

Departamento de Eletrónica, Telecomunicações e
Informática

LECTURE 8 Anomaly detection

Petia Georgieva
(petia@ua.pt)

Outline

1. Anomaly detection
2. Gaussian (Normal) distribution & Density Estimation
3. Multivariate density estimation
4. Univariate vs. Multivariate Gaussian models for Anomaly detection

Popular applications of anomaly detection

Fraud detection - $x^{(i)}$ – vector of the following features of user i

x_1 - how often does the user login

x_2 # of web pages visited / # of transactions

x_3 - the typing speed of the user

How to identify suspicious computer users ?

Manufacturing (e.g. aircraft engine features)

x_1 = heat generated

x_2 =vibration intensity,

x_3, x_4, \dots other features

How to identify anomalous production (engines) for quality control ?

Matrix X	feature x_0	feature x_1	featur e x_n
User1 /Motor1	1	$x^{(1)}$		$x_n^{(1)}$
User2 /Motor2	1	$x^{(2)}$		$x_n^{(2)}$
	1			
User i /Motor i				$x_n^{(i)}$
User m /Motor m	1	$x^{(m)}$		$x_n^{(m)}$

Monitoring computers in data center: $x^{(i)}$ = features of machine i

x_1 =memory use of computer

x_2 =number of disc accesses /sec

x_3 =CPU load

x_4 =network traffic &....other features...

How to identify if a computer is doing something strange and further inspect it?

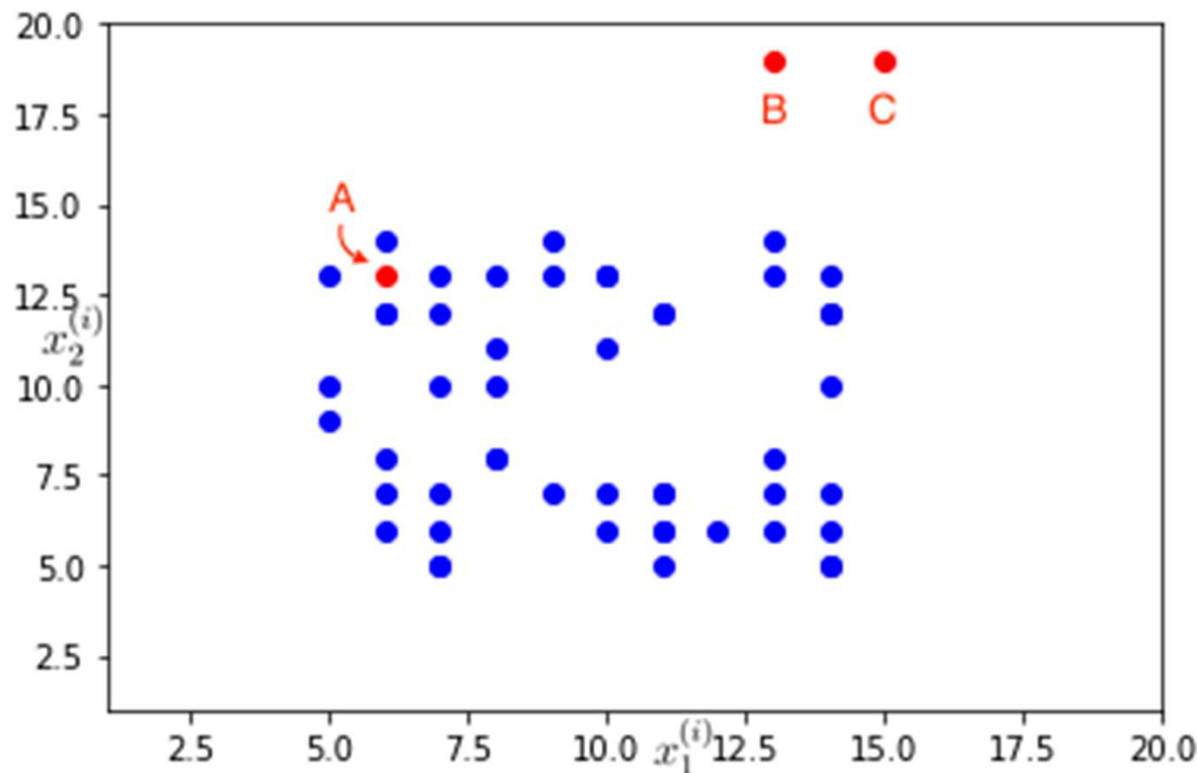
Anomaly detection

We have a dataset of examples (blue points): $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$

Each example has two features x_1 and x_2 .

We get new examples (red points): A, B, C

How to decide that A is not an outlier, B and C are anomalous (outliers) ?



Anomaly detection – How ?

From given regular (not anomalous) data get a model of what is considered as normal. For example – a probability model $p(x)$.

Identify anomalous case by checking if

$$p(x_{test}) < \epsilon \text{ (flag as anomaly)}$$

$$p(x_{test}) \geq \epsilon \text{ (flag as normal)}$$

Gaussian (Normal) distribution

If $x \in \mathbb{R}$, and x follows Gaussian distribution with mean, μ and variance σ^2 , denoted as,

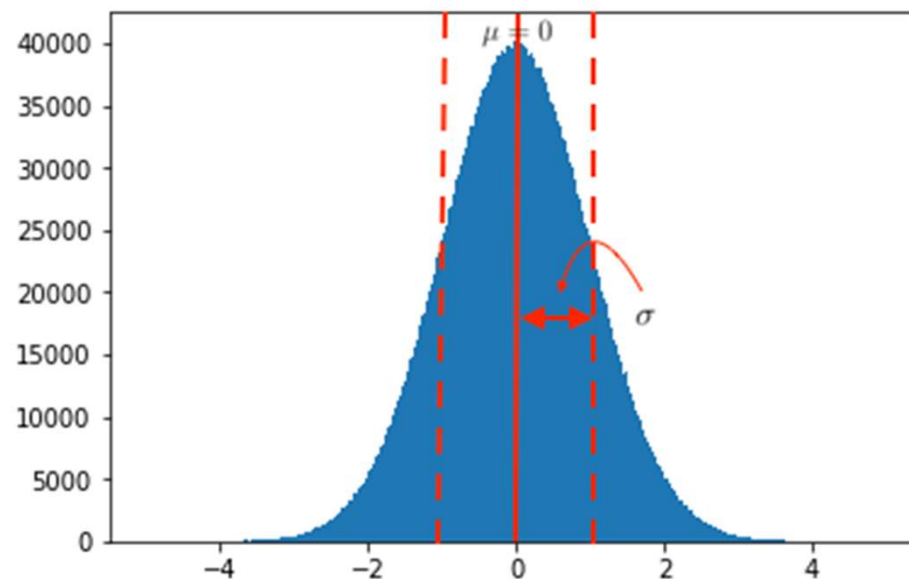
$$x \sim \mathcal{N}(\mu, \sigma^2)$$

Standard normal Gaussian distribution ($\mu=0$, standard deviation $\sigma=1$).

Density is higher around μ and reduces as distance from mean increases.

If we know parameters μ and σ , the probability of x in Gaussian distribution is:

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

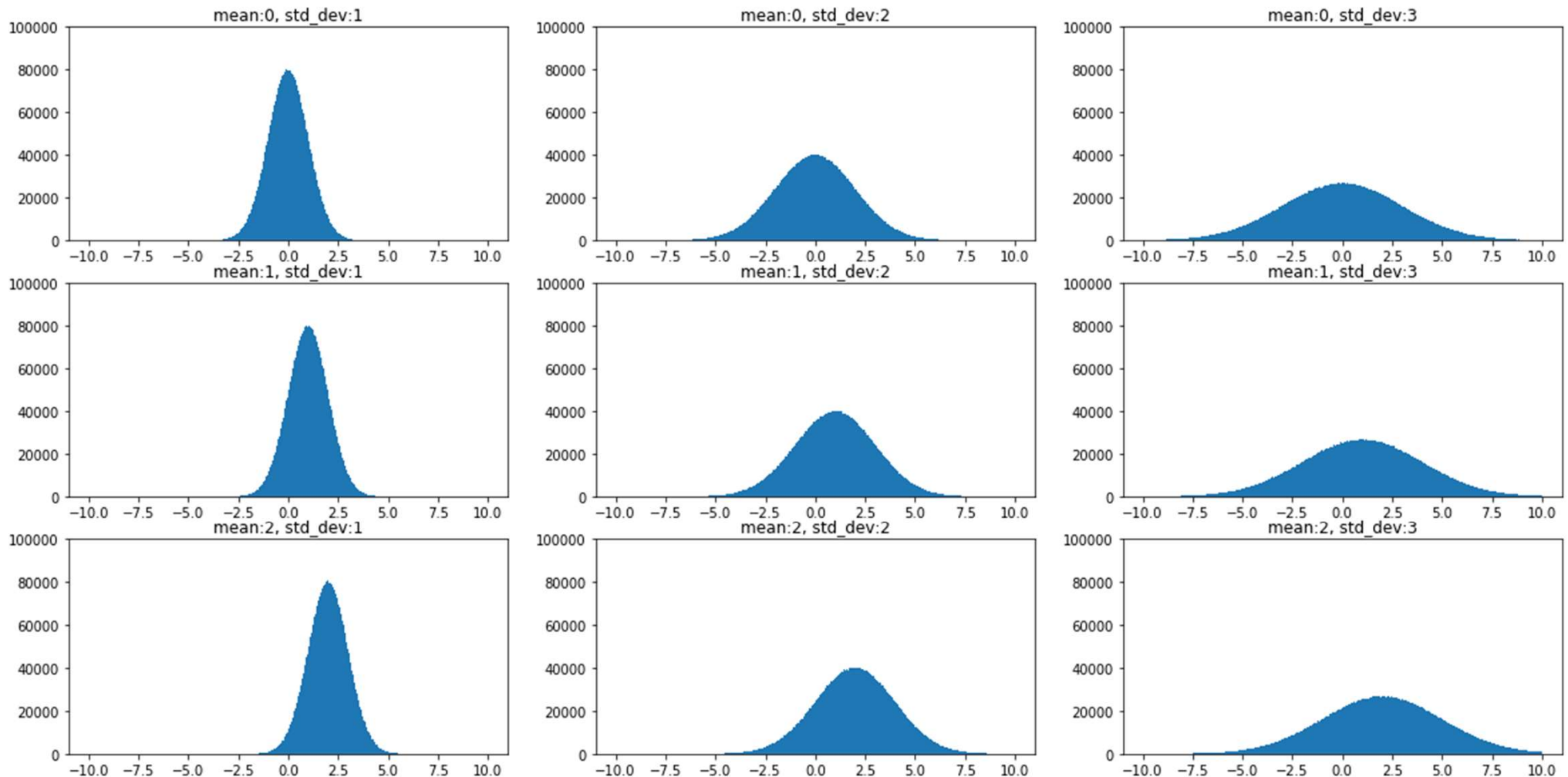


Effect of μ and σ on Gaussian curve

Mean (μ) defines the centering of the distribution.

Standard deviation (σ) defines the spread of the Gaussian distribution.

As the spread increases the height of the plot decreases, because the total area under a probability distribution should be = 1.



Parameter estimation of Gaussian curve

Parameters (μ and σ) of the Gaussian distribution are estimated based on given data

$$\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$$

$$\mu = \frac{1}{m} \sum_{i=1}^m x^{(i)}$$

$$\sigma^2 = \frac{1}{m} \sum_{i=1}^m (x^{(i)} - \mu)^2$$

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

Density Estimation - example

All features have Gaussian distribution (living area and bedrooms)
How to compute the probability (density estimation) of all features $p(x)$?

$$\mu = \frac{1}{m} \sum_{i=1}^m x^{(i)} \quad p(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)$$
$$\sigma^2 = \frac{1}{m} \sum_{i=1}^m (x^{(i)} - \mu)^2$$

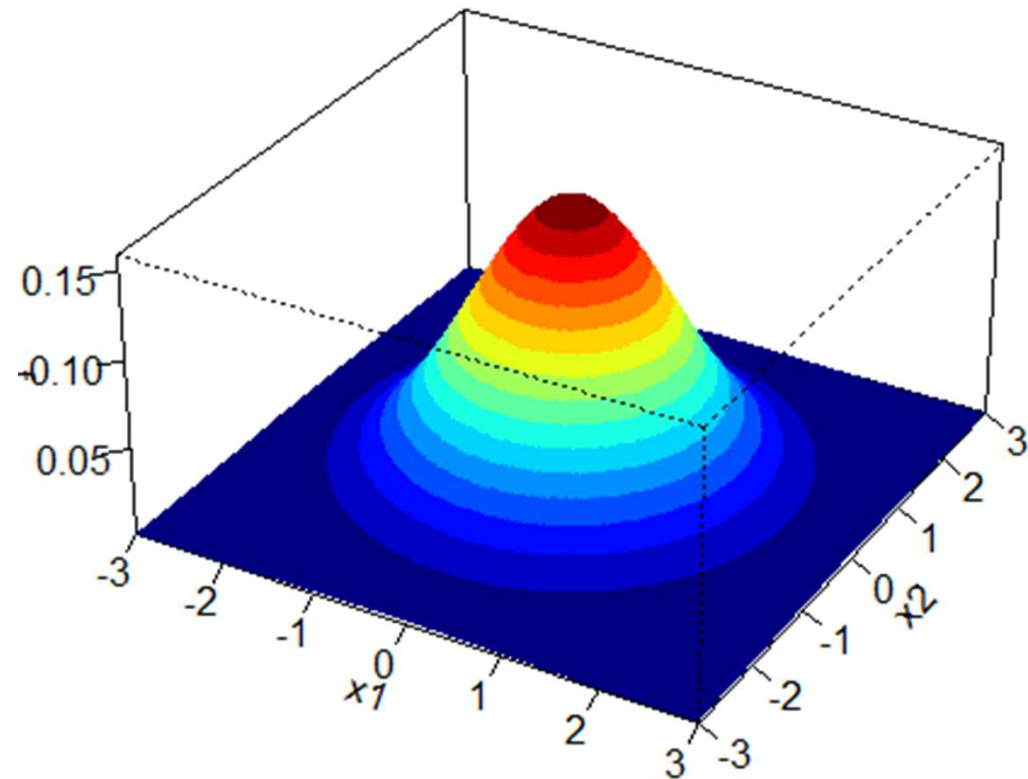
Assumption: features are independent

$$p(x) = p(x_1, \mu_1, \sigma_1) * p(x_2, \mu_2, \sigma_2)$$

Living area (feet ²)	#bedrooms
2104	3
1600	3
2400	3
1416	2
3000	4
⋮	⋮

Gaussian distribution model

Living area (feet ²)	#bedrooms
2104	3
1600	3
2400	3
1416	2
3000	4
⋮	⋮



$$p(x) = p(x_1, \mu_1, \sigma_1) * p(x_2, \mu_2, \sigma_2) \text{ 3D Bell shaped volume}$$

Density Estimation Algorithm

Given data with n features and m examples =>

Major assumptions:

The features have Gaussian distribution and are independent.

Compute μ and σ of each feature.

Compute $p(x_j)$ of each feature.

Compute probability (density estimation) of all features $p(x)$:

$$\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$$

$$\{x_2^{(i)}, x_2^{(i)}, \dots, x_n^{(i)}\}$$

$$x_1 \sim \mathcal{N}(\mu_1, \sigma_1^2)$$

$$x_2 \sim \mathcal{N}(\mu_2, \sigma_2^2)$$

$$\vdots$$

$$x_j \sim \mathcal{N}(\mu_j, \sigma_j^2)$$

$$\vdots$$

$$x_n \sim \mathcal{N}(\mu_n, \sigma_n^2)$$

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

$$p(x) = p(x_1; \mu_1, \sigma_1^2) p(x_2; \mu_2, \sigma_2^2) \cdots p(x_n; \mu_n, \sigma_n^2)$$

$$p(x) = \prod_{j=1}^n p(x_j; \mu_j, \sigma_j^2)$$

Anomaly Detection Algorithm

1. Choose features that you think might be indicative of anomalous examples.

2. Fit Gaussian distribution parameters (μ and σ) for each feature.

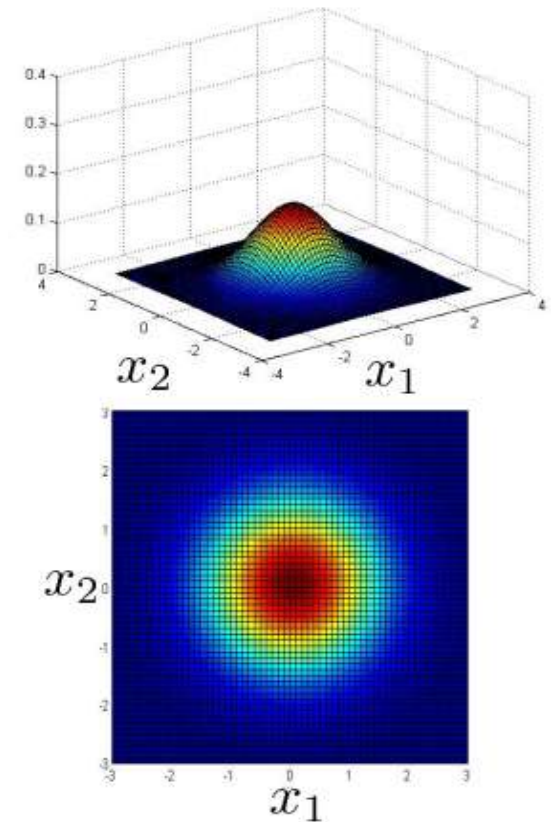
3. Given new example (x_{new}), compute $p(x_{\text{new}})$

$$p(x) = \prod_{j=1}^n p(x_j; \mu_j, \sigma_j^2)$$

4. Anomaly if $p(x_{\text{new}}) < \epsilon$ (some threshold)

x_1, x_2 axis- features

z axis - probability density function $p(x)$



Evaluation of Anomaly Detection System

Let we have some labelled data, of many normal examples and a much less anomalous examples.

Train set (take ONLY normal examples !!!): $\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$

Cross validation (CV) set (normal & anomalous exs.):
 $(x_{cv}^{(1)}, y_{cv}^{(1)}), \dots, (x_{cv}^{(m_{cv})}, y_{cv}^{(m_{cv})})$

Test set (normal & anomalous exs.):
 $(x_{test}^{(1)}, y_{test}^{(1)}), \dots, (x_{test}^{(m_{test})}, y_{test}^{(m_{test})})$

Ex. Manufacturing (e.g. aircraft engine features)

10000 good (normal) engines & 20 anomalous engines

Train set (only good examples): 6000 good engines ($y=0$)

CV set: 2000 good engines ($y=0$), 10 anomalous ($y=1$)

Test set: 2000 good engines ($y=0$), 10 anomalous ($y=1$)

Evaluation of Anomaly Detection System

1) Fit $p(x)$ on train set (ONLY normal examples)

$$\{x^{(1)}, x^{(2)}, \dots, x^{(m)}\}$$

2) Check the performance on cross-validation (CV) set.

From a range of possible values of ϵ , choose the best threshold (ϵ) to optimize some performance metric.

$$p(x_CV) < \epsilon \text{ (anomaly)}$$

$$p(x_CV) > \epsilon \text{ (normal)}$$

$$p(x) = \prod_{j=1}^n p(x_j; \mu_j, \sigma_j^2)$$

Possible performance metrics:

- Precision = $TP / (TP + FP)$
- Recall = $TP / (TP + FN)$
- F1-score = $2(\text{Recall} * \text{Precision}) / (\text{Recall} + \text{Precision})$

Accuracy is not a good perf. measure because data is highly unbalanced (much more normal samples than anomalous).

3) Test the final model on test set.

$$p(x_test) < \epsilon \text{ (anomaly)}$$

$$p(x_test) > \epsilon \text{ (normal)}$$

Anomaly Detection vs. Supervised Learning

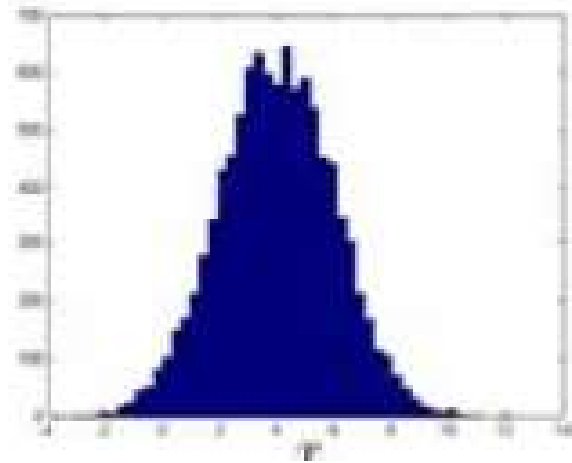
- Very small number of positive (anomalous) examples.
 - Large number of negative (normal) examples.
 - Many different “types” of anomalies. Hard for any algorithm to learn from positive examples what the anomalies look like.
 - Future anomalies may look nothing like any of the anomalous examples seen before.
- Usually large number of both positive and negative examples
 - Enough positive examples for the algorithm to get a sense of what positive examples are like.
 - Future positive examples likely to be similar to ones in training set.

Exs.: fraud detection, monitoring computers in data centers, suspicious computer;

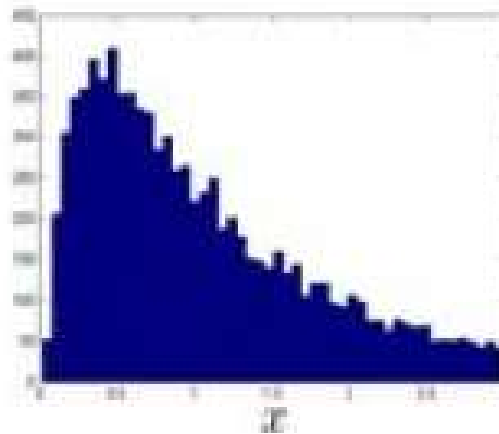
Exs.: Spam/fishing email classification; cancer prediction/classification

Choosing Features

If features have Gaussian distribution =>
apply the anomaly detection algorithm .



If features do not have Gaussian distribution =>
apply some transformation of data to get close to Gaussian curve.

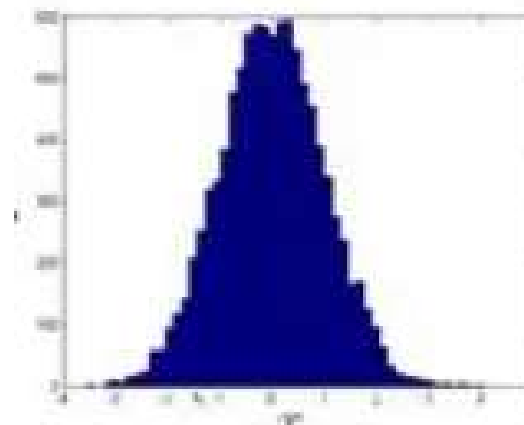
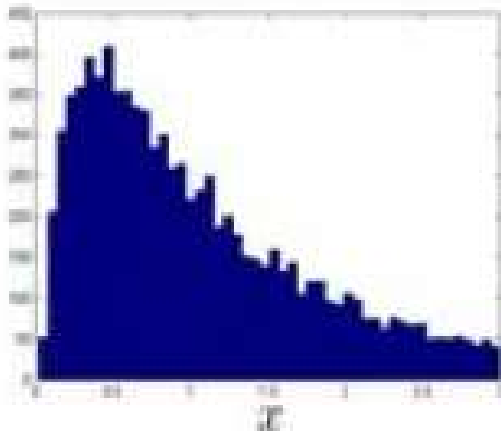


Choosing Features

Popular feature transformations =>

- $\log(x)$
- $\log(x + c)$
- \sqrt{x}

for example: $x \Rightarrow \log(x) \Rightarrow$ much more Gaussian curve



Error Analysis for Anomaly Detection

Want: $p(x)$ large for normal examples x ;
 $p(x)$ small for anomalous examples x .

Most common problem:

$p(x)$ is comparable (say both large) for normal and anomalous examples.

Solution: Make error analysis to create new features

Look at the anomalies the algorithm did not flag correctly (the mistakes) and try to create some new feature that may take unusually different (large or small) values in the event of anomaly and thus distinguish the abnormal ex.

Ex. Monitoring computers in data center

x_1 =memory use of computer

x_2 =number of disc accesses /sec

x_3 =CPU load

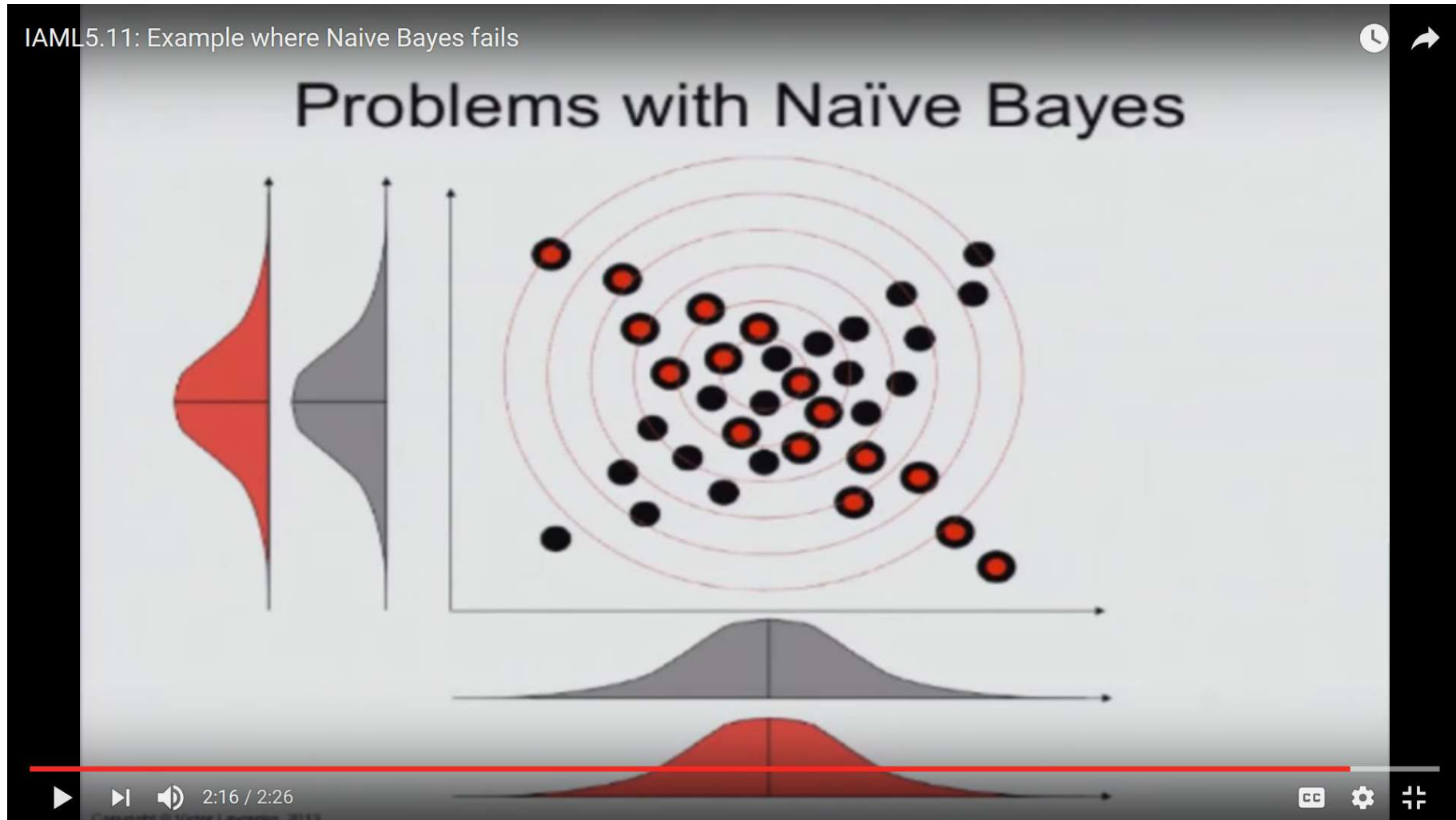
x_4 =network traffic

Feature engineering (new features, e.g. to detect when comp. is stuck in infinite loop)

x_5 =CPU load / network traffic

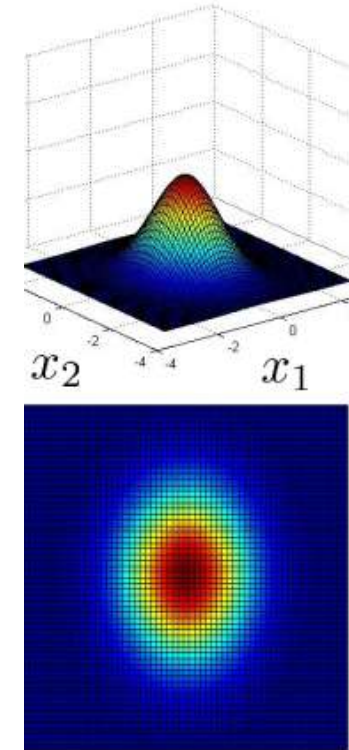
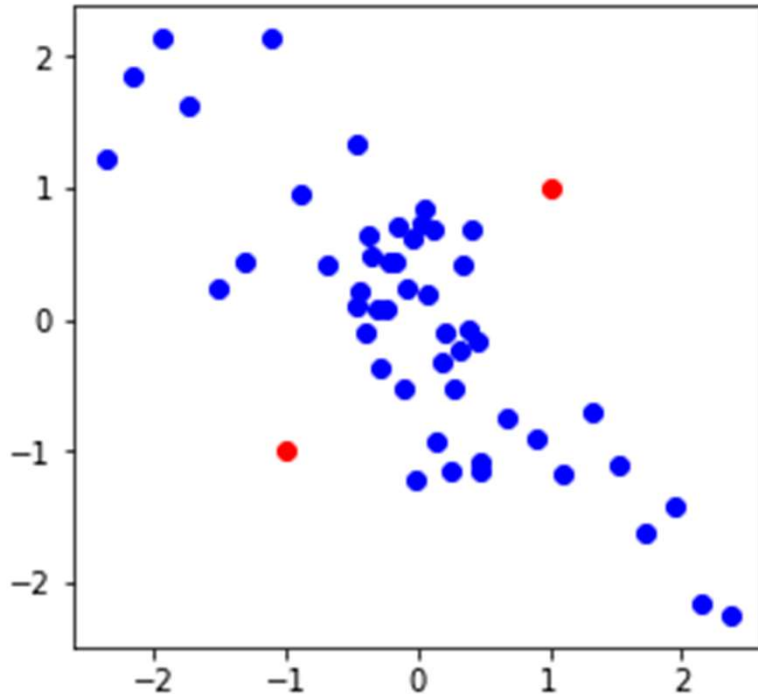
x_6 = (CPU load)² / network traffic

Naïve Bayes will not be able to separate the red from the black points, why ?



Multivariate Gaussian Distribution

$$p(\mathbf{x}) = \prod_{j=1}^n p(x_j; \mu_j, \sigma_j^2)$$



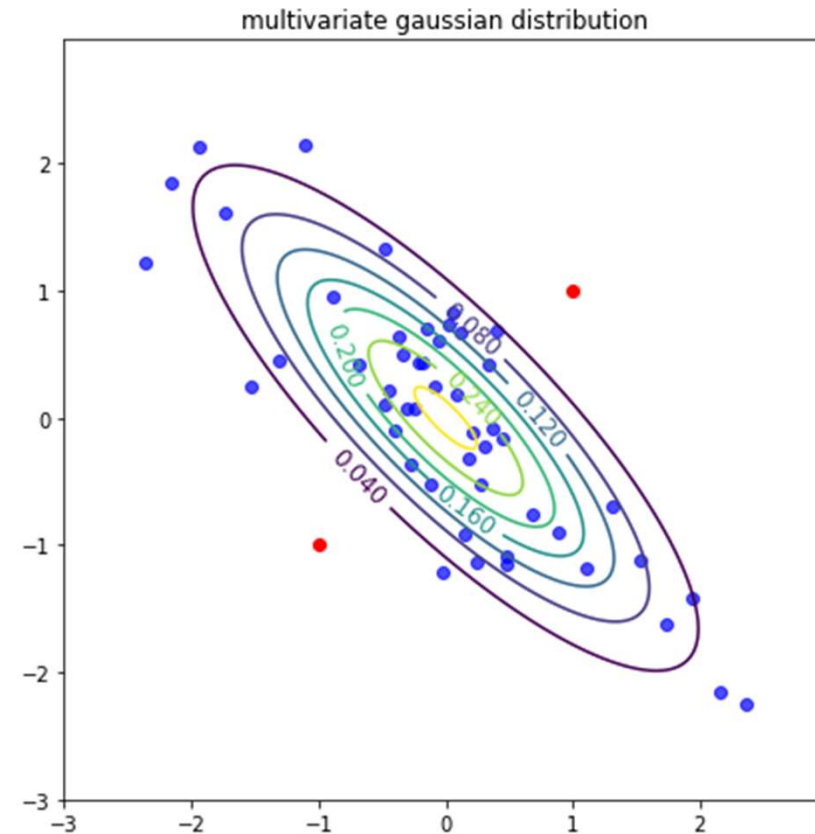
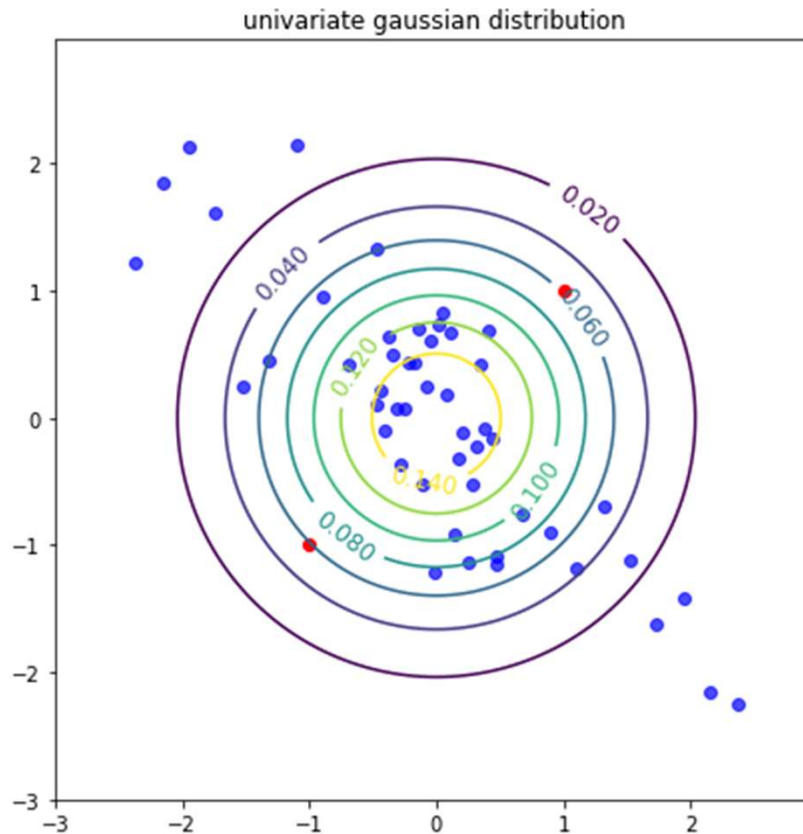
If we use univariate Gaussian distribution for this data, the contour plots (curves with the same probability value) will be circles (if both variances are the same) or axes aligned elipces (if the variances are different) . The red points will have relatively high probability => not flaged as outliers.

But features x_1 and x_2 are negatively correlated (one increases, the other decreases). The assumption of independance is violated.

Red points are outliers.

Univariate vs. Multivariate Gaussian Distribution

$$p(x) = \prod_{j=1}^n p(x_j; \mu_j, \sigma_j^2)$$



Univariate Gaussian distribution considers separate probability models for each $p(x_1)$, $p(x_2)$ => it will not flag the red points as outliers.

Better use Multivariate Gaussian distribution.

Multivariate density estimation

Given training data, estimate μ ($n \times 1$ vector) and Σ (**$n \times n$ covariance matrix**):

$$\mu = \frac{1}{m} \sum_{i=1}^m x^{(i)}$$

$$\Sigma = \frac{1}{m} \sum_{i=1}^m (x^{(i)} - \mu)(x^{(i)} - \mu)^T$$

For a new example x , compute:

$$p(x; \mu, \Sigma) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp \left(-\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right)$$

Flag as anomaly if $p(x) < \epsilon$.

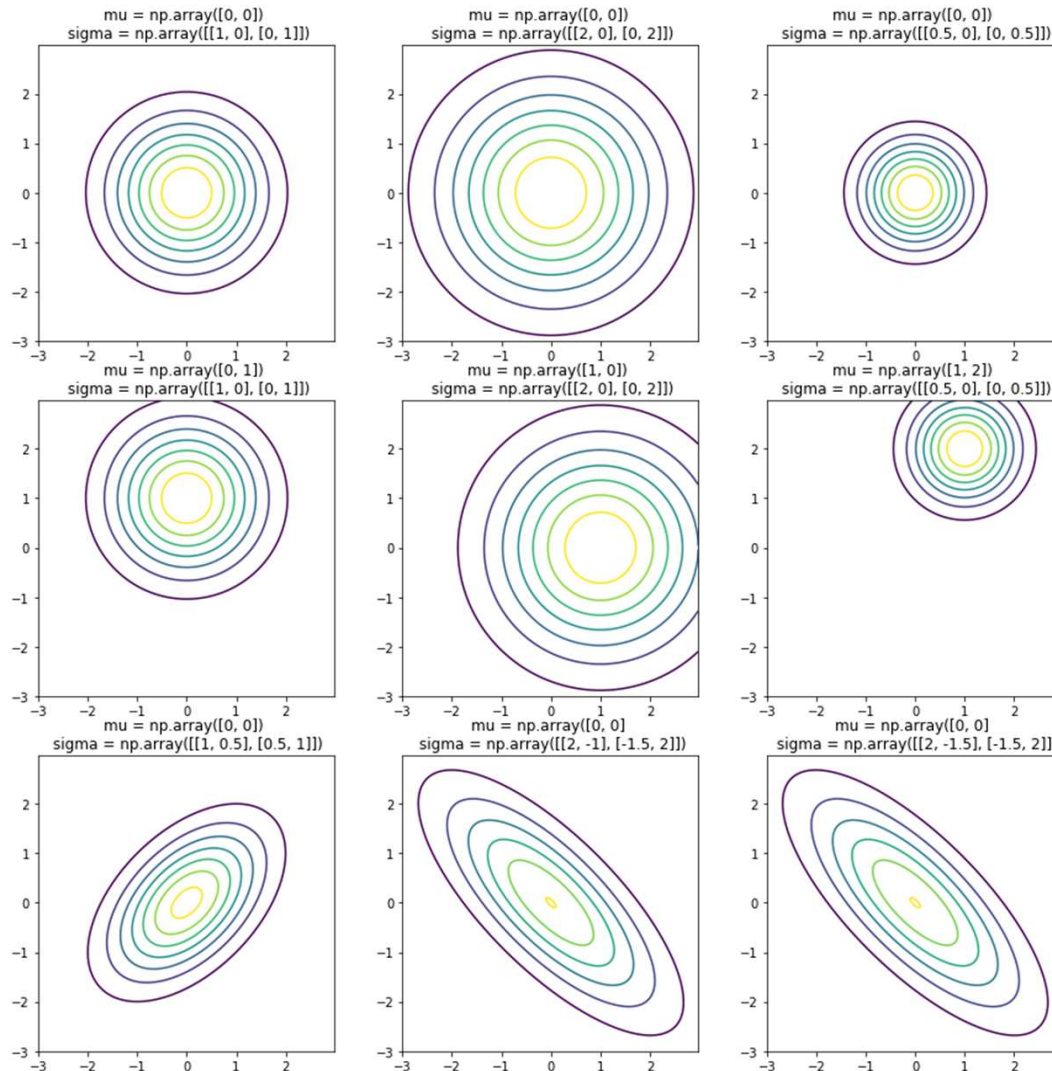
Σ – $n \times n$ covariance matrix

$|\Sigma|$ – determinant of matrix Σ .

Σ – symmetric about the main diagonal.

Σ - major difference between univariate and multivariate Gaussian !!!

Effect of Mean and Covariance Matrix Shifting



μ shifts the center of the distribution.

Diagonal elements of Σ vary the spread of the distribution along the corresponding features

Off-diagonal elements of Σ show the correlation among the features:

Positive off-diagonal values of Σ
=> positive correlation

Negative off-diagonal values of Σ
=> negative correlation

Univariate Gaussian distribution is a special case when off-diagonal values of Σ are 0.

Original vs. Multivariate Gaussian models for Anomaly detection

Multivariate Gaussian

Gaussian model with independent features

$$\mu = \frac{1}{m} \sum_{i=1}^m x^{(i)}$$

$$\sigma^2 = \frac{1}{m} \sum_{i=1}^m (x^{(i)} - \mu)^2$$

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

$$p(x) = p(x_1; \mu_1, \sigma_1^2) p(x_2; \mu_2, \sigma_2^2) \cdots p(x_n; \mu_n, \sigma_n^2)$$

Manually create features to capture anomalies
(e.g. x_{new} =CPU load / network traffic)

Computationally cheaper, scales better to large number of features (n)

OK even if the training set size (m) is small

$$\mu = \frac{1}{m} \sum_{i=1}^m x^{(i)}$$

$$\Sigma = \frac{1}{m} \sum_{i=1}^m (x^{(i)} - \mu)(x^{(i)} - \mu)^T$$

$$p(x; \mu, \Sigma) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(x - \mu)^T \Sigma^{-1} (x - \mu)\right)$$

Automatically captures correlations between features

Computationally more expensive, takes time to compute inverse of Σ if number of features (n) is large

Must have training set size (m) \gg number of features (n), otherwise Σ is singular and not invertible.

In practice $m > 10 \cdot n$

Distribution Types

