Machine Learning

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Chapter 06: Dimensionality Reduction

(and Anomaly Detection)

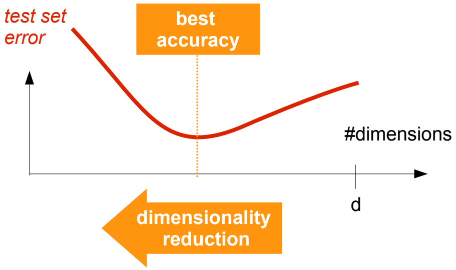
Prof. Adrian Ulges
Masters "Computer Science"
DCSM Department
University of Applied Sciences RheinMain

Outline

Dimensionality Reduction: Motivation

The Challenge

- **Reminder**: In machine learning, we are usually given **d-dimensional** samples $\mathbf{x}_1, ..., \mathbf{x}_n \in \mathbb{R}^d$
- The number of features d can be high!



- **Goal: Reduce d** while preserving (or even improving) discriminativity

Why?

- **Efficiency**: faster training, faster application, less storage
- Avoid **overfitting**: overcoming the curse of dimensionality
- Better **interpretability** (and maybe visualization) of data

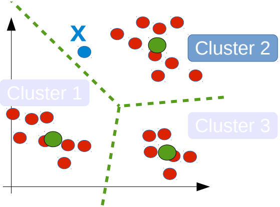
Dimensionality Reduction: Overview

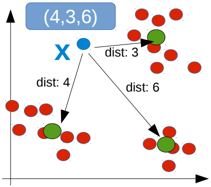
Approaches

- **feature selection**
- **feature derivation**, typically, by applying transformations

Example: K-Means for Feature Derivation

- **Approach**: map samples $\mathbf{x}$ to clusters *(vector quantization)*
- **Alternative 1**: store only the cluster number *(1 dimension!)*
- **Alternative 2**: store the distances to all centers *(K dimensions) (see* `sklearn` $>$ `KMeans` $>$ `transform()`*)*





Outline

Feature Selection: Strategies

- **Goal**: Find a **subset of features** $\mathcal{F} \subseteq \{1, ..., d\}$ for which we can solve our machine learning problem 'best' *(for example: minimizing classification error)*
- This is a **search problem** *(brute-force effort: $O(2^d)$)*
- There are **three common approaches**: **wrappers**, **filters**, and **embedded methods**

1. Wrappers

- Wrappers use an explicit evaluation of feature subsets *(training and validating classifiers)*
- Search can be done in a **greedy** fashion (adding or removing the 'best' features to the feature set), or by **backtracking**
- Benefit: It takes the **underlying classifier** into account!
- Usually the most reliable way, but very slow

Feature Selection: Strategies

2. Filters

- Assess feature quality by a **proxy measure**
  - example: *mutual information* between feature X and class labels C

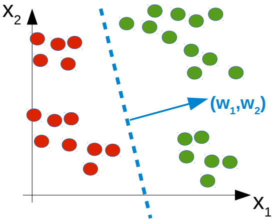
$$I(X, C) = \sum_{x \in X} \sum_{c \in C} p(x, c) \cdot \log_2 \left(\frac{P(x, c)}{P(x) \cdot P(c)} \right)$$

- **Search strategy**: rank features by their quality, pick the K top ones *(K determined via cross-validation)*
- Filters are cheaper than wrappers, but not as accurate

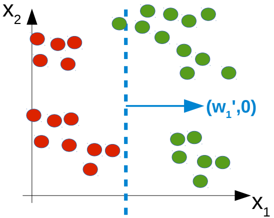
Feature Selection: Strategies

3. Embedded Methods

- ... treat feature selection as a part of **model construction** (i.e., we find classifier and features in the *same process*)
- Optimization is driven towards models with **few features**
- **Example**: logistic regression with **regularization**
  - the classifier penalizes feature weights, shrinking them to zero
  - features with weight zero are “filtered”!



no L_1-Regularization



with L_1-Regularization (feature x_2 has weight 0)

Outline

Principal Component Analysis (PCA)

Idea (unsupervised!)

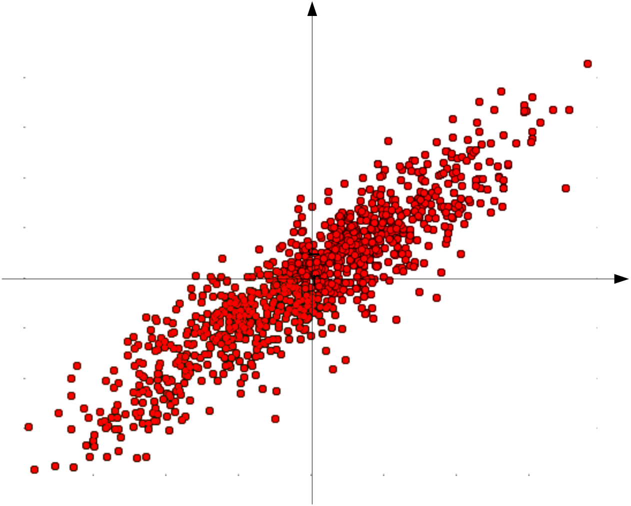
- The dataset exhibits a large stretch along some directions. These are the *important* directions.
- Along other directions, there is only little variation. These directions are merely *noise* and can be discarded.
- PCA is about finding the *important* directions *(or* **principal components***)* of the data

Principal Components: Formalization

- In the following, we assume our data points to be centered around the origin (otherwise, we simply shift the data beforehand)
- What is the *most important direction*? What is the *second most important* direction, etc.?

PCA: Illustration

What are the Principal Components here?



Principal Components: Derivation

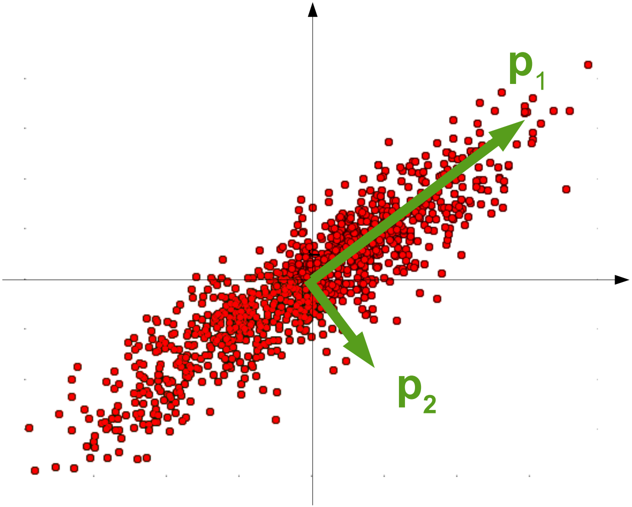
Obviously, the principal components seem to be related to the data's **covariance matrix**. Let's find out how[1]

[1] cmp. Marsland, page 228f

Principal Components: Derivation

Principal Components: Derivation

Principal Components: Illustration



PCA: Training

```
function PCA_TRAIN(x_1, ..., x_n, K)  // given: samples x_1, ..., x_n ∈ R^d
    μ := 1/n Σ_i x_i
    for i = 1, ..., n:
        x_i := x_i − μ               // shift the samples to mean zero
    stack the samples into an n × d data matrix X
    Σ := 1/n (X^T · X)               // covariance matrix
    compute Σ's eigenvalues λ_1, ..., λ_d and eigenvectors p_1, ..., p_d
     (sorted in descending order of the eigenvalues)
    stack p_1, ..., p_K as rows into a K × d-Matrix P_K
    return P_K, μ
```

Remarks

- **Training**: Compute the top K eigenvectors of the data's covariance matrix
- **Application**: reduces the samples from d to K dimensions

```
function PCA_APPLY(x)                // given: a new sample x
    return P_K · (x − μ)             // dimension of return value: K
```

PCA: Remarks

- Heuristic for choosing K: Preserve α (e.g., 90%) of the eigenvector's total energy

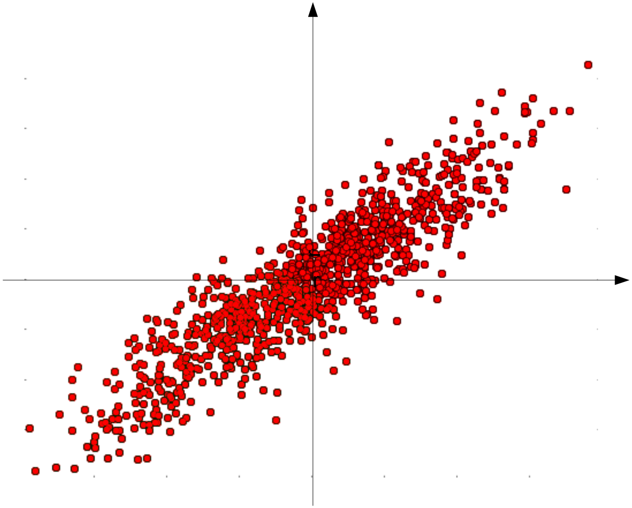
$$K := \min_{K \in \{1,...,d\}} \text{ such that } \sum_{k=1}^{K} \lambda_k \geq \alpha \cdot \sum_{k=1}^{d} \lambda_k$$

- Given a reduced K-dimensional feature $\mathbf{y} = (y_1, ..., y_K)$, we can reconstruct $\mathbf{x}$ (to some extent) from $\mathbf{x}'$:

$$\mathbf{x}' = \mu + y_1 \cdot \mathbf{p}_1 + y_2 \cdot \mathbf{p}_2 + ... + y_K \cdot \mathbf{p}_K$$

- We call $||\mathbf{x} - \mathbf{x}'||$ the **reconstruction error**.

PCA: Illustration



From PCA to Whitening

We learned above: Given a feature vector $\mathbf{x}$ (and the $d \times d$ matrix P with Σ's eigenvectors as rows), by applying the transformation $P \cdot \mathbf{x}$, the **covariance matrix** of the data becomes

$$\begin{pmatrix} \lambda_1 & 0 & & ... & 0 \\ 0 & \lambda_2 & 0 & ... & 0 \\ ... & ... & ... & ... & ... \\ 0 & ... & ... & 0 & \lambda_d \end{pmatrix}$$

Each value λ_i is a variance within one dimension. We turn these variances into 1, simply by dividing by the standard deviation $\sqrt{\lambda_i}$. This leads to the **whitening** transform *(see Chapter 'Features')*:

$$Diag(\frac{1}{\sqrt{\lambda_1}}, \frac{1}{\sqrt{\lambda_2}}, ..., \frac{1}{\sqrt{\lambda_d}}) \cdot P \cdot \mathbf{x}.$$

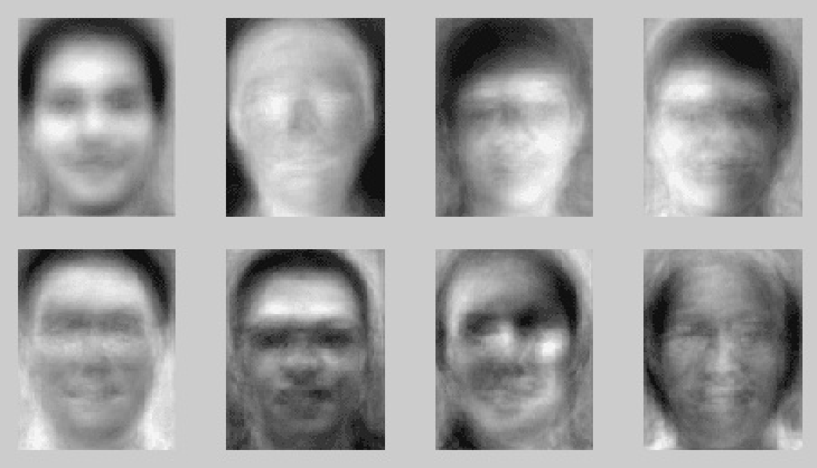
Applying this transformation turns the data's covariance matrix into the identity I and decorrelates the features.

Outline

Example: Applying PCA to Images

- We can apply PCA to **images**, simply by scaling images to a standard resolution (say, $N \times M$) and stacking all pixel values into sample vectors of dimension $d = N \times M$
- Note: The principal components are $(N \cdot M)$-dimensional, too! (i.e., we can *visualize them as images*)
- Example: PCA for **face recognition** → "eigenfaces" *(apply PCA to lots of face images)*

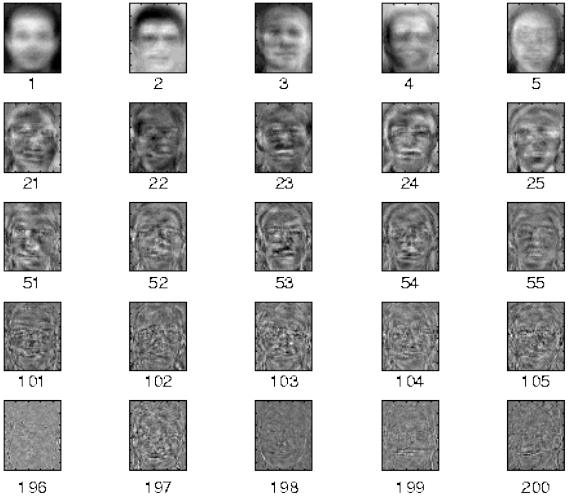
Example: Applying PCA to Images



Mean face (top left) and the first 7 principal components (=eigenfaces)

Example: Applying PCA to Images

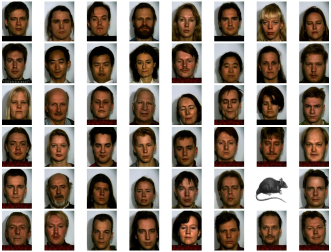
Some eigenfaces from a different face dataset



Example: Applying PCA to Images

Reconstruction of a face using $0, 8, 16, \ldots$ eigenfaces

Example: Applying PCA to Images



- Which of these images does not show a human face?
- Approach: Compare the **original image** with its **PCA reconstruction**

faces are <u>well</u> reconstructed

non-faces are <u>poorly</u> reconstructed

Eigenfaces: Discussion

The Eigenfaces approach for **face detection** is **simple and powerful**, but it has some shortcomings:

- The results depend strongly on *illumination*, *shadows*, and *local changes*, e.g. glasses or beards
  - include those effects in the training set
  - learn smaller components (eye, mouth, ...)
  - (illumination): normalize all images
- Only faces of *fixed size* are detected
  - create scaled versions of the input image before searching
- Already small *rotations* of the head change the result
  - include rotated faces into the training set.
  - try to make the image upright before the applying PCA

Since eigenfaces [8], there have been at least two generations of more elaborate face detection methods [9, 7].

PCA: Discussion

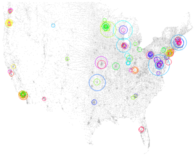
Outline

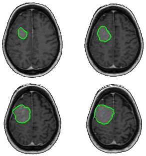
Anomaly Detection: Mission Statement images from [1] [3] [2]

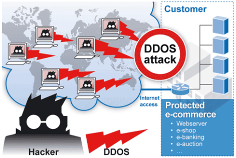
Goal: identify samples that do not conform to an expected pattern, or to other samples in the dataset [6].

Applications

- credit card fraud detection
- detecting tumours in imagery
- detecting technical failures
- finding errors in text
- network intrusion detection

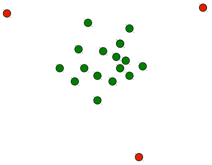




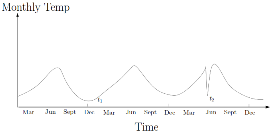


Anomaly Detection: Types of Anomalies image from [6]

1. **point anomalies**: individual samples that are unusual (typically, in high distance) to the flock



2. **contextual anomalies**: Samples are described by contextual features (e.g., location) and behavioral features (e.g., the temperature). An anomaly occurs if the behavioral features are unusual *given the contextual ones* (e.g., the temperature is unusually high *given the location*).



3. **collective anomalies**: a **combination** of samples that is unusual (whilst the individual samples are not necessarily). **Example**: ... `http-web smtp-mail buffer-overflow ssh ftp` ...

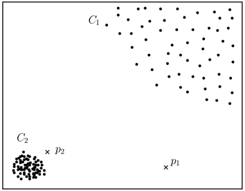
Our focus here will be on **point anomalies**.

Anomaly Detection: Characteristics

Learning Setups

- Usually, there are two labels: *normal* vs. *abnormal*
- Labeled training data can be really difficult to find!
- **supervised** techniques: Training data from both classes given *(but often highly imbalanced)*
- **semi-supervised** techniques: Training data only for the *normal* class
- **unsupervised** techniques: training data without labels *(there may be anomalies, but we do not know when/where)*

Absolute Distance as an Anomaly Criterion? image from [6]



Anomaly Detection: Methods

There is a plethora of anomaly detection methods [6]

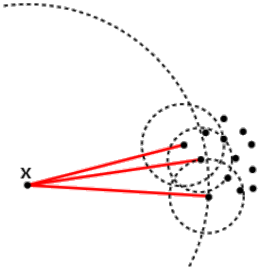
- ... some using regular classifiers
- ... some using density-based modeling
- ... some using rule mining
- ...

We will only look at two of the most prominent ones:

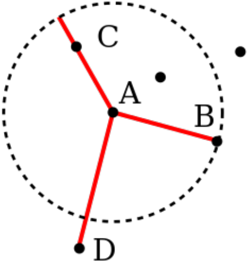
- a density-based method ("local outlier factor")
- a classification-based method ("one-class SVMs") $\rightarrow$ later

Local Outlier Factor (LOF) [5] image from [4])

- **Idea**: A sample $\mathbf{x}$ is a point anomaly if the point density in its surrounding is lower than in its nearest neighbors' surroundings.
- **Anomaly Measure**: Measure the distance to $\mathbf{x}$'s neighbors, measure the same distance for each neighbor, and compare.

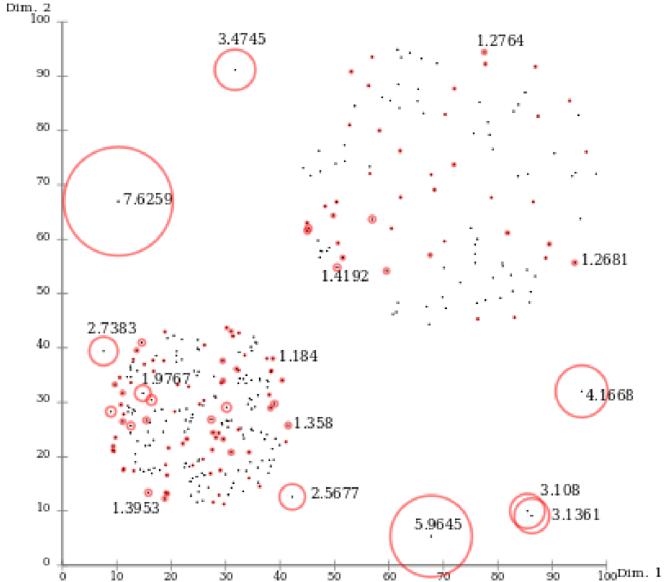


Derivation



LOF: Derivation

LOF: Example 2 image from [4]



LOF: Discussion

References

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