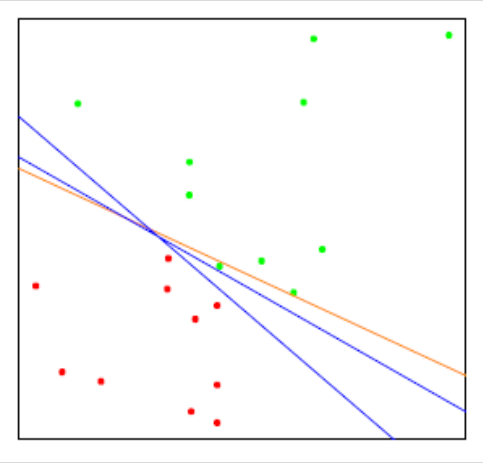

Big Data Analytics

Basic concepts of analyzing very large amounts of data

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LECTURE BDA1

Support Vector Machines

2014-01-24 (v4)
Online Material

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

JÜLICH
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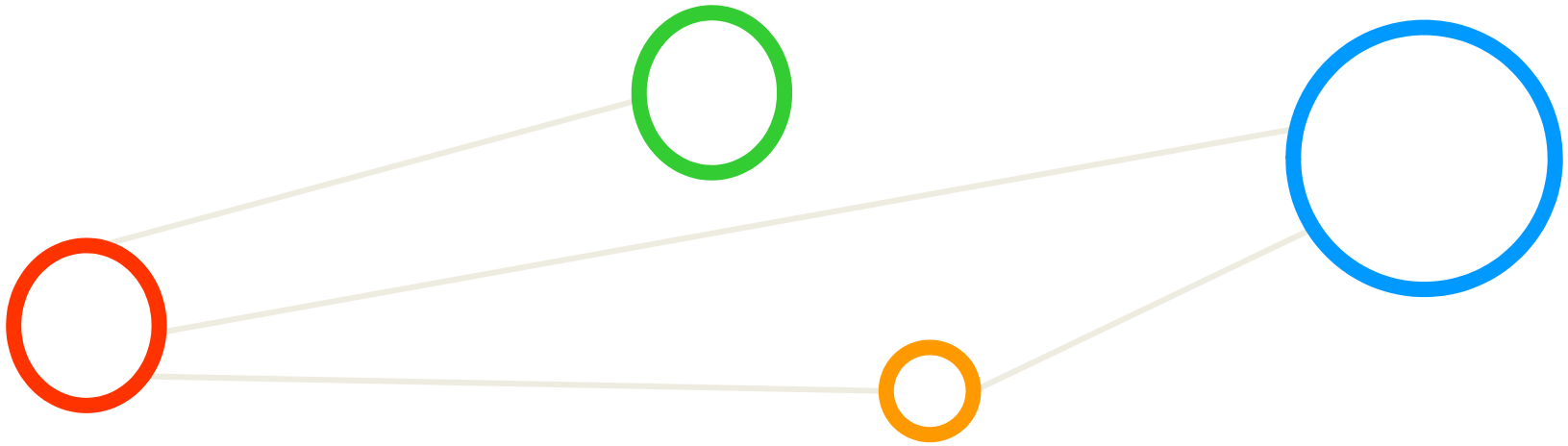
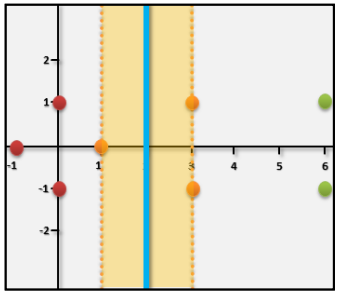
Outline

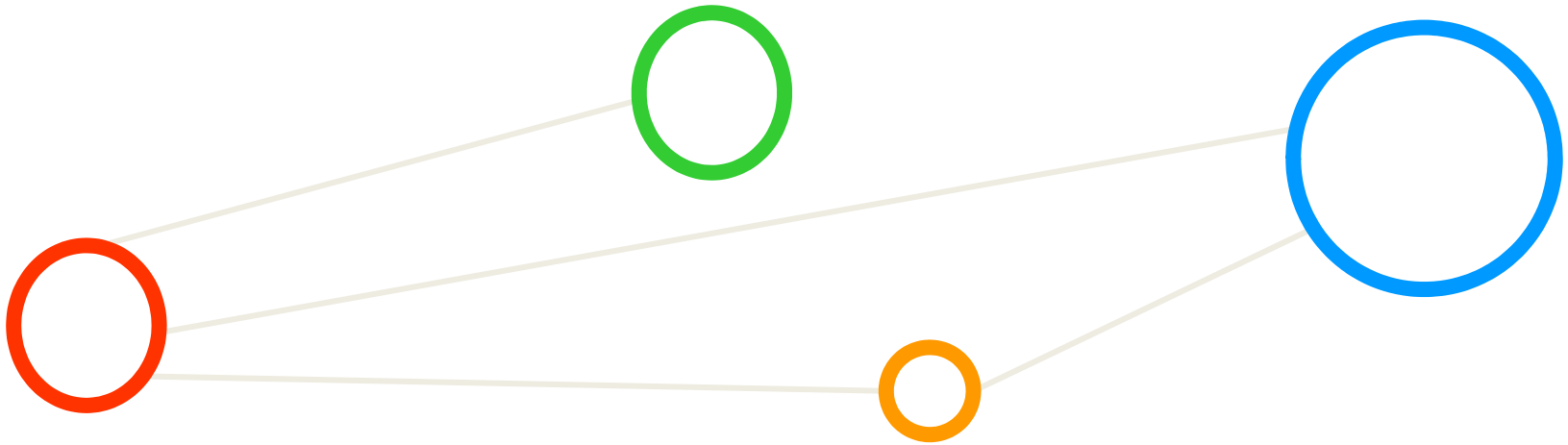


Outline

- SVMs
  - General Information
  - Need for Labelled Data
  - Advantages / Disadvantages
  - Linear Example
- Step-Wise Approach
  - Categorical feature transformations
- Application Areas
  - Text Categorization
  - Bioinformatics
  - Image Processing



Support Vector Machines (SVMs)



General Information

- Support Vector Machines (SVMs)
  - Appeared in the early 1990s
  - Standard methodology in computer science and engineering communities
- Optimal margin classfiers
  - In the context of 'statistical learning theory'
- Operate within the framework of 'regularization theory'
  - Minimizing an 'empirical risk' in a well-posed and consistent way
- Compromise and Kernel Functions
  - Between the parametric and the pure nonparametric approaches
  - As in linear classiers: SVMs estimate a linear decision function
  - With the particularity that a previous mapping of the data into a 'higher-dimensional feature space' may be needed
  - Mapping is characterized by the choice of a class of functions (known as kernels)

Need for Labelled Data

- Sample Dataset $\{(\mathbf{x}_i, \mathbf{y}_i) \in X \times Y\}_{i=1}^{n}$

- Goal is to learn the relationship between the **x** and **y** variables
- The main goal in this context usually is 'predictive accuracy'
  - In most cases it is not possible to assume a parametric form for the probability distribution p(**x**, **y**)

Advantages / Disadvantages

- Advantages
  - Sparse solutions to classication and regression problems are obtained
  - Only a few samples are involved in the determination of the classication (or regression functions)

Literature

- Books
  - ‘Introduction to SVMs’, Cristianini and Shawe-Taylor

[2] Introduction to SVMs

SVM Foundations

- **SVM make use of a (nonlinear) mapping function ϕ that transforms data in input space to data in feature space in order to render a problem linearly separable**
- **SVM then automatically discovers the optimal separating hyperplane**
- **When mapped back into input space via ϕ^{-1} , this plane can be a complex decision surface**

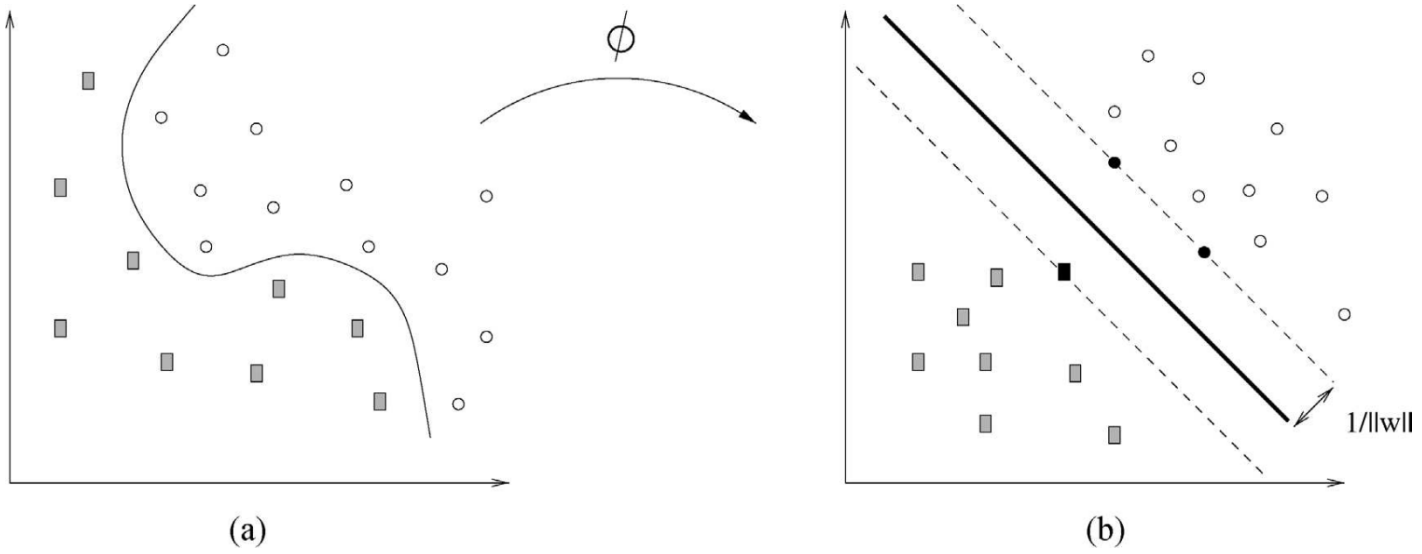
- Support Vector Machines (SVMs)
  - Represent a popular classification technique
  - Based on a sound theoretical basis
  - Have state-of-the-art success in real-world applications

SVM Principles

- Classification problem
  - Discriminant function is nonlinear
  - (a) Original data in the input space
  - (b) Mapped data in the feature space – e.g. two possible classes (mapping function ϕ such that the data becomes linearly seperable)

$$\{(\Phi(\mathbf{x}_i), y_i)\}_{i=1}^{n}$$

$$y_i \in \{-1, +1\}$$

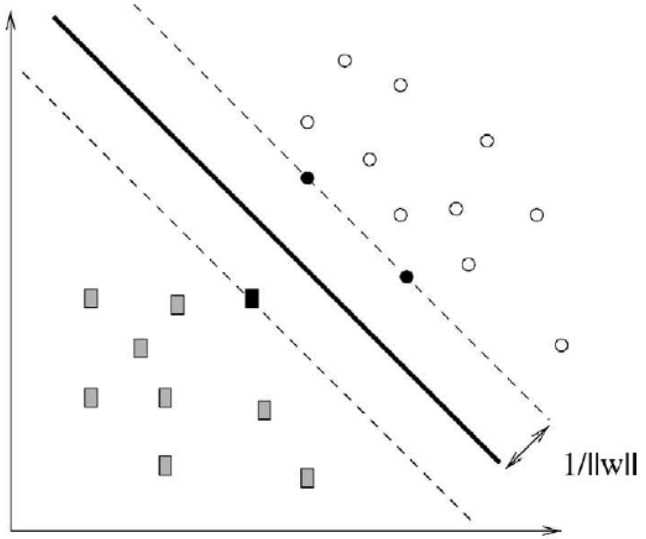


[1] SVMs with Applications

Optimal (Maximal) Margin Hyperplane

- There is an infinite number of existing separating hyperplanes
- Separating hyperplane in the space of the mapped data:
  - (equidistant to the nearest point in each class)

$$\mathbf{w}^T \Phi(\mathbf{x}) + b = 0$$



- Rescale

$$|\mathbf{w}^T \Phi(\mathbf{x}) + b| = 1$$

every $i \in \{1, \ldots, n\}$

  - (assuming separability) for those points in each class nearest to the hyperplane

$$\mathbf{w}^T \Phi(\mathbf{x}_i) + b \begin{cases} \geq 1, & \text{if } y_i = +1 \\ \leq -1, & \text{if } y_i = -1. \end{cases}$$

- **SVMs pick the separating hyperplane that lies furthermost both clases**
- **The separating plane is called optimal (maximal) margin hyperplane**

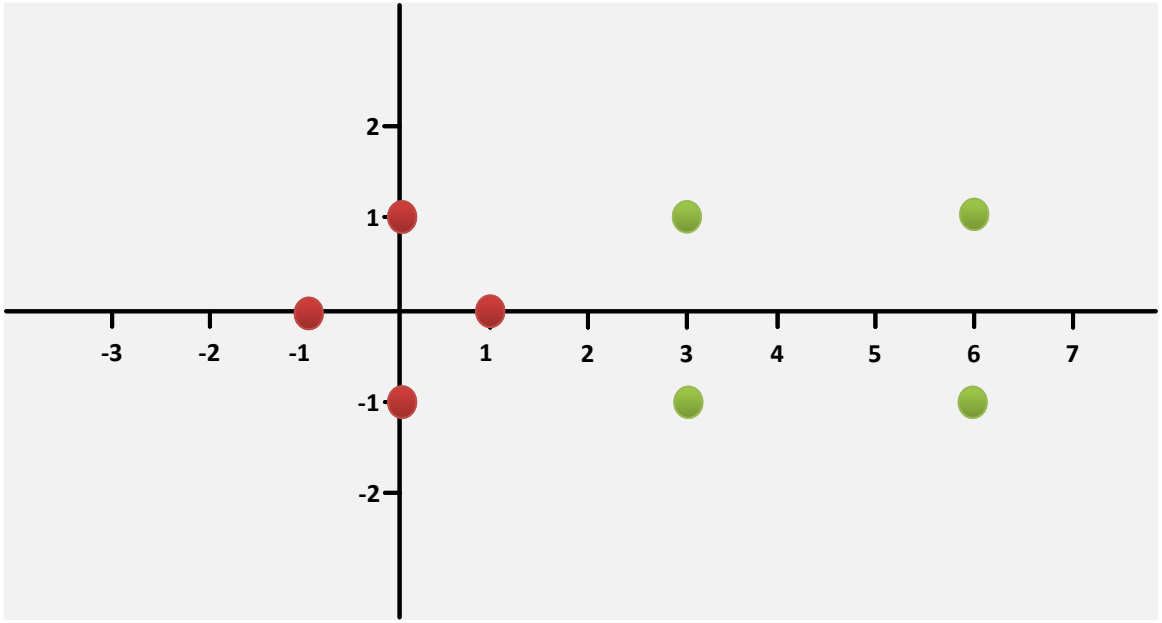
Linear SVM Example (1)

- Given: positively labelled data points in $\mathbb{R}^2$: red (class -1)

$$\left\{\begin{pmatrix}3\\1\end{pmatrix},\begin{pmatrix}3\\-1\end{pmatrix},\begin{pmatrix}6\\1\end{pmatrix},\begin{pmatrix}6\\-1\end{pmatrix}\right\}$$

- Given: negatively labelled data points in $\mathbb{R}^2$: green (class +1)

$$\left\{\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix},\begin{pmatrix}0\\-1\end{pmatrix},\begin{pmatrix}-1\\0\end{pmatrix}\right\}$$



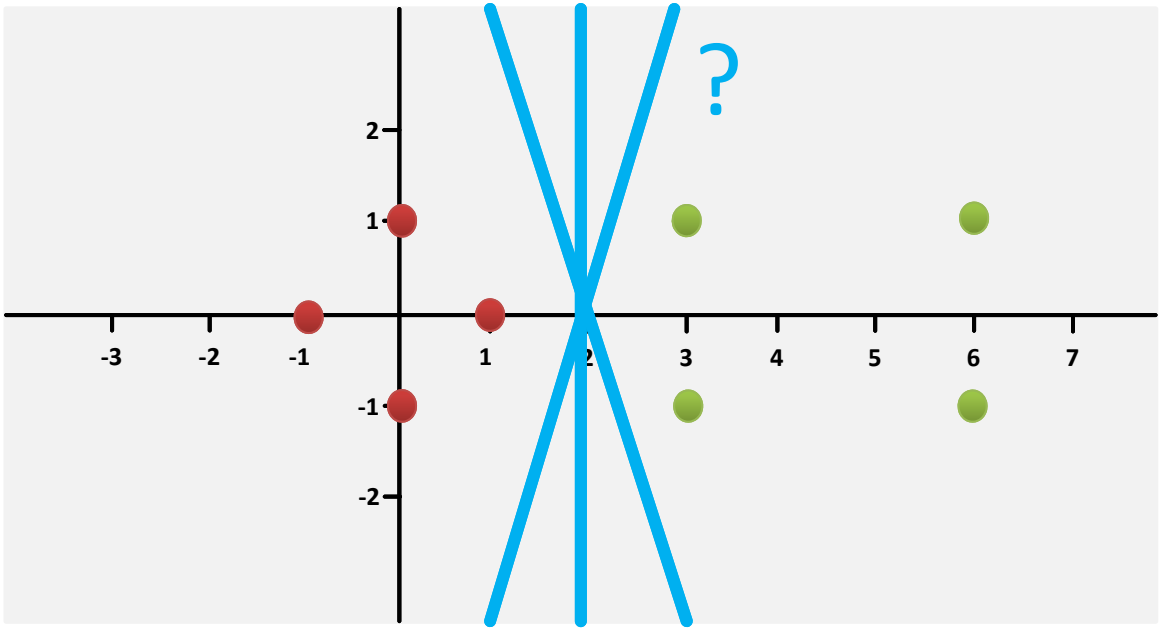
- $\mathbb{R}$: **Real numbers can be represented as points on an infinitely long number line**
- **Real numbers include all the rational numbers, irrational numbers, & Pi**

[3] SVM Example

Linear SVM Example (2)

- **A 'Linear SVM' is a SVM whose mapping function ϕ() is the identity function**
- **The 'identity function' is a function that always returns the same value that was used as ist argument: e.g. f (x) = x**

- Goal: Discover a SVM that accurately discriminates two classes
- Simple Analysis of Input Space:
  - Data is linear separable → Linear SVM should be ok (finds optimal plane)



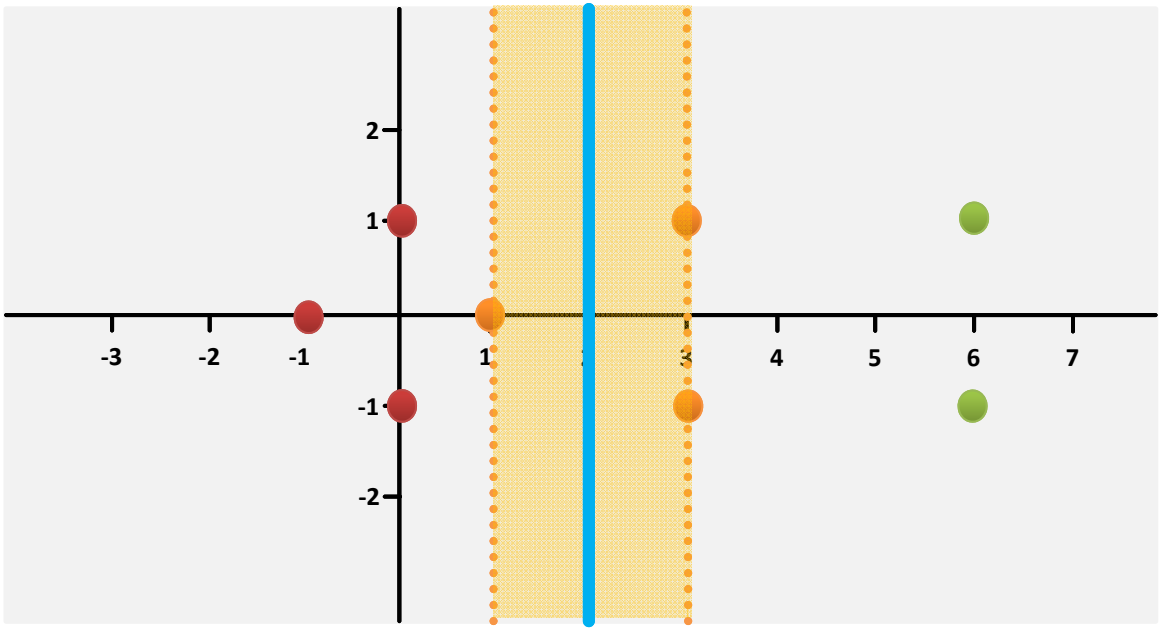
[3] SVM Example

Linear SVM Example (3)

- **Support Vectors lie directly on the margin and satisfy $y_i = (w \cdot x_i - b) = 1$**

- (Manual) Inspection of the data
  - Three support vectors (orange)

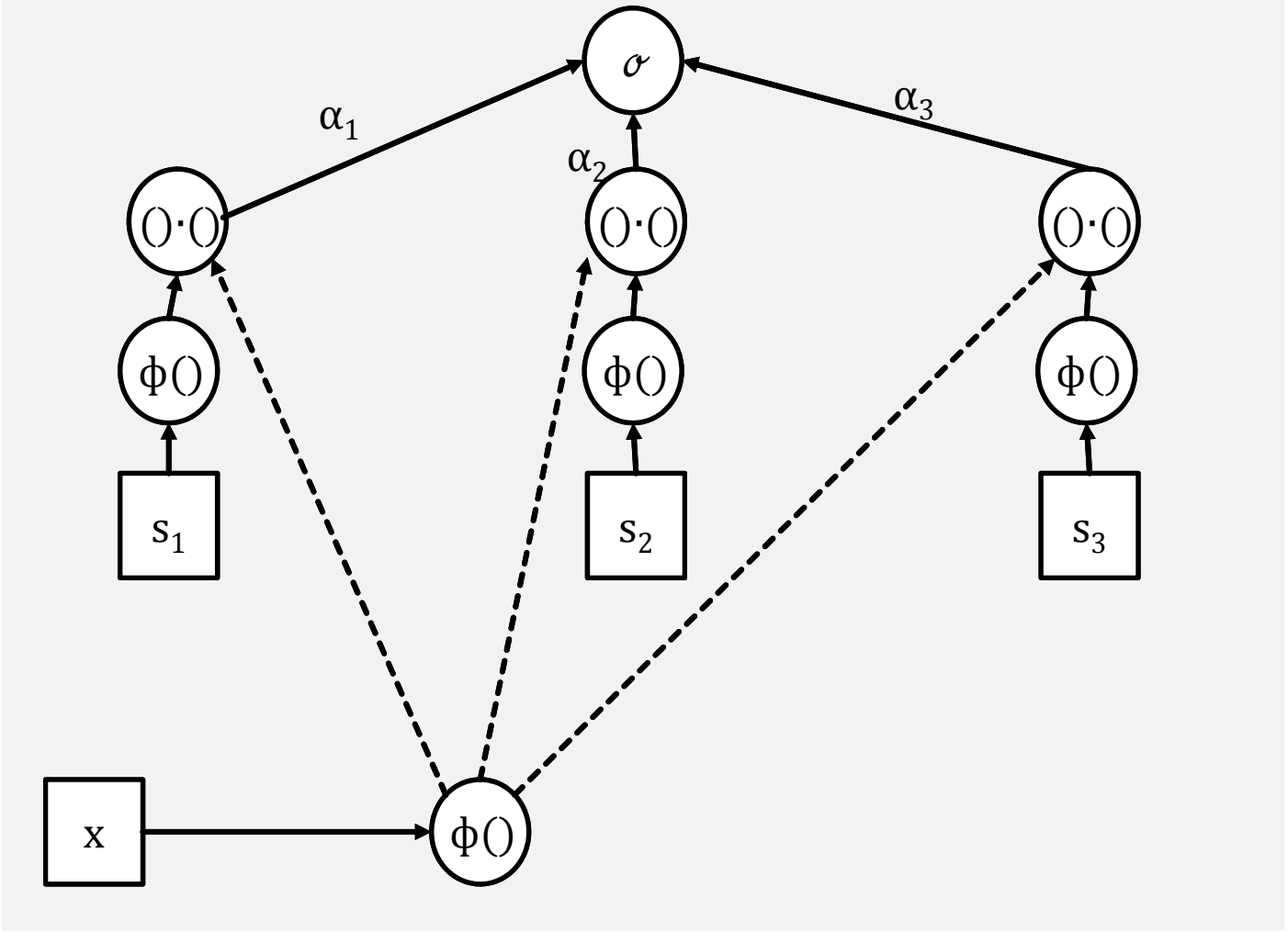
$$\left\{s_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, s_2 = \begin{pmatrix} 3 \\ 1 \end{pmatrix}, s_3 = \begin{pmatrix} 3 \\ -1 \end{pmatrix}\right\}$$



[3] SVM Example

Linear SVM Example (4)

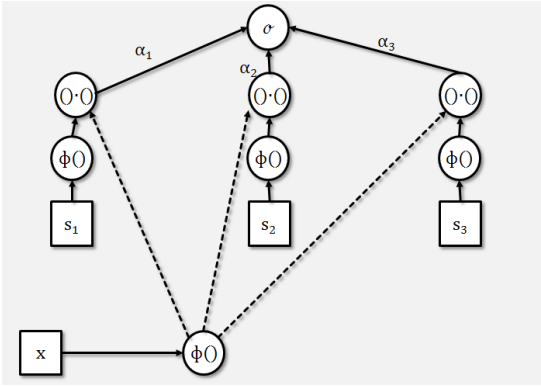
- The ‘SVM Architecture‘



[3] SVM Example

Linear SVM Example (5)

- Use vectors augmented with a 1 as a bias input
  - Differentiated with over-tilde
  - E.g. $s_1 = (10)$, with bias $\tilde{s}_1 = (101)$



- Goal: Find values for α_i so that:

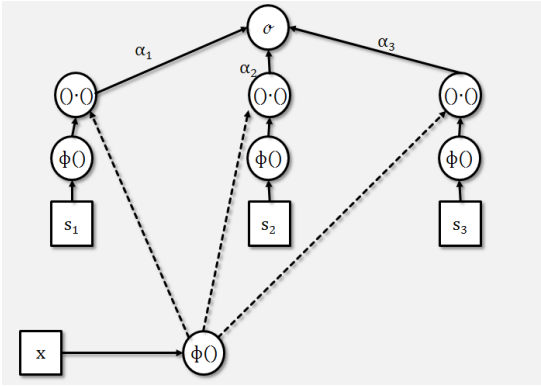
$$\begin{aligned}
\alpha_1 \phi(s_1) \cdot \phi(s_1) + \alpha_2 \phi(s_2) \cdot \phi(s_1) + \alpha_3 \phi(s_3) \cdot \phi(s_1) &= -1 \\
\alpha_1 \phi(s_1) \cdot \phi(s_2) + \alpha_2 \phi(s_2) \cdot \phi(s_2) + \alpha_3 \phi(s_3) \cdot \phi(s_2) &= +1 \\
\alpha_1 \phi(s_1) \cdot \phi(s_3) + \alpha_2 \phi(s_2) \cdot \phi(s_3) + \alpha_3 \phi(s_3) \cdot \phi(s_3) &= +1
\end{aligned}$$

- **Sometimes it is required that the hyperplane pass through the origin of the coordinate system for simplicity ('unbiased hyperplane')**
- **General hyperplanes not necessarily passing through the origin ('biased hyperplane')**

[3] SVM Example

Linear SVM Example (6)

- Using $\phi() = I$
  (Identity function, because linear SVM)
  - Adding bias for $s\sim_i$



$$\begin{aligned}
\alpha_1 s\sim_1 \cdot s\sim_1 + \alpha_2 s\sim_2 \cdot s\sim_1 + \alpha_3 s\sim_3 \cdot s\sim_1 &= -1 \\
\alpha_1 s\sim_1 \cdot s\sim_2 + \alpha_2 s\sim_2 \cdot s\sim_2 + \alpha_3 s\sim_3 \cdot s\sim_2 &= +1 \\
\alpha_1 s\sim_1 \cdot s\sim_3 + \alpha_2 s\sim_2 \cdot s\sim_3 + \alpha_3 s\sim_3 \cdot s\sim_3 &= +1
\end{aligned}$$

- Recall: Given three points with added bias

$$\left\{ \boldsymbol{s}\sim_1 = \begin{pmatrix} \mathbf{1} \\ \mathbf{0} \\ \mathbf{1} \end{pmatrix}, \boldsymbol{s}\sim_2 = \begin{pmatrix} \mathbf{3} \\ \mathbf{1} \\ \mathbf{1} \end{pmatrix}, \boldsymbol{s}\sim_3 = \begin{pmatrix} \mathbf{3} \\ \mathbf{-1} \\ \mathbf{1} \end{pmatrix} \right\}$$

- Computing the dot product

$$\begin{aligned}
2\,\alpha_1 + 4\,\alpha_2 + 4\,\alpha_3 &= -1 \\
4\,\alpha_1 + 11\,\alpha_2 + 9\,\alpha_3 &= +1 \\
4\,\alpha_1 + 9\,\alpha_2 + 11\,\alpha_3 &= +1
\end{aligned}
\quad \xrightarrow{\textit{linear algebra}} \quad
\begin{aligned}
\alpha_1 &= -3.50 \\
\alpha_2 &= +0.75 \\
\alpha_3 &= +0.75
\end{aligned}$$

[3] SVM Example

Linear SVM Example (7)

$$\tilde{w} = \sum_i \alpha_i \tilde{s}_i$$

- α_i relates to the discriminating hyperplane with w:

$$w^T \phi(x) + b = 0$$

- Computing w~ using given points with bias and α_i :

$$\tilde{w} = -3.5 \begin{pmatrix}1\\0\\1\end{pmatrix} + 0.75 \begin{pmatrix}3\\1\\1\end{pmatrix} + 0.75 \begin{pmatrix}3\\-1\\1\end{pmatrix}$$

$$\tilde{w} = \begin{pmatrix}1\\0\\-2\end{pmatrix}$$

$$\alpha_1 = -3.50$$
$$\alpha_2 = +0.75$$
$$\alpha_3 = +0.75$$

$$\left\{ \tilde{s}_1 = \begin{pmatrix}1\\0\\1\end{pmatrix}, \tilde{s}_2 = \begin{pmatrix}3\\1\\1\end{pmatrix}, \tilde{s}_3 = \begin{pmatrix}3\\-1\\1\end{pmatrix} \right\}$$

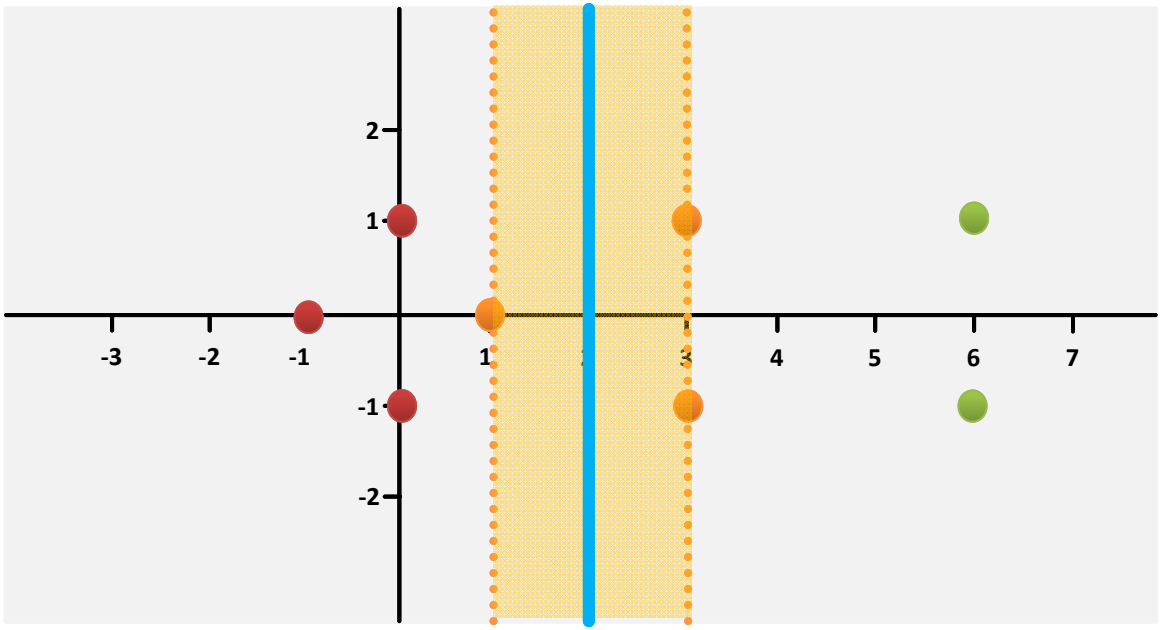
[3] SVM Example

Linear SVM Example (8)

- Context of linear hyperplane equation (linear function):

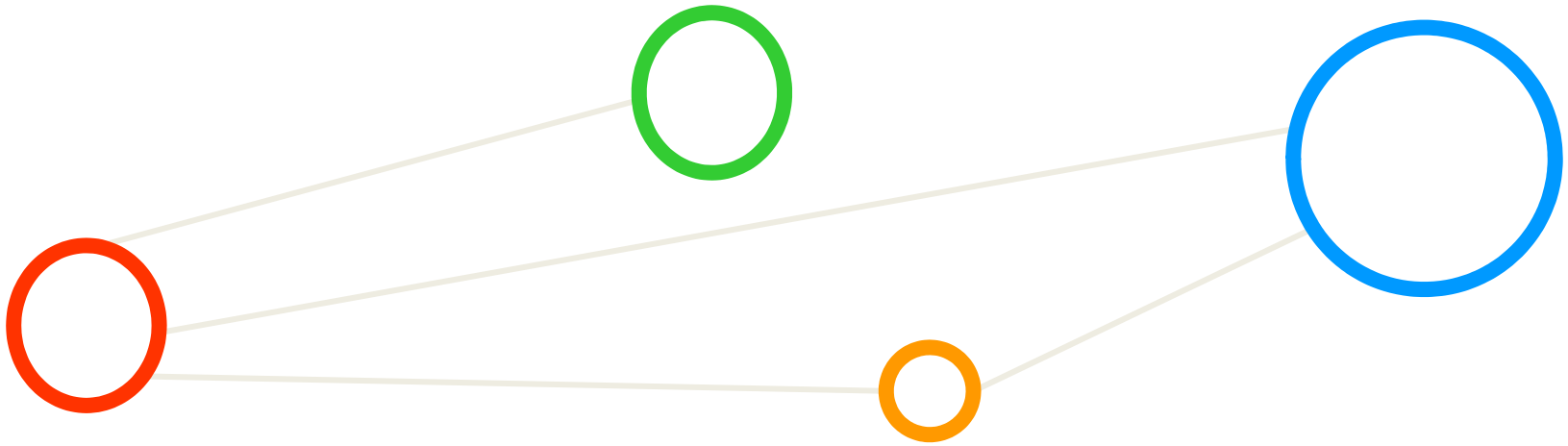
$$y = w\,x + b$$

$\tilde{w} = \begin{pmatrix} 1 \\ 0 \\ -2 \end{pmatrix}$ *bias b from vector* → $w = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, b = - 2



[3] SVM Example

Step-Wise Approach



Step-Wise Approach

- **SVM beginners often get unsatisfactory results, because they miss some easy but significant steps**

1. Transform data to SVM package format **Preprocessing**
2. Conduct simple ‘scaling‘ on the data **Preprocessing**
3. Consider the ‘Radial Basis Function (RBF)‘ Kernel K

$$K(x, y) = e^{-\Upsilon \, || \, x - y \, ||^2}$$

Model Selection

4. Use cross-validation to find best parameter C and ϒ **Model Selection**
5. Use C and ϒ to train the whole training set **Training**
6. Test **Testing**

[4] SVM Guide

Step 1: Categorical Feature

Preprocessing

- **SVM requires that each data instance is represented as a vector of real numbers**

- Problematic: Categorical attributes
  - Need to convert into a numeric data representation
- Example
  - Use m numbers to represent an m-category attribute
  - Only one of the m numbers is 1, others are 0

three-category attribute: {red, green, blue}

represented as

(0,0,1), (0,1,0), (1,0,0)

- Experience: if number of values in an attribute is not too large, this coding might be more stable than using a single number

[4] SVM Guide

Step 2: Simple Scaling (1) Preprocessing

- **Scaling before applying SVM is a very important process**
- **Scaling avoids attributes in greater numeric ranges dominating those in smaller numeric ranges**
- **It further avoids numerical dificulties during the calculation**

- Input data is often represented as vector
  - Apply ‘rescaling or normalization‘ of them (used term depend on field)
- Rescaling of vectors
  - Add/subtract a constant – then multiply/divide by a constant
- Normalizing a vector
  - Divide by a norm of the vector
    (e.g. make the Euclidean length of the vector equal to one)
  - Often refers to rescaling by the minimum and range of the vector
    (e.g. to make all the elements lie between 0 and 1)

[4] SVM Guide

[5] AI FAQ

Step 2: Simple Scaling (2) Preprocessing

- Scaling avoids numerical difficulties
  - Kernel values depend on inner products of feature vectors (e.g. the linear kernel and the polynomial kernel)
  - Especially large attribute values might cause numerical problems
- Ranges
  - ‘Linearly scaling‘ each attribute to certain ranges: [-1 ; +1] or [0 ; 1]
- Data Scaling
  - Use the same method to scale both training and testing data
- Example
  - Scale first attribute of training data from [-10; +10] to [-1; +1]
  - Then scale first attribute of testing data from [-11; +8] to [-1,1; +0,8]

[4] SVM Guide

Step 3: Radial Basis Function

Model Selection

- **Model selection for SVMs means to choose one of four possible ones: linear, polynomial, radial basis function, sigmoid**
- **Often recommended Kernel is Radial basis function**

- Linear

$$K(x_i, yj) = xiTxj$$

ϒ, r, d are kernel parameters

- Polynomial

$$K(x_i, yj) = (\Upsilon\, xiTxj + r)^d, \Upsilon > 0$$

- Sigmoid

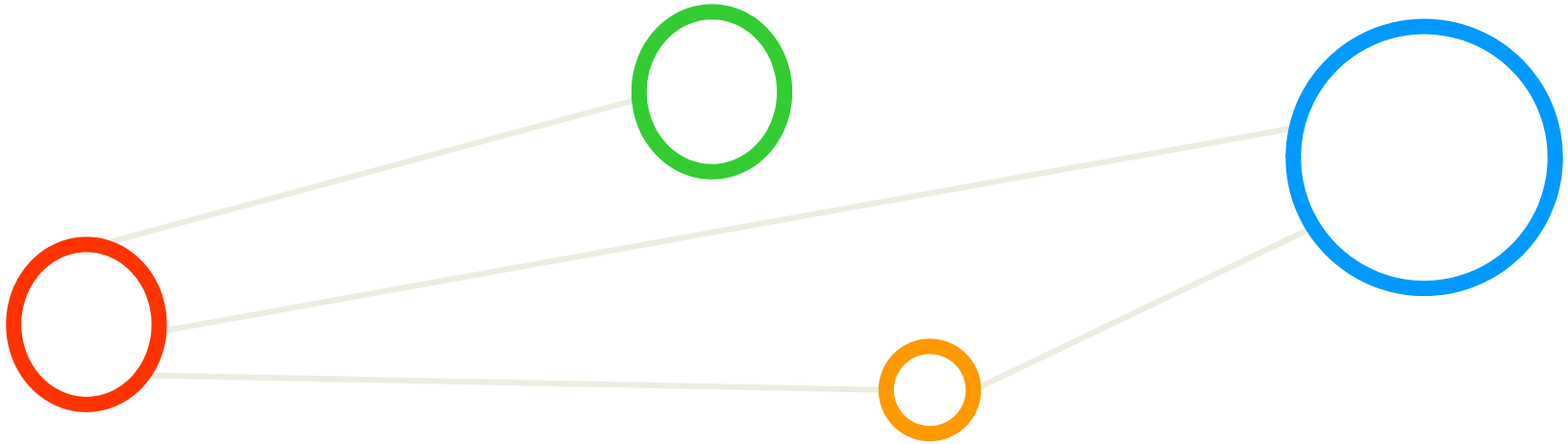
$$K(x_i, yj) = \tanh(\Upsilon\, xiTxj + r)$$

- Radial Basis Function (RBF)

$$K(x_i, yj) = e^{-\Upsilon\ ||\ xi - yj\ ||^2} = \exp(-\Upsilon\ ||\ x_i - y_j\ ||^2), \Upsilon > 0$$

[4] SVM Guide

Application Areas



Application Areas

- Only a few samples are involved in the determination of the classication (or regression functions)
  - This facilitates the application of SVMs to problems that involve a large amount of data (aka ‘big data’)
- Typical Application Areas
  - Text processing applications, e.g. text categorization
  - Bioinformatics tasks
  - Image recognition
- Application communities
  - Often involved in the solution of consulting
  - ‘Industrial data analysis’ problems

[1] SVMs with Applications

Text Categorization (1)

- Goal: Consists of the classication of documents into a predefined number of given categories
  - Used by many Internet search engines, e.g. to select Web pages related to user queries.
- Example: News Messages
  - Document collection made up of Usenet News messages
  - Organized in ‘predefined classes’: computation, religion, statistics, etc.
- Key Benefit: Automation of Classification Process
  - Input: new document
  - Task: conduct the ‘category assignment’ in an automatic way

[1] SVMs with Applications

Text Categorization (2)

- Mathematical Representation
  - Documents are represented in a vector space of 'dimension equal to the number of different words' in the vocabulary
  - Text categorization problems involve 'high-dimensional inputs' and the data set consists of a 'sparse document by term matrix'

[1] SVMs with Applications

Text Categorization (3)

- Data Set: Reuters data base
  - Text collection composed of 21,578 documents and 118 categories
  - The data space has dimension 9947
    (the number of different words that describe the documents)
- Example of SVM Performance
  - Results obtained using a SVM with a linear kernel
- First Measure: Average Rate of Success
  - SVM is 87%, Naive Bayes (72%), Bayesian Networks (80%), Classification Trees (79%), and *k*-nearest neighbors (82%)

- **Results for SVM with a linear kernel in text categorization are consistently better along categories than those obtained with four widely used classification methods (Naive Bayes, Bayesian networks, Classication trees, *k*-nearest neighbors)**

[1] SVMs with Applications

Text Categorization (4)

- **SVM text classifiers training time is most impressive benefit**
- **Much faster than other classification methods such as Naive Bayes or Classification Trees**

- Second Measure: Training Time
  - 4x faster than Naive Bayes
  - 35x faster than Classification Trees
- Reasons for extraordinary performance
  - Algorithms take advantage of 'sparsity in the document by term matrix'
- Other Methods Not Useful
  - Methods that involve the 'diagonalization of large and dense matrices'
  - E.g. like the 'criterion matrix in Fisher flexible discriminant analysis'
  - Out of consideration for text classication, because of their expensive computational requirements

[1] SVMs with Applications

Bioinformatics Tasks

- Goal: Analyzing microarray data
  - Analyzing ‘biological samples’ using their genetic expression profiles

- SVMs have been applied to:
  - E.g. tissue classication
  - E.g. gene function prediction
  - E.g. protein subcellular location prediction
  - E.g. protein secondary structure prediction
  - E.g. protein fold prediction

- **SVM outperform other classification methods (or in worst case are at least similiar to the best non-SVM method)**

[1] SVMs with Applications

Bioinformatics: Protein Subcellular Location Prediction

- Goal
  - Predict protein subcellular positions from 'prokaryotic sequences'
- Categories
  - Three possible location categories
  - [cytoplasmic, periplasmic, extracellular]
- Approach
  - Classification: the problem reduces to classifying 20-dimensional vectors into three (highly unbalanced) classes
- Measure: Prediction Accuracy
  - SVMs (with Gaussian Kernel) is 91.4%
  - Neural Networks is 81%
  - First-order Markov Chain is 89.1%

Image Processing (1)

- Example: Handwritten Digit Identification
  - U.S. Postal Service data base contains 9298 samples of digits
  - Divided into 7291 training samples and 2007 samples for testing
  - Obtained from real-life zip codes
  - Digit is represented by a 16 × 16 gray level matrix
  - Each data point is represented by a Vector in R256
  - Manual: Human classication error for this problem is known to be 2.5%
  - Automated: Error rate for a standard SVM is 4%
    (with a third degree polynomial kernel)

[1] SVMs with Applications

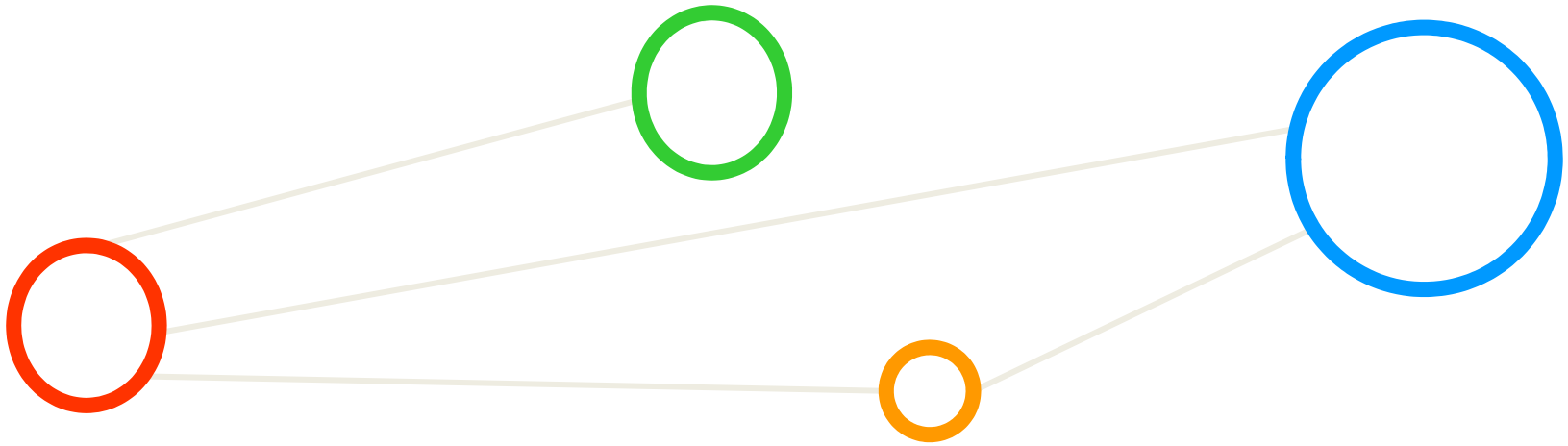
Image Processing (2)

- Example: Face Recognition
  - E.g. Used for ‘gender detection’
  - The data contain 1755 face images (1044 males and 711 females),
  - Overall error rate for a SVM with a Gaussian kernel is 3.2%

  - E.g. another application of SVMs is the ‘detection of human faces’ in gray-level images
  - Determine in an image the location of human faces
  - If there are any, return an encoding of their position
  - Detection rate for a SVM with a second degree polynomial kernel is 97.1%

[1] SVMs with Applications

Lecture Bibliography



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