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Support Vector Machines

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Quick Recap

- Supervised Learning
  - Given training data with true labels, learn a model to predict label
  - So far, we have learnt about
    - Decision Trees
    - Neural Networks
    - Logistic Regression

Web Document Classification

- Very large number of features (words)
- Relatively low number of labelled training samples available
- Highly sparse data
- In such situations, employing Boosted Decision Trees may not be a good idea
  – Usually works well until around 4K features
- In this talk, we will focus on SVMs
  – Known to perform very well even with very low training data
  – Training scales well with large number of features!

Outline of the Talk

- Maximum Margin Classifiers
- Basic Formulation of Linear SVMs
- Dealing with Noisy Data
- Non-linear Decision Boundaries
- Practical Advice on SVMs

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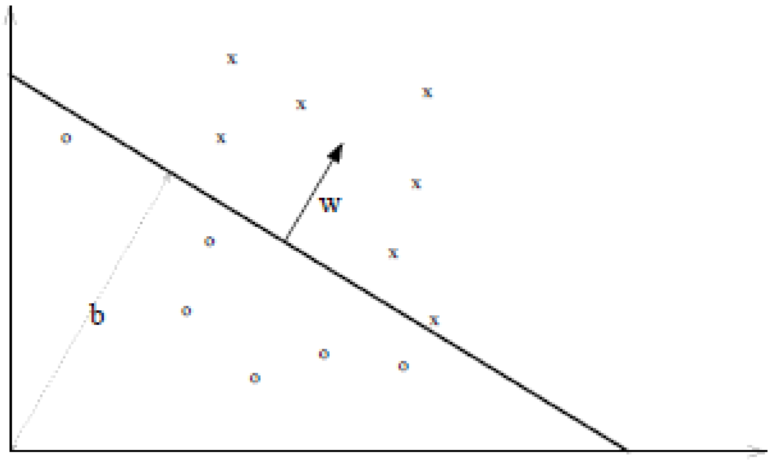
Linear Classifiers

Inner product between vectors

$$\langle \bar{x}, \bar{z} \rangle = \sum_i x_i z_i$$

Hyperplane:

$$\langle w, x \rangle + b = 0$$



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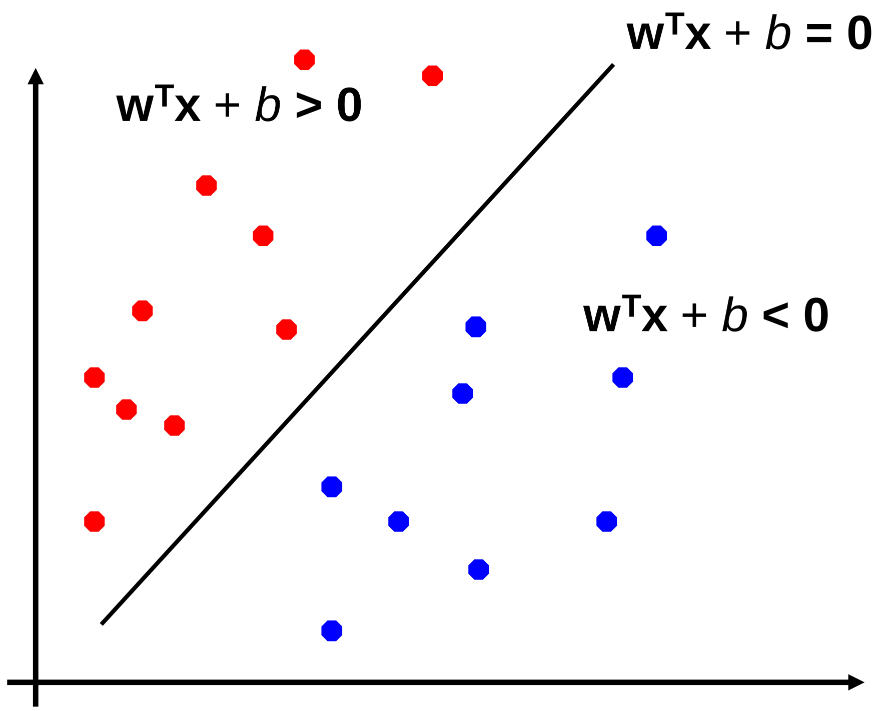
Linear Classifiers

- Binary classification can be viewed as the task of separating classes in feature space:



$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$$

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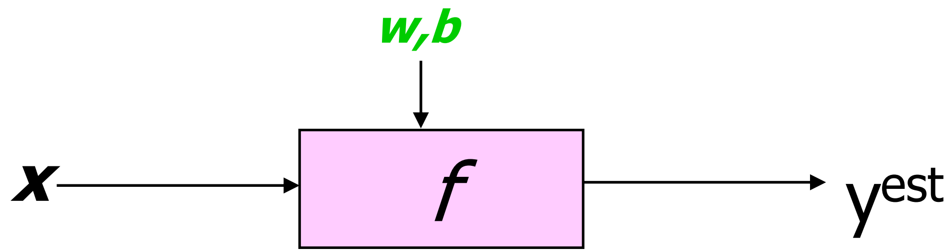
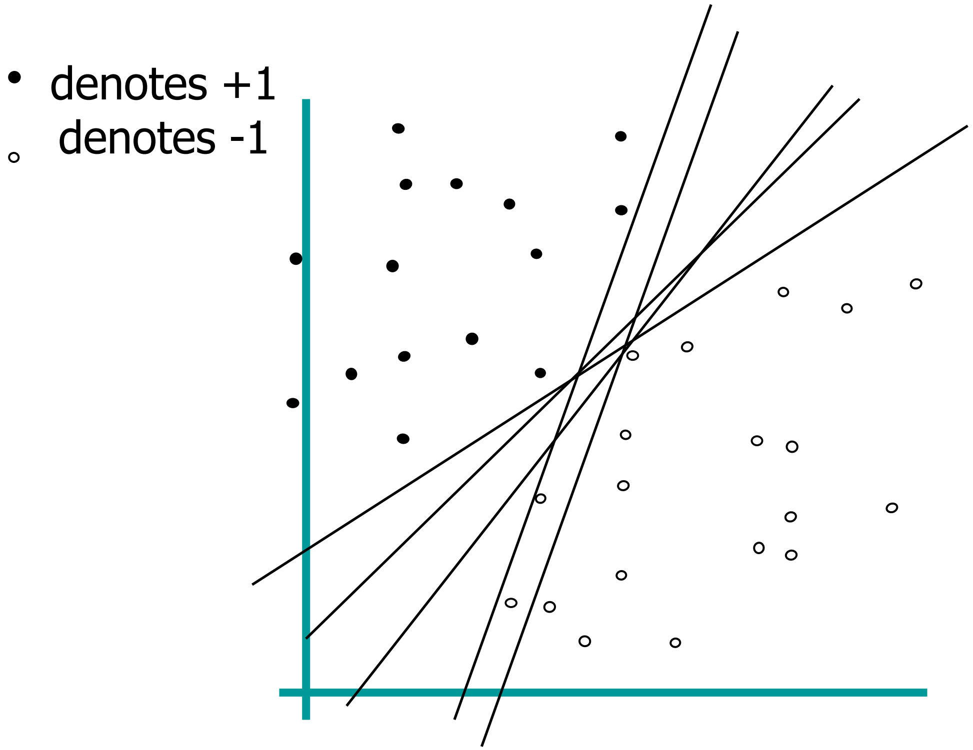
Linear Classifiers



$$f(\mathbf{x}, \mathbf{w}, b) = sign(\mathbf{w} \cdot \mathbf{x} - b)$$

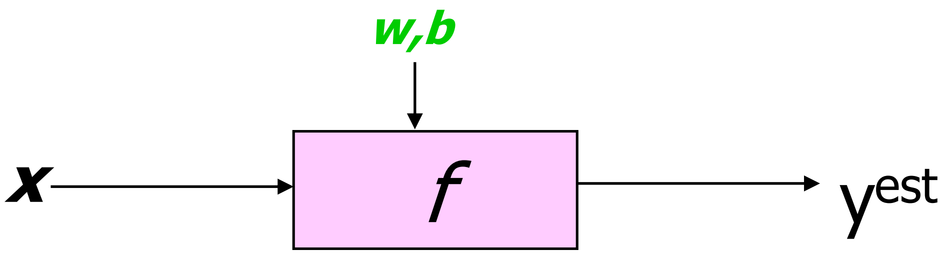


How would you classify this data?

Any of these would be fine..

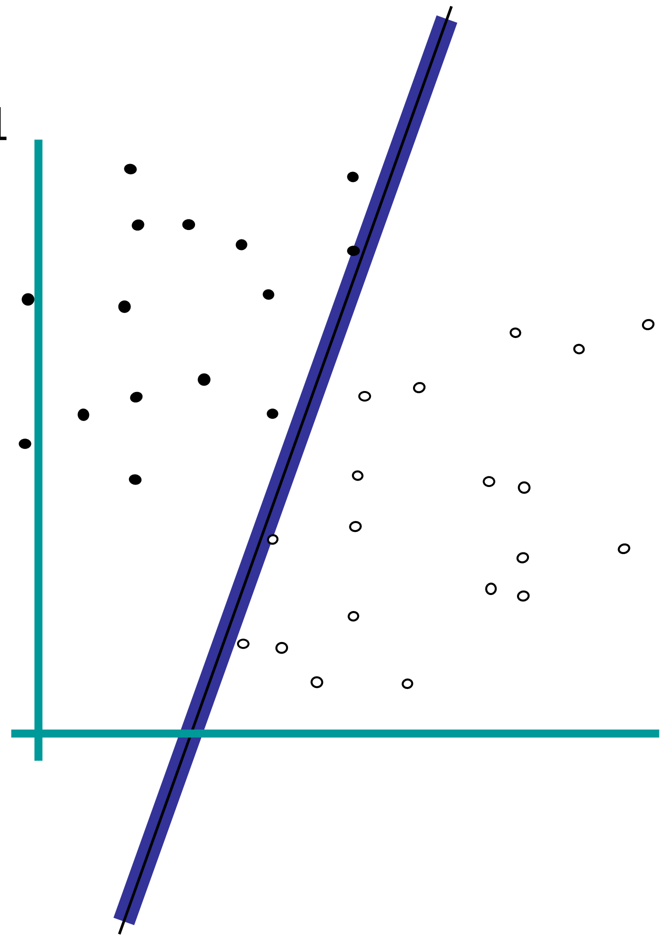
..but which is best?

Margin of a Classifier



$f(\mathbf{x},\mathbf{w},b) = sign(\mathbf{w}.\ \mathbf{x} - b)$

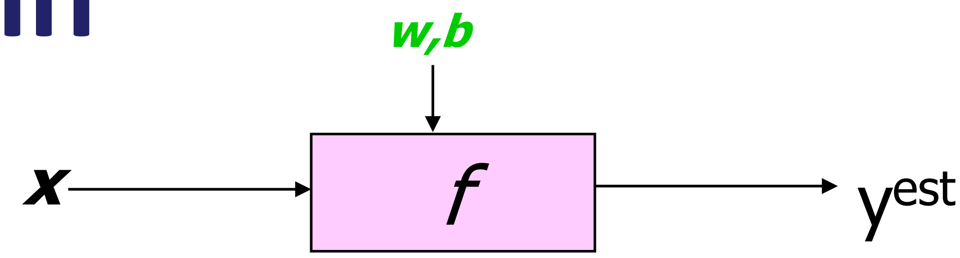
- • denotes +1
- ° denotes -1



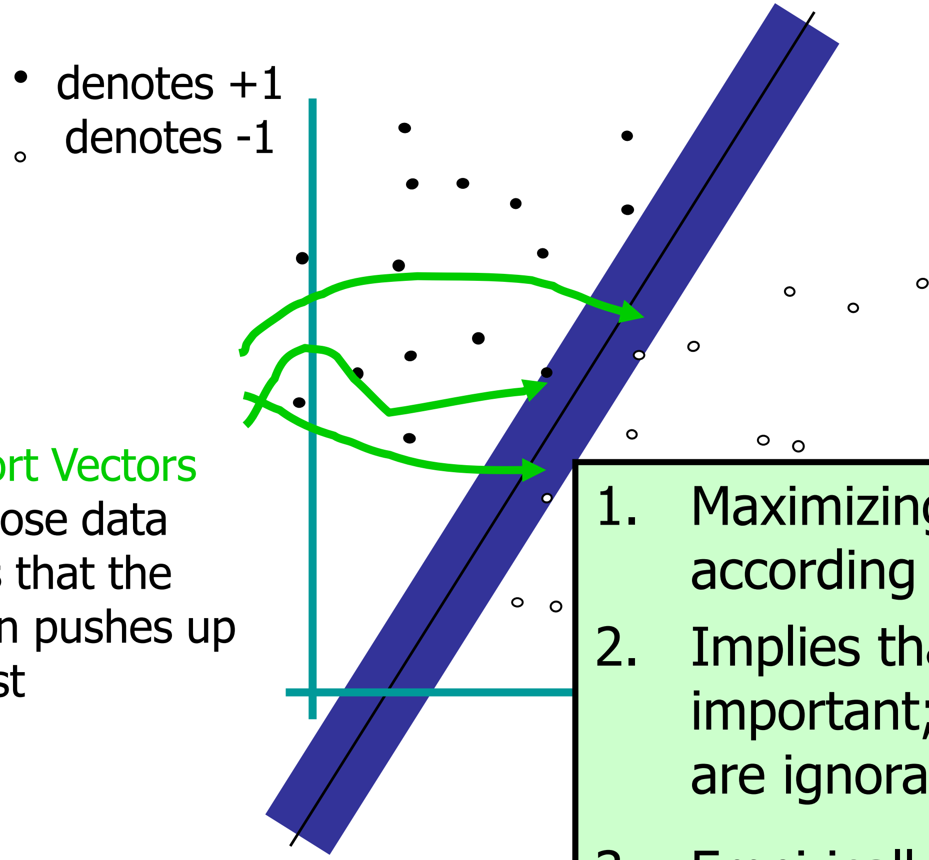
Margin of a Linear Classifier

Width that the boundary could be increased by before hitting a data point.

Maximum Margin



$$f(\mathbf{x},\mathbf{w},b) = \mathrm{sign}(\mathbf{w}\cdot\mathbf{x} - b)$$



Support Vectors are those data points that the margin pushes up against

The maximum margin linear classifier is the linear classifier with the maximum margin.

kind of SVM –

1. Maximizing the margin is good according to intuition and PAC theory
2. Implies that only support vectors are important; other training examples are ignorable.
3. Empirically it works very well.

Computing the Margin Width

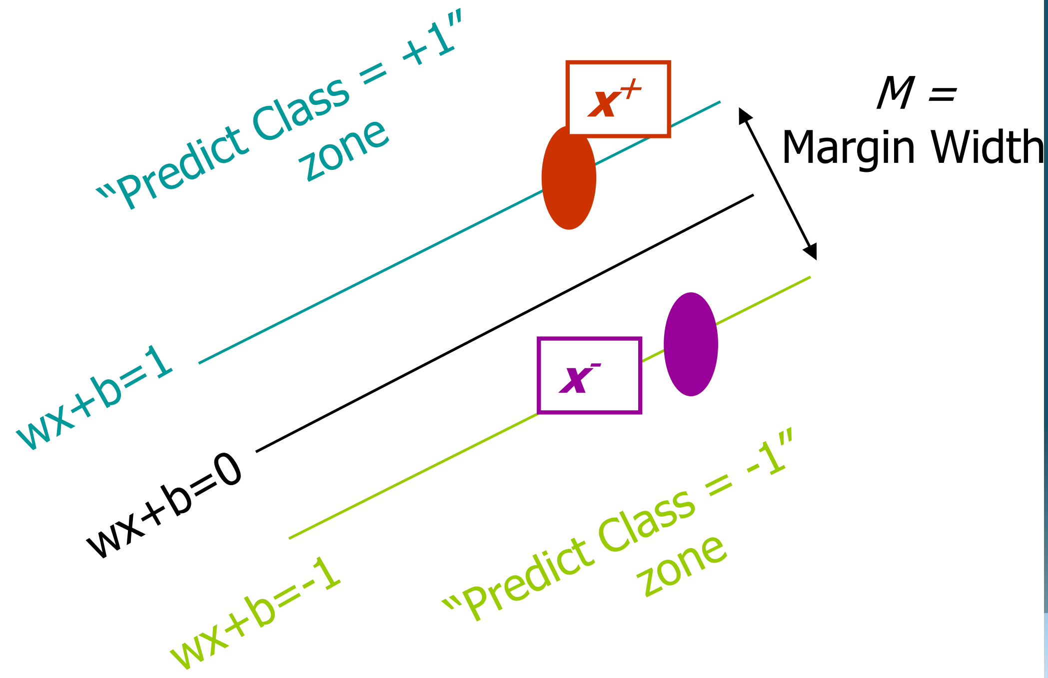
- ***w*** is normal to the separating hyperplane
  - For any two points u, v on the plane
    w .(u – v) = 0

- *M = Projection of (**x**⁺ - **x**⁻) onto unit vector normal to separating plane*

$$M = \frac{w}{||w||}.(x^{+} - x^{-})$$

$$M = \frac{2}{||w||}$$

$$M = \frac{2}{\sqrt{w.w}}$$



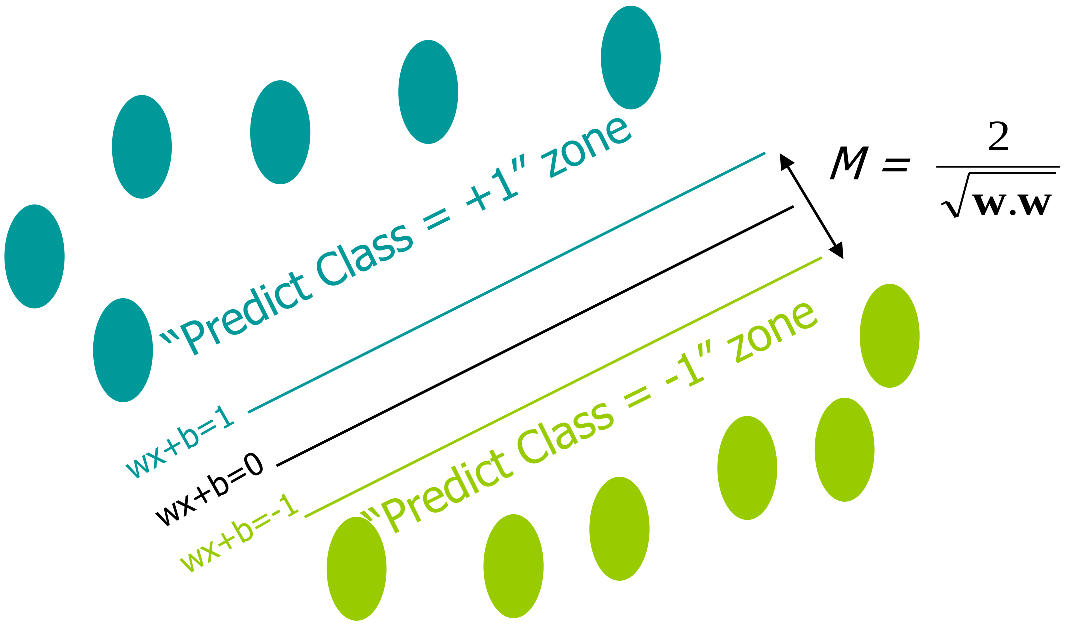
We know that

$\boldsymbol{w} \,.\, \boldsymbol{x}^{+} + b = +1$

$\boldsymbol{w} \,.\, \boldsymbol{x}^{-} + b = -1$

$\boldsymbol{w} \,.\, (\boldsymbol{x}^{+} - \boldsymbol{x}^{-}) = 2$

Learning the Maximum Margin Classifier



Given guess of ***w*** , *b* we can

- Compute whether all data points are in the correct half-planes
- Compute the margin width

Assume *R* datapoints, each $(\mathbf{x}_k, y_k)$ where $y_k = +/- 1$

What should our optimization criterion be?

Minimize ***w.w***

How many constraints will we have?

R

What should they be?

$\mathbf{w} \cdot \mathbf{x}_k + b >= 1 \text{ if } y_k = 1$

$\mathbf{w} \cdot \mathbf{x}_k + b <= -1 \text{ if } y_k = -1$

Formulation of Linear SVM

Minimize **w.w** — **Quadratic Objective Function**

Subject to — **Linear Constraints**

$$\boldsymbol{w} \cdot \boldsymbol{x}_k + b >= 1 \text{ if } y_k = 1$$

$$\boldsymbol{w} \cdot \boldsymbol{x}_k + b <= -1 \text{ if } y_k = -1$$

Solving the Optimization Problem

Primal Problem

Find **w** and b such that

$\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^T\mathbf{w}$ is minimized

and for all $(\mathbf{x}_i, y_i)$, i=1..n : $y_i\,(\mathbf{w}^T\mathbf{x}_i + b) \geq 1$

Dual Problem

Packages are available for efficiently solving the above Quadratic Program (QP) to find the optimal w, b values

Find $\alpha_1 \ldots \alpha_n$ such that

$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ is maximized and

(1) $\Sigma\alpha_i y_i = 0$

(2) $\alpha_i \geq 0$ for all α_i

The Optimization Problem Solution

- Given a solution $\alpha_1 \dots \alpha_n$ to the dual problem, solution to the primal is:

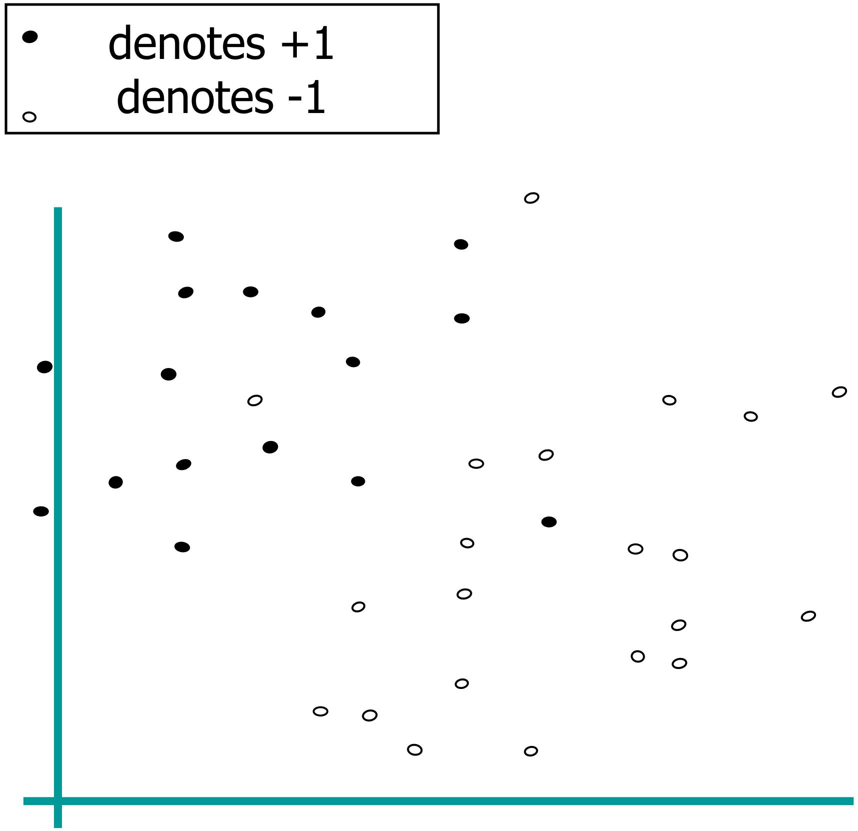
$$\mathbf{w} = \Sigma \alpha_i y_i \mathbf{x}_i \qquad b = y_k - \Sigma \alpha_i y_i \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_k \quad \text{for any } \alpha_k > 0$$

- Each non-zero α_i indicates that corresponding $\mathbf{x}_i$ is a support vector.
- Then the classifying function is (note that we don't need **w** explicitly):

$$f(\mathbf{x}) = \Sigma \alpha_i y_i \mathbf{x}_i^{\mathrm{T}} \mathbf{x} + b$$

- Notice that it relies on an *inner product* between the test point **x** and the support vectors $\mathbf{x}_i$ – we will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products $\mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j$ between all training points.

Welcome to the real world, Neo! ☺



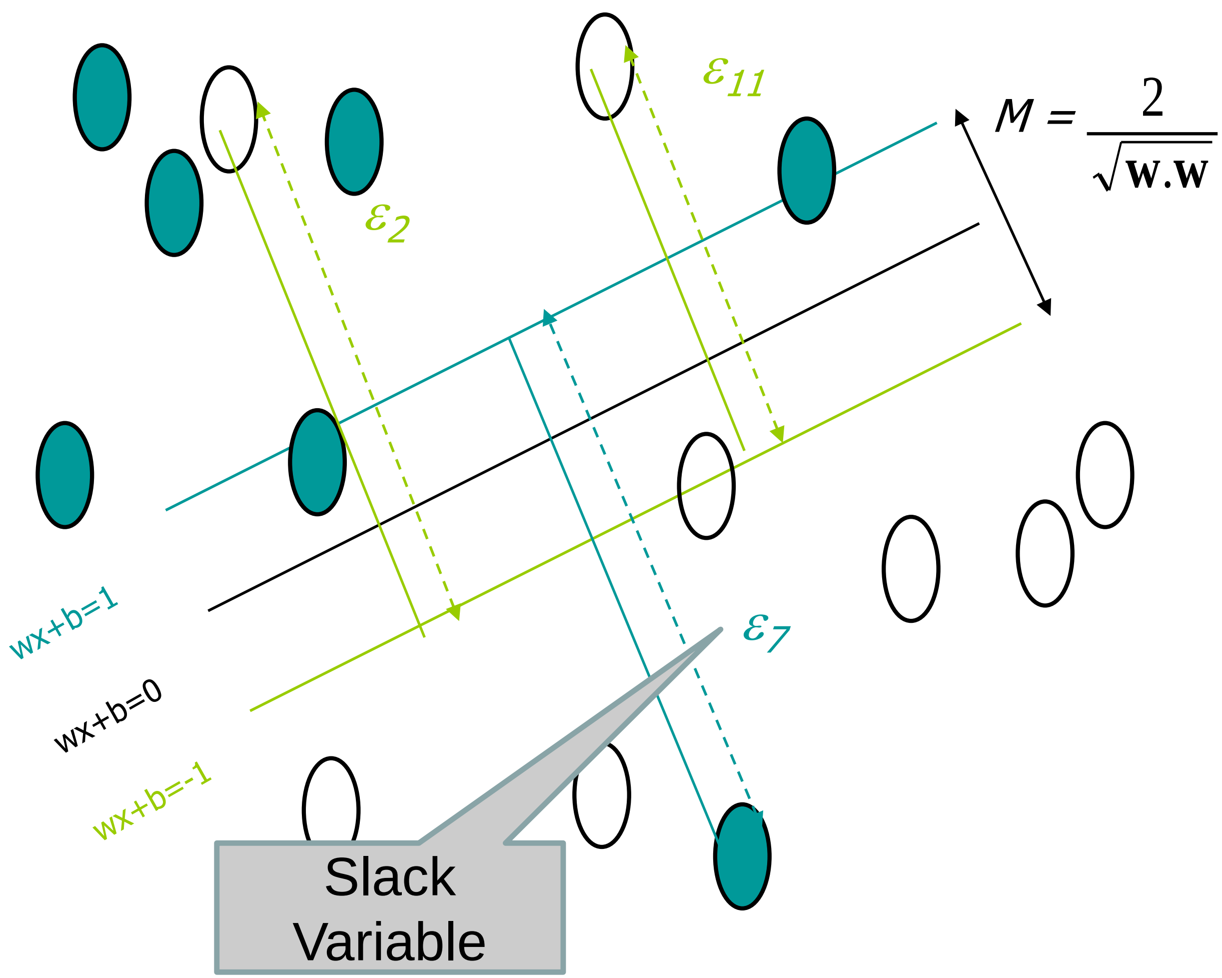
Can we classify this data with the previous formulation?

We can't!

In real world data points are

- Often not linearly separable
- Prone to noise and outliers

Fixing the Formulation to handle Noise



Relaxing Constraints

$\mathbf{w} \cdot \mathbf{x}_k + b \geq 1 - \varepsilon_k$ if $y_k = 1$

$\mathbf{w} \cdot \mathbf{x}_k + b \leq -1 + \varepsilon_k$ if y_k

Slack Constraints

$\varepsilon_k \geq 0$ for all k

Fixing Objective

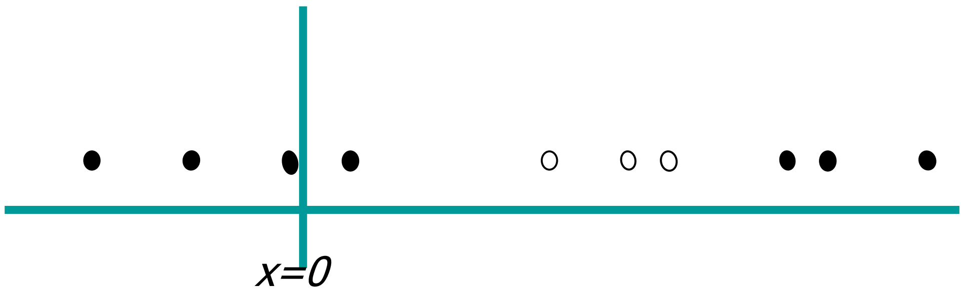
$$Minimize \frac{1}{2}\mathbf{w.w} + C\sum_{k=1}^{R}\varepsilon_k$$

SVM Parameter - C

- Controls training error
- Used to prevent over-fitting
- Lets play with C – Demo Link

Learning Non-Linear Patterns

Yet another challenge to Linear SVM!

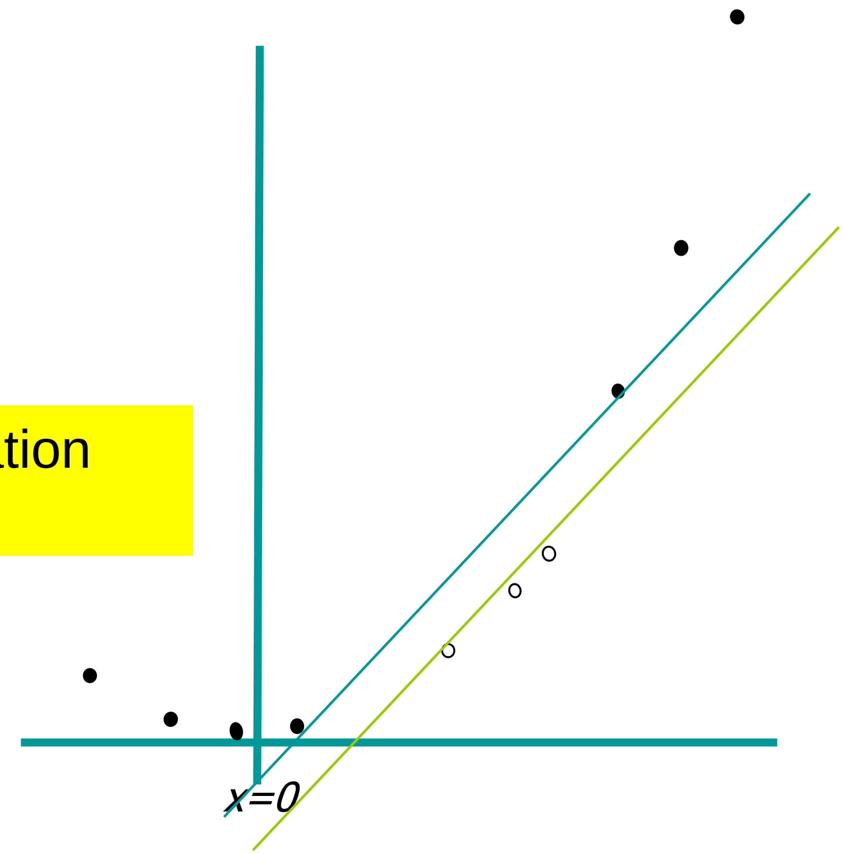


What can be done about this?

Is it time to give up? ☺

Harder 1-dimensional Dataset

Let's map the data points into a higher dimensional space.

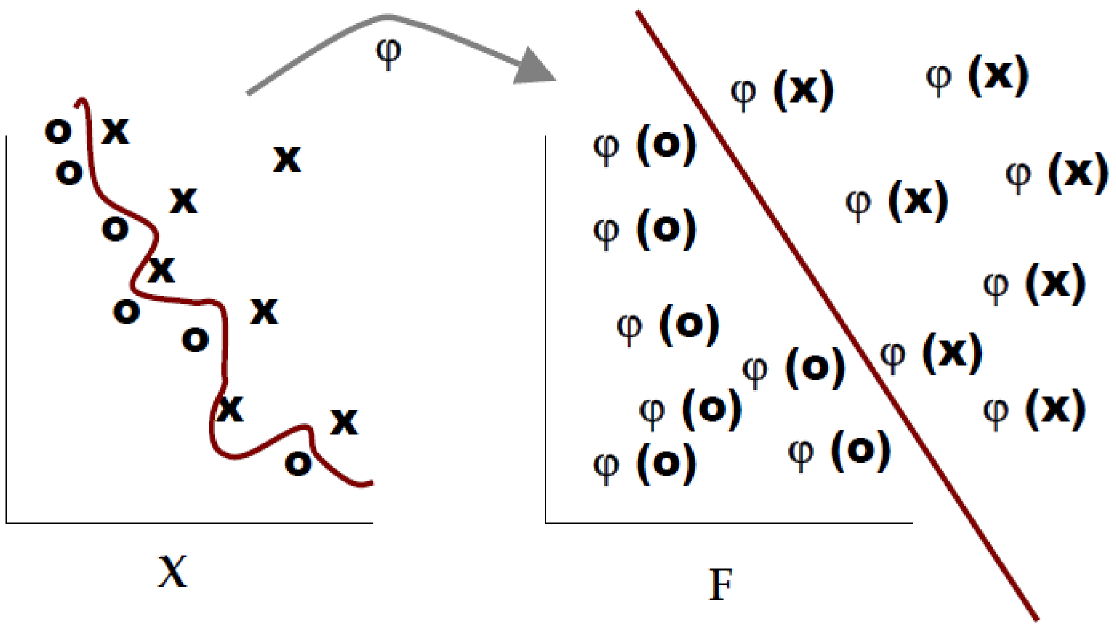


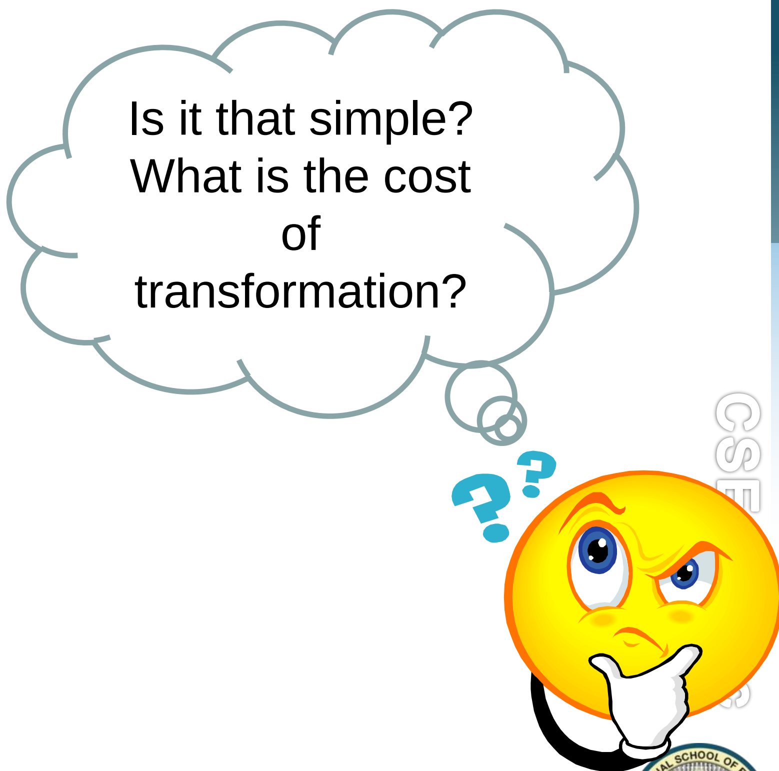
Linear SVM formulation still works! ☺

$$\mathbf{z}_k = (x_k, x_k^2)$$

Non-Linear SVMs: Feature Space Mappings

- Transform the original training samples onto a higher dimensional feature space





Learning Quadratic Functions

$$
\mathbf{\Phi}(\mathbf{x}) = \begin{pmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ \vdots \\ \sqrt{2}x_m \\ x_1^2 \\ x_2^2 \\ \vdots \\ x_m^2 \\ \sqrt{2}x_1x_2 \\ \sqrt{2}x_1x_3 \\ \vdots \\ \sqrt{2}x_1x_m \\ \sqrt{2}x_2x_3 \\ \vdots \\ \sqrt{2}x_1x_m \\ \vdots \\ \sqrt{2}x_{m-1}x_m \end{pmatrix}
\begin{array}{l} \} \text{ Constant Term} \\ \} \text{ Linear Terms} \\ \} \text{ Pure Quadratic Terms} \\ \} \text{ Quadratic Cross-Terms} \end{array}
$$

Constant Term

Linear Terms

Pure Quadratic Terms

Quadratic Cross-Terms

Number of terms (assuming m input dimensions) =

= (m+1)-Choose-2
= (m+1).(m)/2
= $O(m^2/2)$

In general, for degree ‘d’ polynomials:

(d+m-1)-Choose-d
=$O(m^d)$

The Kernel Trick

$$\mathit{Minimize}\ \frac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_{k=1}^{R}\varepsilon_k$$

$\mathbf{w} \,.\, \mathbf{x}_k + b >= 1-\varepsilon_k$ if $y_k = 1$

$\mathbf{w} \,.\, \mathbf{x}_k + b <= -1+\varepsilon_k$ if $y_k = -1$

Original QP

Using optimization theory transformed into Dual Problem

Training examples only occur as dot products of each other and not individually!

Maximize $$\sum_{k=1}^{R}\alpha_k - \frac{1}{2}\sum_{k=1}^{R}\sum_{l=1}^{R}\alpha_k\alpha_l y_k y_l < x_k . x_l >$$

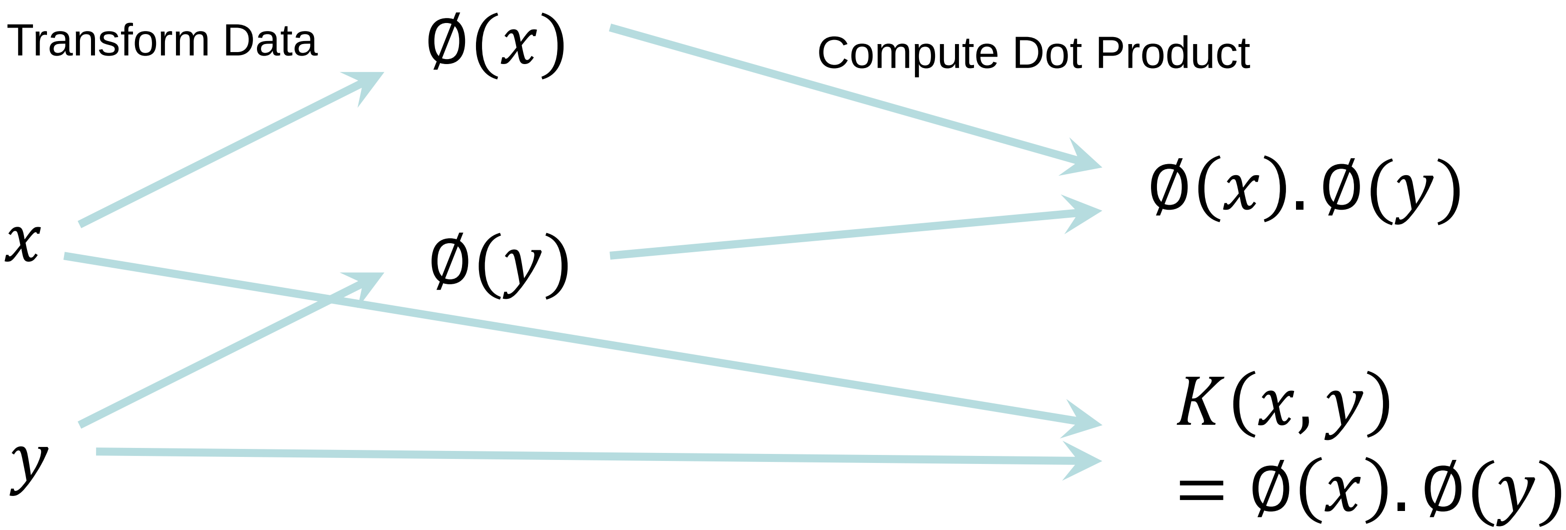
Subject to these constraints: $0 \le \alpha_k \le C \quad \forall k \qquad \sum_{k=1}^{R}\alpha_k y_k = 0$

$$\mathbf{w} = \sum_{k=1}^{R}\alpha_k y_k \mathbf{x}_k$$

$$b = y_K(1-\varepsilon_K) - \mathbf{x}_K . \mathbf{w}_K$$

$$\text{where } K = \arg\max_k \alpha_k$$

The Kernel Trick



K is known as the **Kernel Matrix**

Captures the similarity between training instances x and y

$$\Phi(\mathbf{a}) \bullet \Phi(\mathbf{b}) = \begin{pmatrix} 1 \\ \sqrt{2}a_1 \\ \sqrt{2}a_2 \\ \vdots \\ \sqrt{2}a_m \\ a_1^2 \\ a_2^2 \\ \vdots \\ a_m^2 \\ \sqrt{2}a_1a_2 \\ \sqrt{2}a_1a_3 \\ \vdots \\ \sqrt{2}a_1a_m \\ \sqrt{2}a_2a_3 \\ \vdots \\ \sqrt{2}a_1a_m \\ \vdots \\ \sqrt{2}a_{m-1}a_m \end{pmatrix} \bullet \begin{pmatrix} 1 \\ \sqrt{2}b_1 \\ \sqrt{2}b_2 \\ \vdots \\ \sqrt{2}b_m \\ b_1^2 \\ b_2^2 \\ \vdots \\ b_m^2 \\ \sqrt{2}b_1b_2 \\ \sqrt{2}b_1b_3 \\ \vdots \\ \sqrt{2}b_1b_m \\ \sqrt{2}b_2b_3 \\ \vdots \\ \sqrt{2}b_1b_m \\ \vdots \\ \sqrt{2}b_{m-1}b_m \end{pmatrix}$$

$$1 + \sum_{i=1}^{m} 2a_ib_i + \sum_{i=1}^{m} a_i^2b_i^2 + \sum_{i=1}^{m}\sum_{j=i+1}^{m} 2a_ia_jb_ib_j$$

Define K(**a**,**b**) = $(\mathbf{a}.\mathbf{b}+1)^2$

$$= (\mathbf{a}.\mathbf{b})^2 + 2\mathbf{a}.\mathbf{b} + 1$$

$$= \left(\sum_{i=1}^{m} a_ib_i\right)^2 + 2\sum_{i=1}^{m} a_ib_i + 1$$

$$= \sum_{i=1}^{m}\sum_{j=1}^{m} a_ib_ia_jb_j + 2\sum_{i=1}^{m} a_ib_i + 1$$

$$= \sum_{i=1}^{m}(a_ib_i)^2 + 2\sum_{i=1}^{m}\sum_{j=i+1}^{m} a_ib_ia_jb_j + 2\sum_{i=1}^{m} a_ib_i + 1$$

Both are same!

And K(a,b) is only O(m) to compute!

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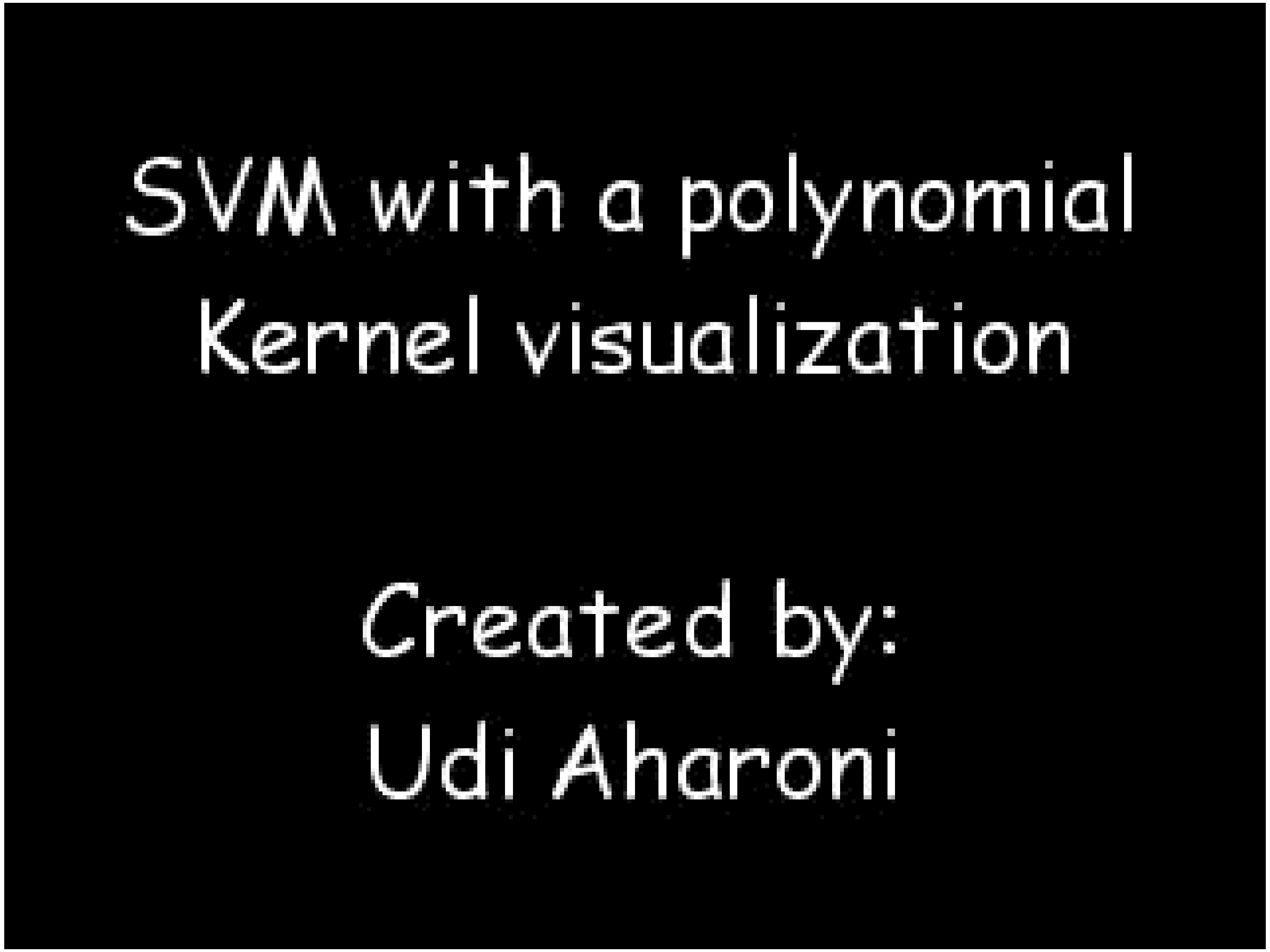
Polynomial Kernel Visualization



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SVM Kernel Functions

- Polynomial Kernel

$$K(\boldsymbol{a}, \boldsymbol{b}) = (\boldsymbol{a}.\boldsymbol{b} + 1)^d$$

- Radial Basis Kernel

$$K(\mathbf{a}, \mathbf{b}) = \exp\left(-\frac{(\mathbf{a}-\mathbf{b})^2}{2\sigma^2}\right)$$

- Hyperbolic Tangent

$$K(\mathbf{a}, \mathbf{b}) = \tanh(\kappa \mathbf{a}.\mathbf{b} - \delta)$$

Project onto infinite dimensional space

SVM Parameter Tuning

- Is very important
- C, Kernel parameters
- Example:

$$-\sigma \ in \ \exp\left(\frac{(\boldsymbol{a}-\boldsymbol{b})^2}{2\sigma^2}\right) \text{ RBF Kernel}$$

- How to select them?

Tuning Steps

- Map categorical features to numerical values
- Re-scale features so that features with high values don't dominate

	height	sex
x_1	150	F
x_2	180	M
x_3	185	M

$$y_1 = 0, y_2 = 1, y_3 = 1$$

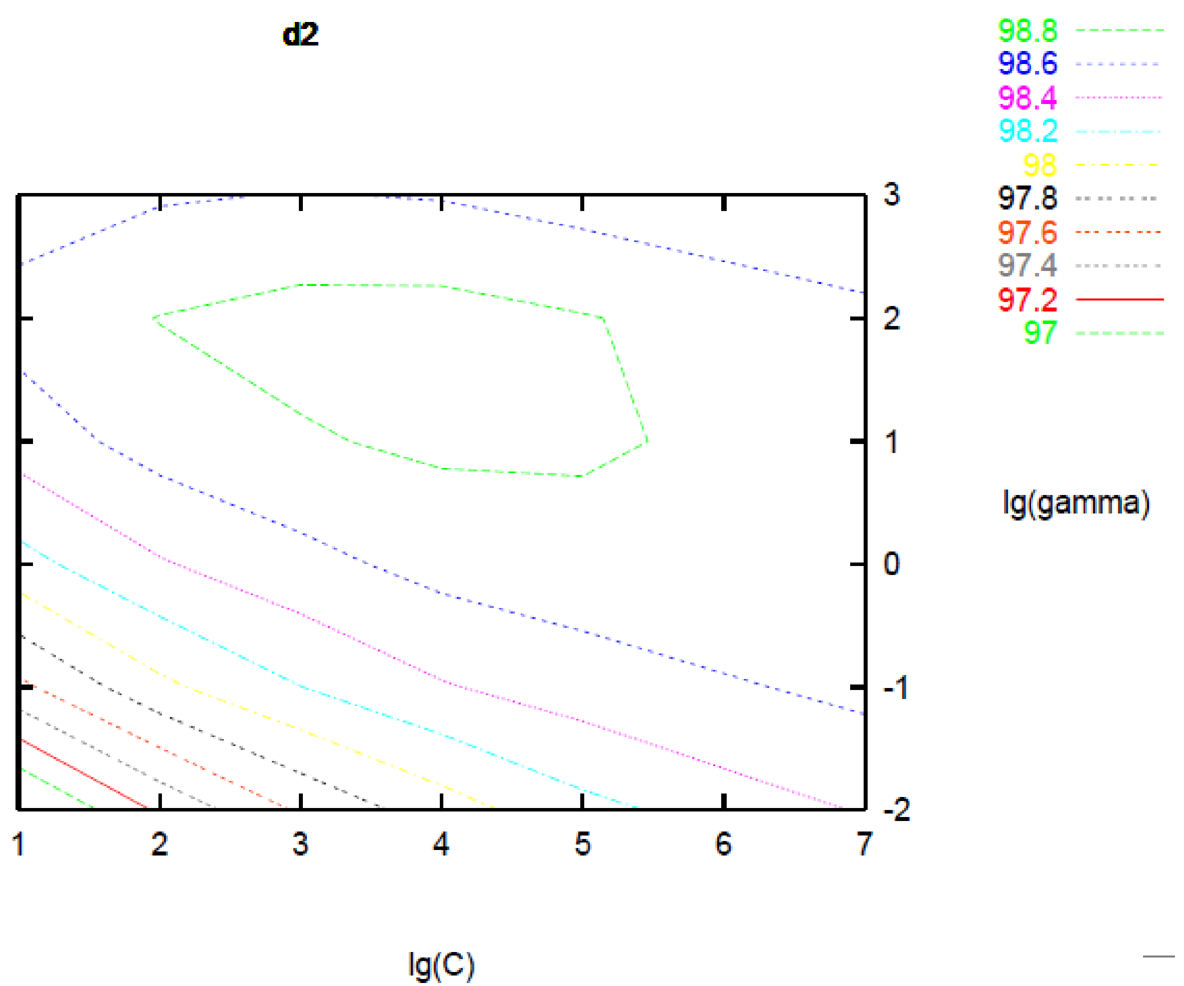
$$height = \frac{height - 150}{185 - 150}$$

	height	sex_m	sex_f
x1	0	0	1
x2	0.857143	1	0
x3	1	1	0

Tuning Steps (Contd..)

- Pre-process (scaling, numerical mapping etc.) training data
- Pick up RBF Kernel
- Use Cross-Validation to find the best C and σ parameter values
- Use the best C, σ to train on the entire training set
- Test

Tuning SVMs (Contd..)



Handling Class Imbalance

- Many practical applications have class imbalance
  - Detecting Fraud Transactions
  - Cancer Detection
- Default SVM formulation will learn highly skewed hyperplanes
- However, we want generalization errors to be equally distributed between positive and negative class

$$\min_{w,b} \frac{1}{2}||w||_2^2 + \frac{C}{N_+} \sum_{j\,:\,y_j=+1} \xi_j + \frac{C}{N_-} \sum_{j\,:\,y_j=-1} \xi_j$$

SVMs – Advantages

- Flexibility in choosing the similarity function (by choosing the kernel)
- Exploits the sparseness of solution when dealing with large datasets
  - Only support vectors specify the hyperplane irrespective of size of dataset
- Can handle large feature sets efficiently
  - Complexity doesn't depend on the dimensionality of feature space
- Good theoretical guarantees
  - Maximum margin generalizes better
  - Convex optimization problem which is guaranteed to converge

SVMs – Shortcomings

- Sensitive to noise and outliers
  - Some noisy or outlier training samples can significantly alter the hyperplane and hence the performance
- SVM doesn’t provide a *posterior probability* which is required for many applications
- Formulation is not clean for multi-labeled classification problems
  - For ‘m’ classes, train ‘m’ One vs. Rest Binary Classifiers
    - Input can be assigned to multiple classes
    - Results in class imbalance
  - Train m (m-1)/2 different binary classifiers on pairs of classes
    - Classify test points based on which class receives highest votes
    - For large ‘m’ requires significantly larger training time

Summary

- Support Vector Machines (SVMs) work very well in practice for a large class of classification problems
- SVMs work on the principle of learning a maximum margin hyperplane which results in good generalization
- The basic linear SVM formulation could be extended to handle noisy and non-separable data
- The Kernel Trick could be used to learn complex non-linear patterns
- For better performance, one has to tune the SVM parameters such as C, kernel parameters using validation set

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