) outlier score
- Outlier scores can be analyzed with (multivariate) extreme-value methods





## Probabilistic and Statistical Models



- Data is modeled as closed-form probability distribution
- The parameters of this model are learned
- Key assumption: choice of data distribution
- The likelihood fit of a data point to a generative model is the outlier score

#### **Example:**

Gaussian PDF:

$$g(x; \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

• "Fit" the parameters  $\mu$ ,  $\sigma$  to the data  $x_i$ 

$$\mu = \frac{1}{n} \sum_{i=1}^{n} x_i, \sigma = \sqrt{\frac{\sum_i (x_i - \mu)^2}{n-1}}$$





#### Example (cont.):

#### Approach:

- Choose Gaussian (Normal)
   Distribution Probability Density
   Function
- 2. "Fit" parameters to dataset
- 3. Calculate the likelihood fit for a data point
- 4. Convert the likelihood fit to an outlier score (e.g. negative log likelihood)

#### **Example:**

1. Gaussian PDF:

$$g(x; \mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

2. "Fit" the parameters  $\mu$ ,  $\sigma$  to the data  $x_i$ 

$$\mu = \frac{1}{n} \sum_{i=1}^{n} x_i, \sigma = \sqrt{\frac{\sum_{i} (x_i - \mu)^2}{n-1}}$$

- 3. Likelihood for  $\hat{x}$ :  $g(\hat{x}; \mu, \sigma)$
- 4.  $NLL(\hat{x}) = -\log(g(\hat{x}; \mu, \sigma))$

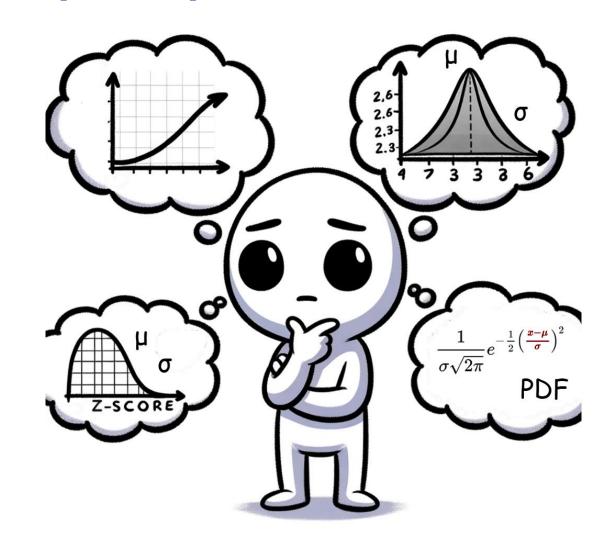




#### Example (cont.):

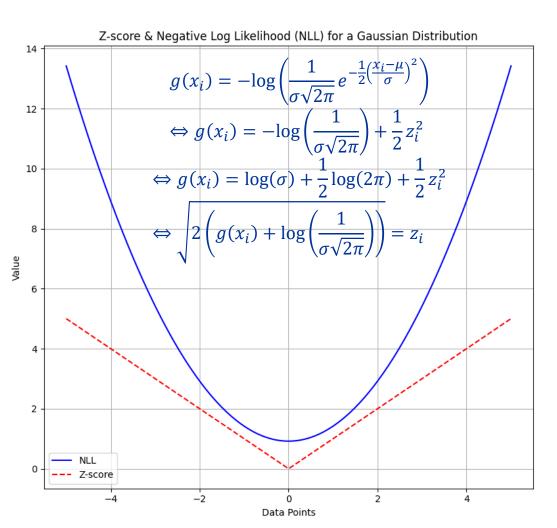
#### Approach:

- Choose Gaussian (Normal)
   Distribution Probability Density
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- 2. "Fit" parameters to dataset
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```
import numpy as np
import matplotlib.pyplot as plt
mu = 0
sigma = 1
x = np.linspace(-5, 5, 400)
                                # Generate data points
# Calculate Z-scores for these data points
z \cdot scores = abs(x - mu) / sigma
# Calculate the PDF likelihood for these data points
pdf_likelihood = (1 / (np.sqrt(2 * np.pi) * sigma)) * \
           np.exp(-0.5 * ((x - mu) / sigma)**2)
plt.figure(figsize=(8, 7.5))
plt.plot(x, -np.log(pdf likelihood), label='NLL', color='blue')
plt.plot(x, z scores, label='Z-score', color='red', linestyle='--')
plt.xlabel('Data Points')
plt.ylabel('Value')
plt.title('Z-score & Negative Log Likelihood (NLL) for a Gaussian
Distribution')
plt.legend()
plt.grid(True)
plt.tight layout()
plt.show()
```



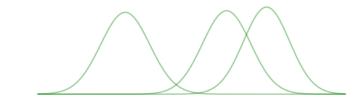


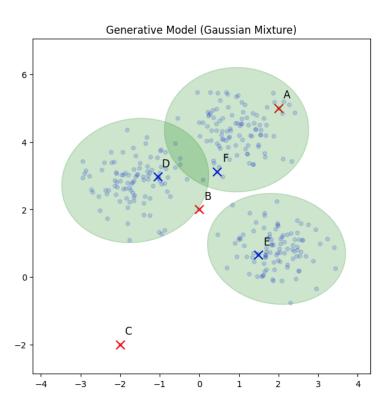
#### **Gaussian Mixture Models**

- Probabilistic model
- Assumption: Data is generated from a mixture of Gaussians
- Data is described as combination of K Gaussians

$$p(x; \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{k=1}^{K} \pi_k g(x; \mu_k, \Sigma_k)$$

Parameters are learned via EM algorithm











Gaussian Mixture Modelling Example: <a href="http://localhost:8888/notebooks/AD02-S94-GMM">http://localhost:8888/notebooks/AD02-S94-GMM</a> Example.ipynb