Machine Learning using Matlab

Lecture 11 PCA and anomaly detection

Outline

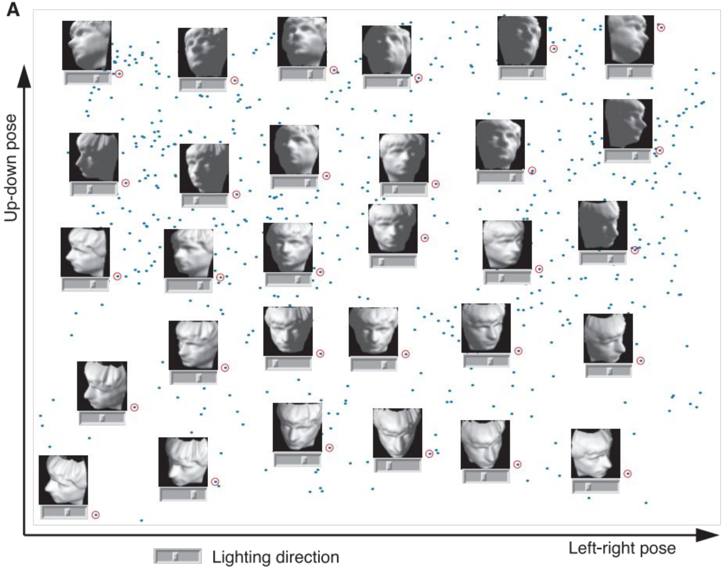
- Dimensionality reduction
- Principal Component Analysis (PCA)
- Anomaly detection
    - Univariate Gaussian distribution
    - Multivariate Gaussian distribution
    - Gaussian mixture model (GMM)
    - One-class Support Vector Machine

Curse of dimensionality

- Data become sparse with increase of dimensionality
- Redundant features, more noise
- Hard to interpret and visualize
- Hard to store and process data (computationally challenging)

Dimensionality reduction

Given a set of $\{x^{(1)}, x^{(2)}, \ldots, x^{(m)}\}$ with n features (m << n) , dimensionality reduction aims to find a set of $\{y^{(1)}, y^{(2)}, \ldots, y^{(m)}\}$ with k features, where k << n, and preserve some properties of the original data set, such as variance, distance, etc



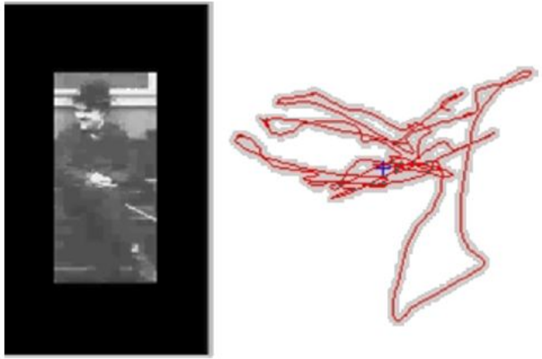


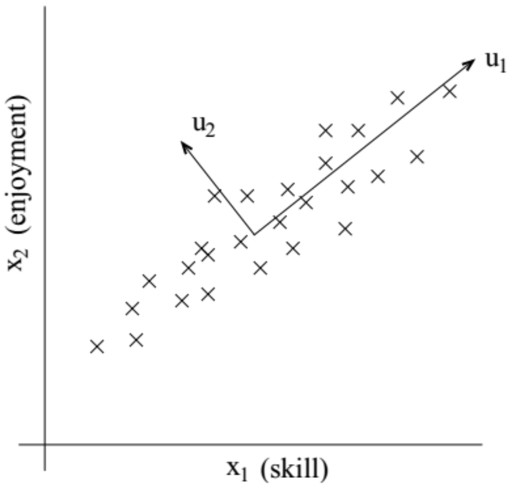
Figure 1: A frame from a short video clip of Charlie Chaplin in a skit where his hat lifts from his head three times, and he fixes it once. This paper considers the problem of creating "video trajectories" — a representation of changes in a video sequence, based upon the non-linear dimensionality reduction technique called Isomap.

Dimensionality reduction

- Dimensionality reduction can be applied:
  - Compression
  - Visulization
  - Face detection
  - ...
- Dimensionality reduction algorithms can be divided into:
  - Linear: PCA, Locality Preserving Projections (LPP), …
  - Non-linear: Isometric feature mapping (Isomap), Laplacian Eigenmaps (LE), ...

PCA - intuition

- Consider a dataset from a survey of pilots for radio-controlled helicopters, where x_1 is the pilot skill, and x_2 captures how much he/she enjoys flying
- The two attributes are strongly correlated, i.e., truly enjoy flying become good pilots
- We try to find some diagonal axis capturing the intrinsic piloting “karma” of a person, with only a small amount of noise lying off this axis



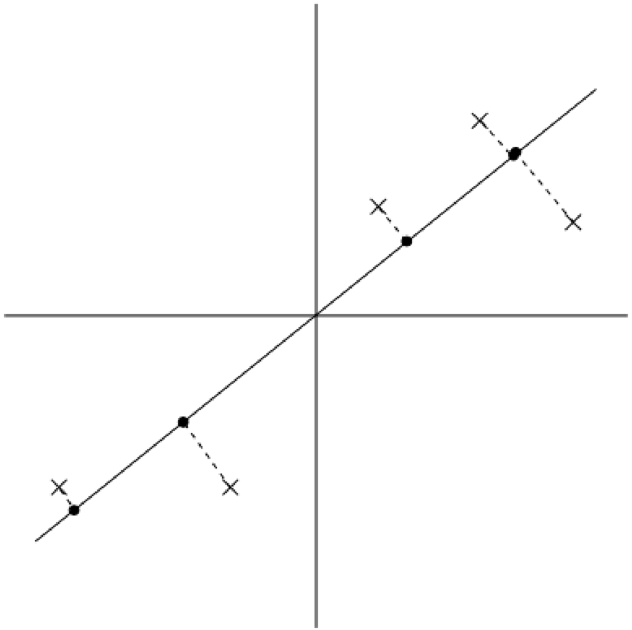
PCA

- Objective: to reduce from n-dimension to k-dimension, PCA aims to find k unit vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error
- Minimize the projection error is equivalent to maximize the variance of the projected data
- Note the difference between PCA and linear regression

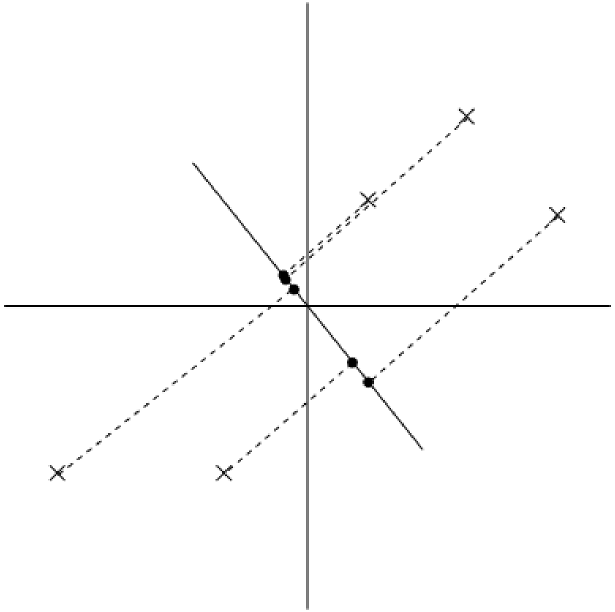
Data preprocessing

- Normalize mean and variance
  1. Let
  $$\mu = \frac{1}{m} \sum_{i=1}^{m} x^{(i)}$$
  2. Replace each $x^{(i)}$ with $x^{(i)} - \mu$
  3. Let
  $$\sigma_j^2 = \frac{1}{m} \sum_{i} (x_j^{(i)})^2$$
  4. Replace each $x_j^{(i)}$ with $x_j^{(i)} / \sigma_j$
- Step 3 and 4 may be omitted if we have apriori knowledge that the different attributes are all on the same scale

Q: which projection is better?



Large variance, small projection error



Small variance, large projection error

PCA

- Optimization objective:

$$\max_u \frac{1}{m}\sum_{i=1}^{m}((x^{(i)})^T u)^2 \quad \Rightarrow \quad \max_u u^T\Bigg(\underbrace{\frac{1}{m}\sum_{i=1}^{m}x^{(i)}(x^{(i)})^T}_{\Sigma}\Bigg)u$$

$$\text{s.t. } ||u||=1 \qquad\qquad \text{s.t. } ||u||=1$$

- Using Lagrange multiplier λ, one may solve the following eigenvalue problem:

$$\Sigma u=\lambda u$$

- Extend the first principal component to k principal components:

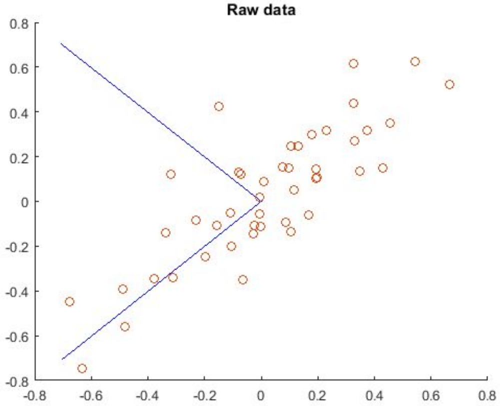
$$\Sigma U=\lambda U$$

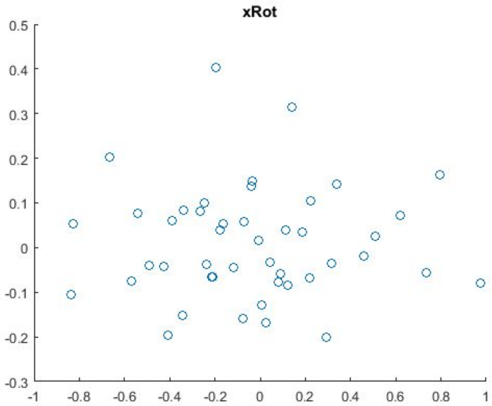
PCA

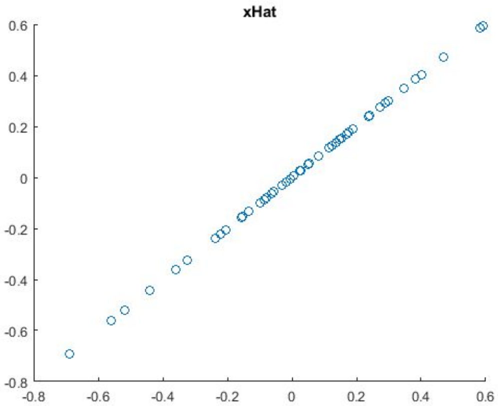
- Algorithm:
  - Preprocess data, i.e., zero mean and scale variance if need
  - Compute the covariance matrix of normalized data
  - Compute the eigenvectors and eigenvalues of the covariance matrix
  - The first top k eigenvectors correspond to the first k principal components
  - Project the data into the k-dimensional subspace
- Matlab implementation:
  - m = size(x,2); mu = mean(x,2); x = x - repmat(mu,1,m);
  - Sigma = x * x' / size(x, 2);
  - [U,S,V] = svd(Sigma);
  - Ureduce = U(:,1:k); y = Ureduce’*x;

Reconstruction from compressed representation

- $x^{(i)}_{approx} = UU^T x^{(i)}$
- xHat = u(:,1:k)*u(:,1:k)' * x;







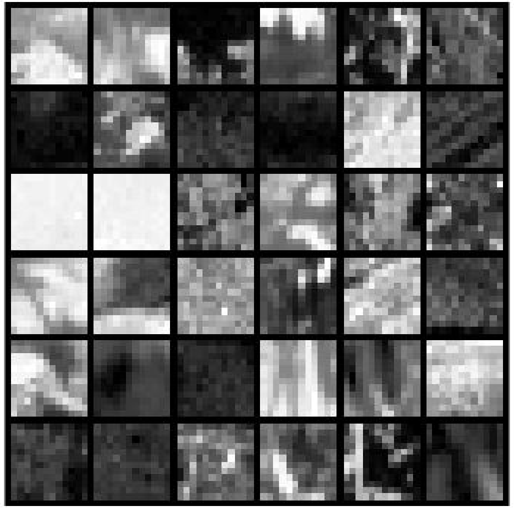
k = 1

Number of components k to retain

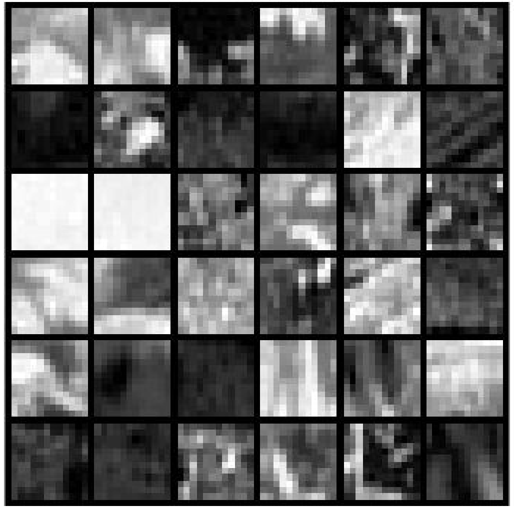
- If k is too large, we won’t be compressing the data much
- if k is too small, we may lose too much information
- To decide how to set k, we will look at the ”‘percentage of variance retained”’ for different values of k.
- Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of covariance matrix (sorted in descending order), if we retain k principal components, the percentage of variance retained is given by:

$$\frac{\sum_{j=1}^{k} \lambda_j}{\sum_{i=1}^{n} \lambda_i} \geq \delta$$

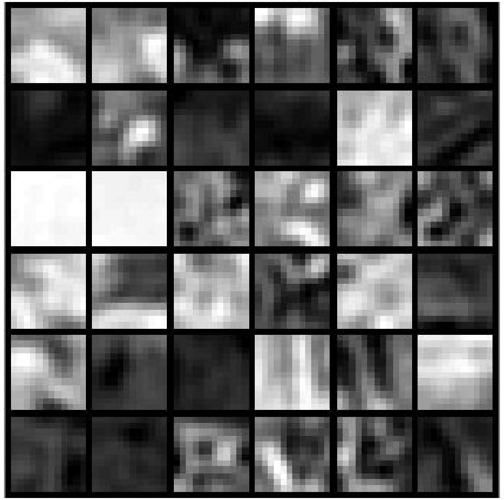
Number of components k to retain



PCA processed images (88 / 144 dimensions) 0.99



PCA processed images (31 / 144 dimensions) 0.95



PCA summary

- Visualization (k = 2 or 3)
- Compression (k is obtained by computing the percentage of variance retained)
  - Reduce memory/disk needed to store data
  - Reduce correlation between features
  - Speed up learning algorithm
- Noise reduction - eigenface [Turk 1991]
- Suggestion: before implementing PCA, first try running whatever you want to do with the original/raw data. Only if that doesn't do what you want, then implement PCA and consider using the projected data

Anomaly detection

- **Anomalies** and **outliers** are essentially the same thing: objects that are different from most other objects
- **Anomaly detection** refers to the problem of finding patterns in data that do not conform to expected behavior. [Chandola 2009]
- Historically, the field of statistics tried to find and remove outliers as a way to improve analyses.
- There are now many fields where the outliers/anomalies are the objects of greatest interest.

Causes of anomalies

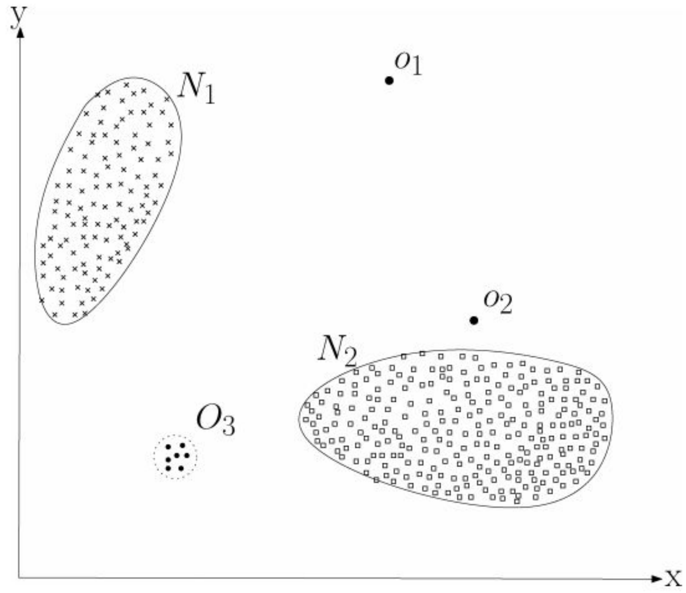
- Data from different class of object or underlying mechanism
  - disease vs. non-disease
  - fraud vs. non-fraud
- Natural variation
  - tails on a Gaussian distribution
- Data measurement and collection errors

Structure of anomalies

- Point anomalies
- Contextual anomalies
- Collective anomalies

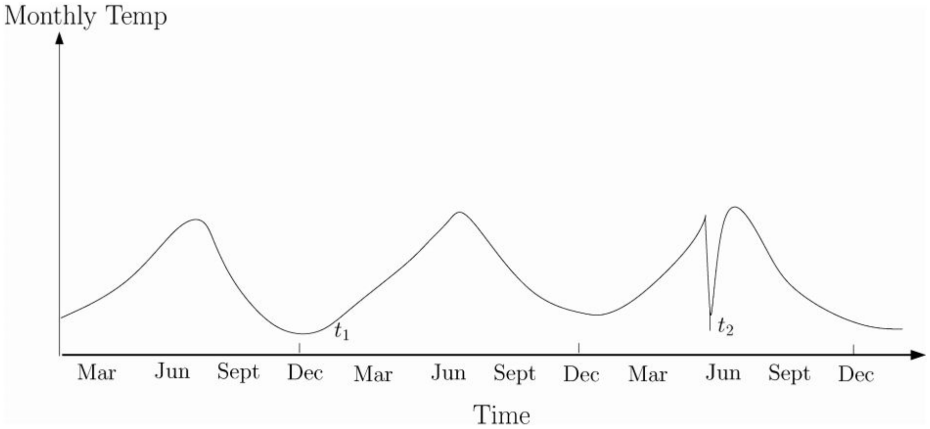
Points anomalies

- An individual data instance is anomalous with respect to the data



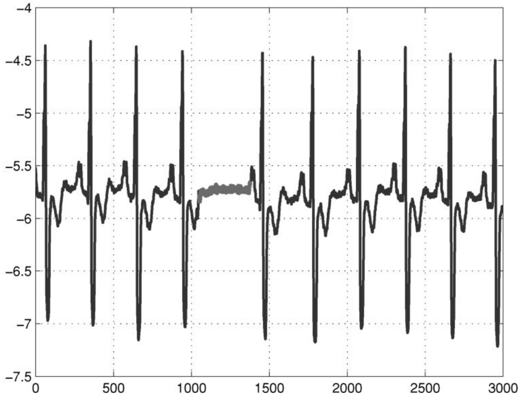
Contextual anomalies

- An individual data instance is anomalous within a context
- Requires a notion of context
- Also called “conditional anomalies”



Collective anomalies

- A collection of related data instances is anomalous
- Requires a relationship among data instances
  - Sequential data
  - Spatial data
  - Graph data
- The individual instances within a collective anomaly are not anomalous by themselves



Applications of anomaly detection

- Network intrusion
- Insurance/credit card fraud
- Healthcare informatics/medical diagnostics
- Image processing/video surveillance
- …

Fraud detection

- Detection of criminal activities occurring in commercial organizations.
- Malicious users might be:
  - Employees
  - Actual customers
  - Someone posing as a customer (identity theft)
- Types of fraud
  - Credit card fraud
  - Insurance claim fraud
  - Mobile/cell phone fraud
- Challenges
  - Fast and accurate real-time detection
  - Misclassification cost is very high

Healthcare informatics

- Detect anomalous patient records
  - Indicate disease outbreaks, instrumentation errors, etc.
- Key challenges
  - Only normal labels available
  - Misclassification cost is very high
  - Data can be complex: spatio-temporal

Image processing

- Detecting outliers in a image monitored over time
- Detecting anomalous regions within an image
- Used in
  - video surveillance
  - satellite image analysis
- Key Challenges
  - Detecting collective anomalies
  - Data sets are very large
  - Adaptive to concept drift and real-time detection

Use of data labels in anomaly detection

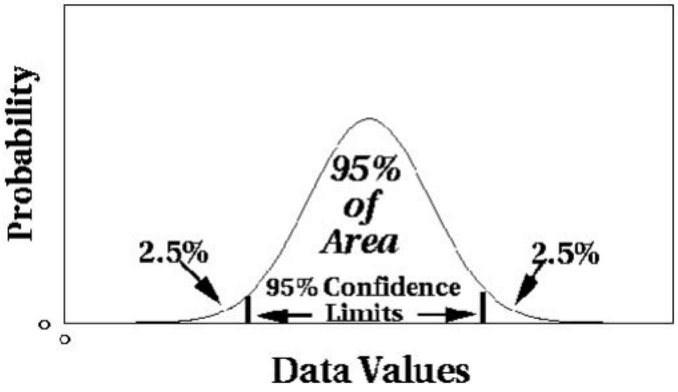
- Supervised anomaly detection
  - Labels available for both normal data and anomalies
  - Similar to classification with high class imbalance
- Semi-supervised anomaly detection
  - Labels available only for normal data
- Unsupervised anomaly detection (Common in application)
  - No labels assumed
  - Based on the assumption that anomalies are very rare compared to normal data

Unsupervised anomaly detection

- No labels available
- Based on assumption that anomalies are very rare compared to “normal” data
- General steps
  - Build a profile of “normal” behavior
    - summary statistics for overall population
    - model of multivariate data distribution
  - Use the “normal” profile to detect anomalies
    - anomalies are observations whose characteristics differ significantly from the normal profile

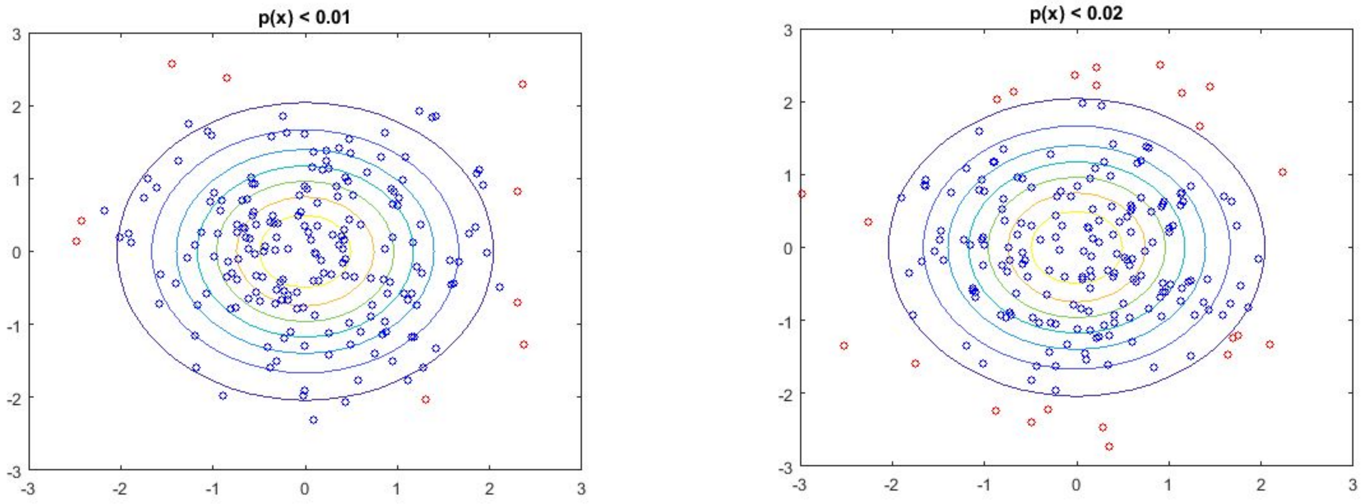
Univariate Gaussian distribution

- Anomalies are defined by z-score > threshold



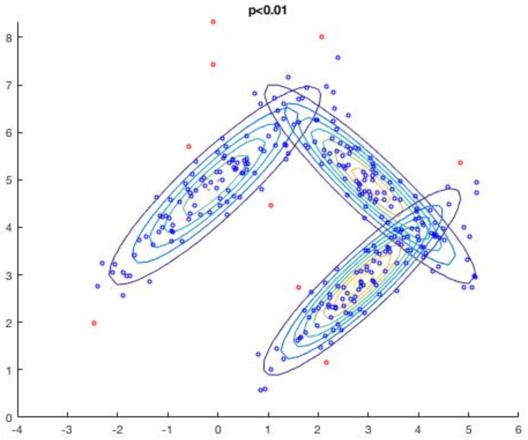
Multivariate Gaussian distribution

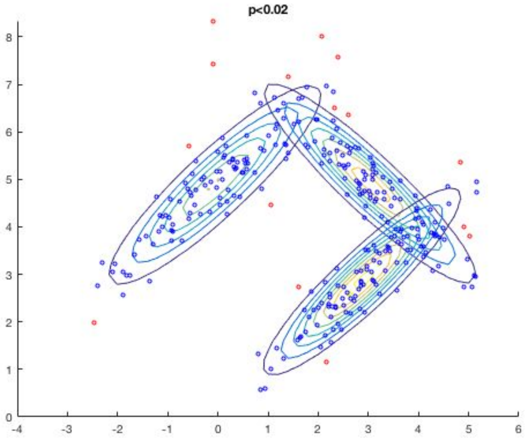
- If the distribution is well defined by multivariate Gaussian distribution
- Outliers are defined by probability < threshold or Mahalanobis distance > threshold



GMM

- Select number of Gaussian models k, run the GMM algorithm to obtain the optimal parameters
- For a new data, if its probability for each Gaussian model is less than a threshold, it is detected as an anomaly





Statistical anomaly detection

- Pros
  - Statistical tests are well-understood and well-validated.
  - Quantitative measure of degree to which object is an outlier.
- Cons
  - Data may be hard to model parametrically.
    - multiple modes
    - variable density
  - In high dimensions, data may be insufficient to estimate true distribution.

One-Class Support Vector Machine (OCSVM)

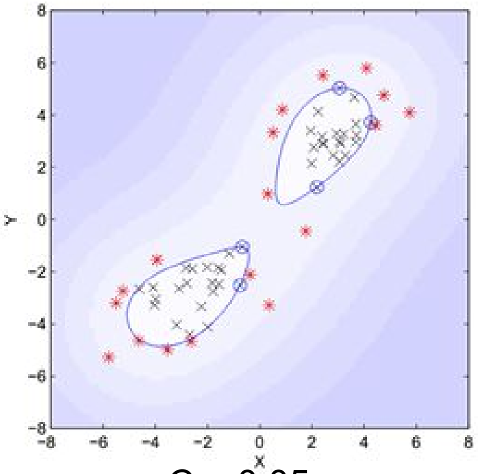
- Given a set of unlabelled train data $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$, OCSVM [Scholkopf 2001] aims to find an optimal separating function $f(x) = w \cdot \Phi(x) - \rho$ to contain most of the training data in a compact region.
- To obtain the optimal parameter w and ρ, one can solve the following quadratic programming problem:

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

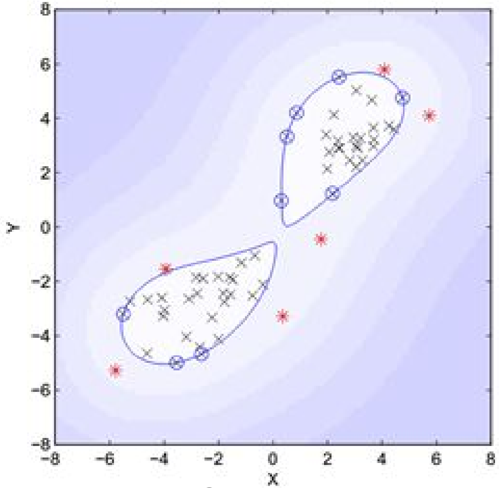
$$\text{s.t. } \; w \cdot \Phi(x^{(i)}) \geq \rho - \xi_i, \;\; \xi_i \geq 0$$

- OCSVM is similar to SVM, so most SVM optimization can be applied to it straightforwardly.

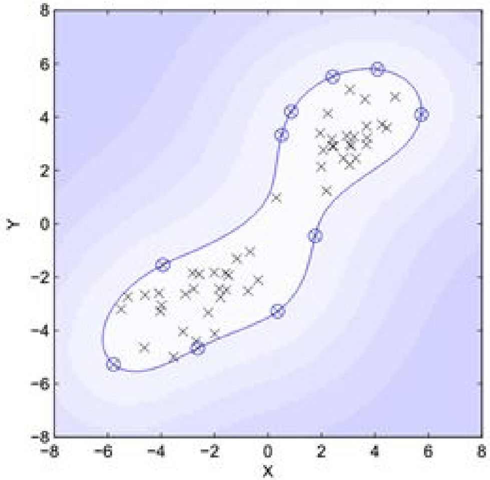
OCSVM example



C = 0.05



C = 0.1



C = 0.4

OCSVM anomaly detection

- Pros:
  - Non-linear by kernel method
  - Quantitative measure of degree to which object is an outlier
- Cons:
  - Time consuming when training set is quite large
  - Must choose parameters, C and sigma

Evaluating an anomaly detection system

- Aircraft engines motivating example: 10,000 good (normal) engines, 20 flawed engines (anomalous)
  - Training set: 6,000 good engines (y=0)
  - Validation set: 2000 good engines (y=0), 10 anomalous (y=1)
  - Test set: 2000 good engines (y=0), 10 anomalous (y=1)
- Possible evaluation metrics to choose threshold:
  - True positive, false positive, false negative, true negative
  - Precision/Recall
  - F1-measure

Anomaly detection vs. supervised learning

- Very small number of positive examples (y=1)
- Large number of negative examples
- Many different “types” of anomalies. Hard for any examples what the anomalies look like
- Future anomalies may look nothing like any of the anomalous

- Large number of positive and negative examples
- Enough positive examples for algorithm to get a sense of what positive examples are like, future positive examples are likely to be similar to ones in training set