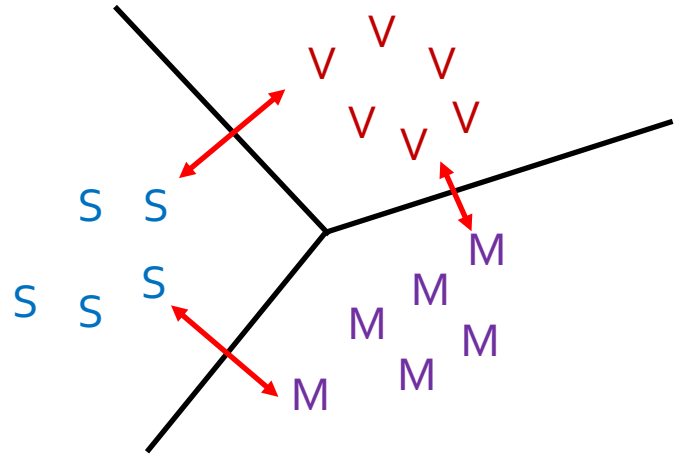
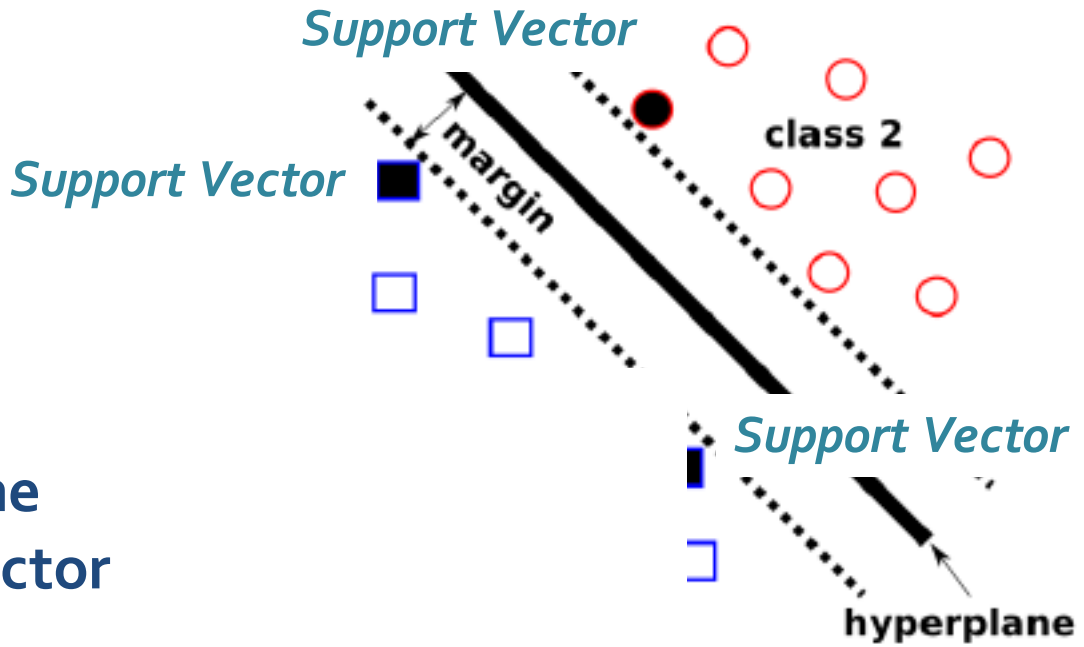


Chapter 9. Advanced Classification: Support Vector Machines (SVMs)

Meng Jiang

CSE 40647/60647 Data Science Fall 2017

Concepts



Quick start:

1. **Hyperplane**
2. **Supper Vector**
3. **Margin**
4. **SVMs**
5. **Maximize Margin Width**
6. **Non-linear SVMs: Kernel Function**

A Classification Problem

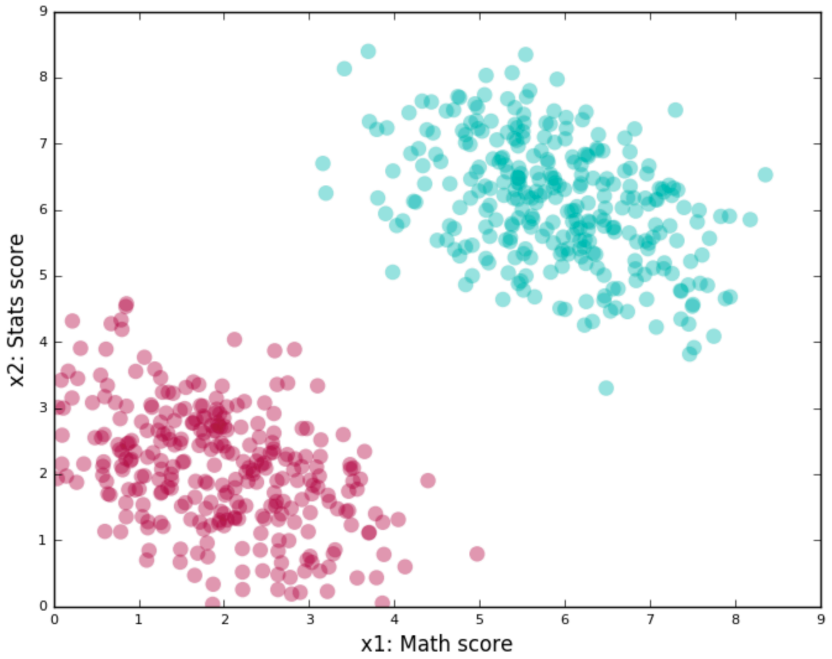
- Dataset
  - Suppose **data science** course instructors have observed that students get the *most out of the course* if they are good at *Math* or *Stats*.
  - Over time, they have recorded the *scores* of the enrolled students in these subjects.
  - Also, for each of these students, they have a *label* depicting their performance in the data science course: "*Good*" or "*Bad*".

A Classification Problem (cont.)

- Research problem
  - Now they want to determine the *relationship* between Math and Stats *scores* and the *performance (label)* in the ML course.
- Application
  - Perhaps, based on what they find, they want to specify a *prerequisite for enrolling in the course*.

A Classification Problem (cont.)

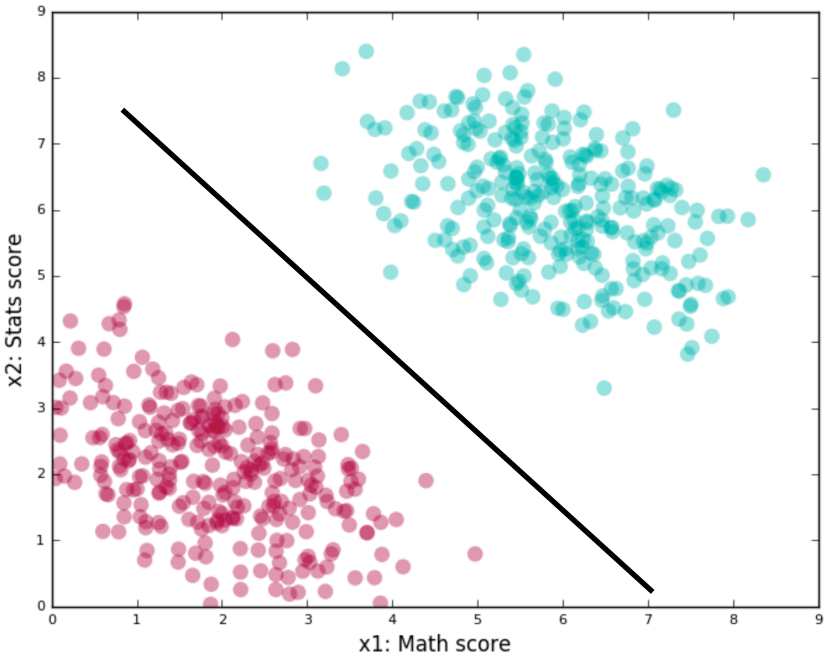
- Data Preprocessing + Visualization
  - Draw a two-dimensional *scatter plot*, where one axis represents scores in Math, while the other represents scores in Stats.
  - A *student* with certain scores is shown as a *point* on the graph.
  - The color of the point – *green* or *red* – represents how he/she did on the data science course: "*Good*" or "*Bad*" respectively.



Training data

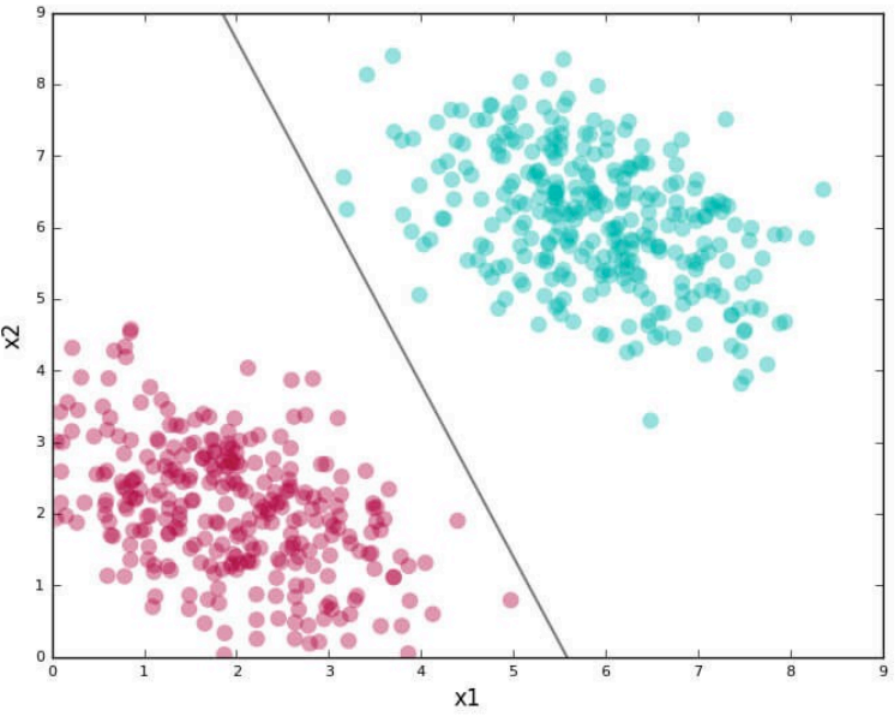
A Classification Problem (cont.)

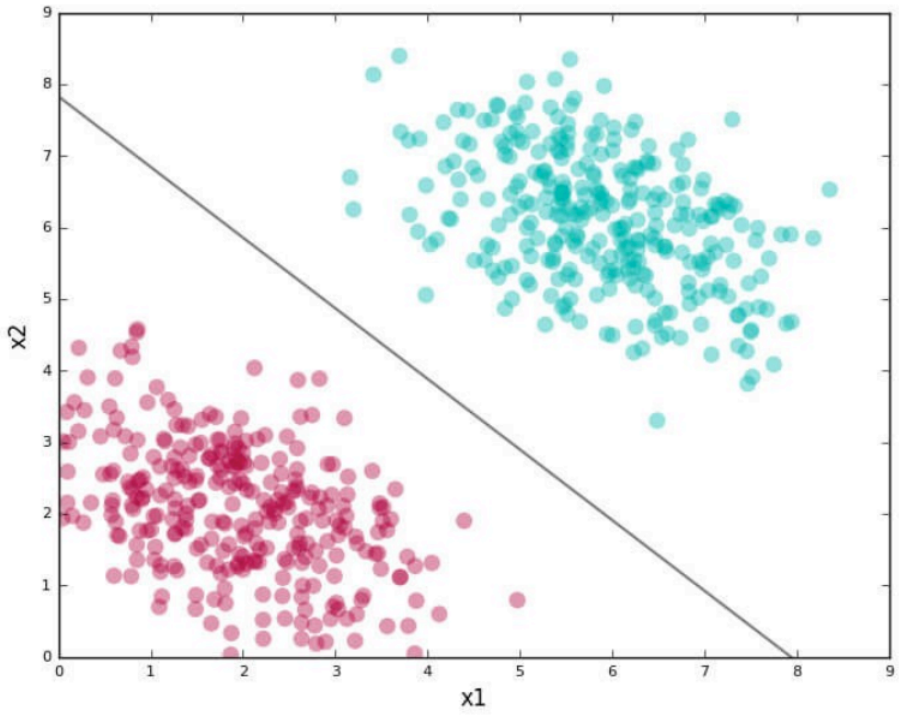
- Goal
  - Finding a ***line*** that passes between the red and green clusters, and then *determining which side* of this line a score tuple lies on, is a good algorithm.



A Classification Problem (cont.)

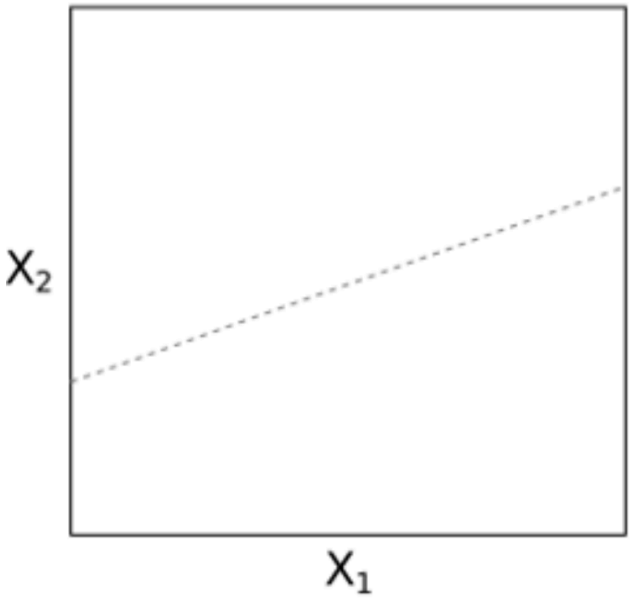
- The ***line*** is our *separating boundary* (because it separates out the labels) or *classifier* (we use it classify points).
- Two classifiers:

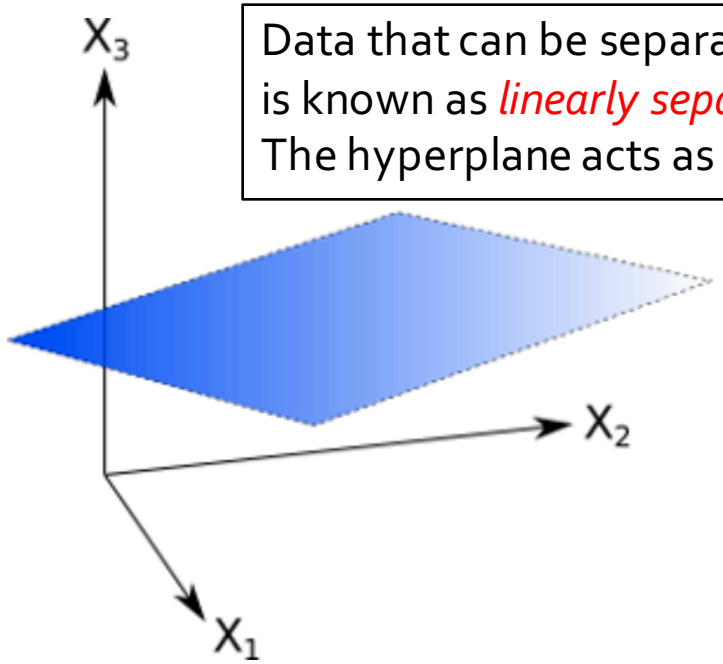




Concept 1: Hyperplane

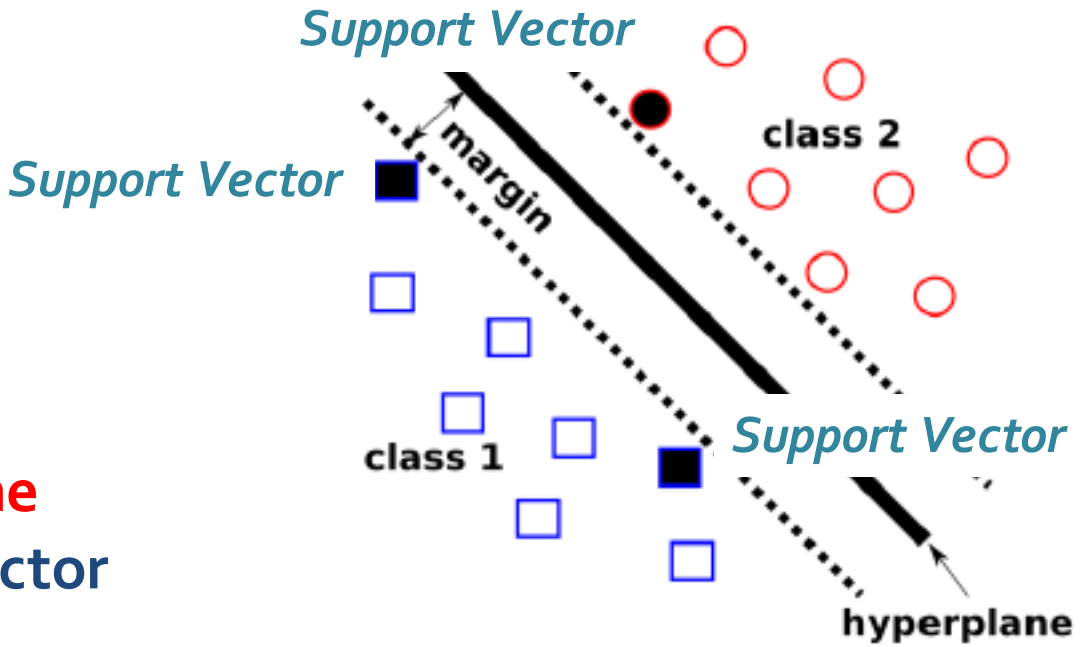
- In two dimensions we find a *line*.
- In three dimensions we find a *plane*.
- In high dimensions we find a *hyperplane* – a generalization of the two-dimensional line and three-dimensional plane to an *arbitrary number of dimensions*.





Data that can be separated by a hyperplane is known as *linearly separable* data.
The hyperplane acts as a *linear classifier*.

Concepts



Quick start:

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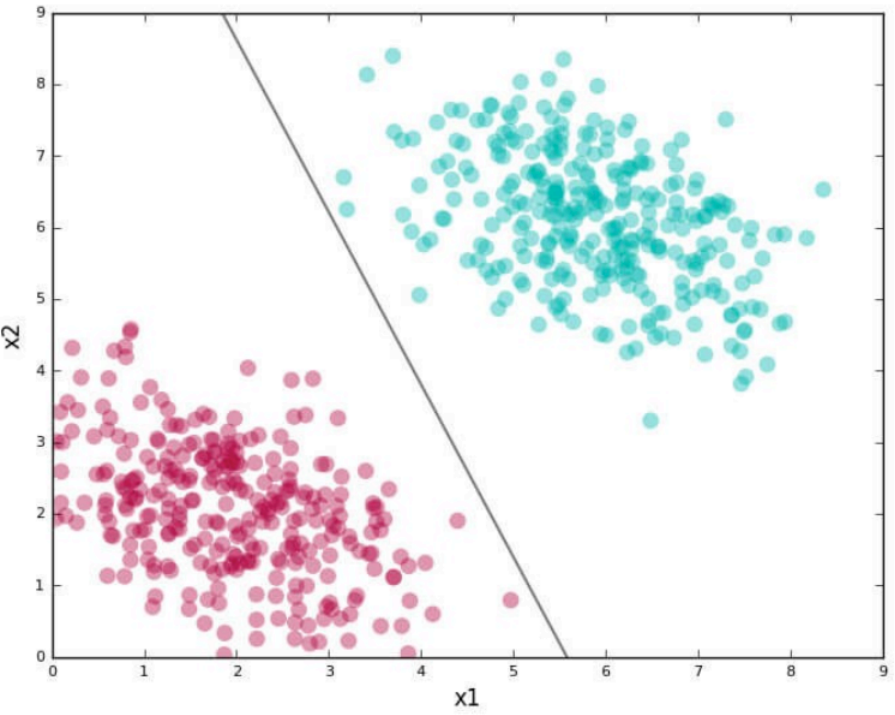
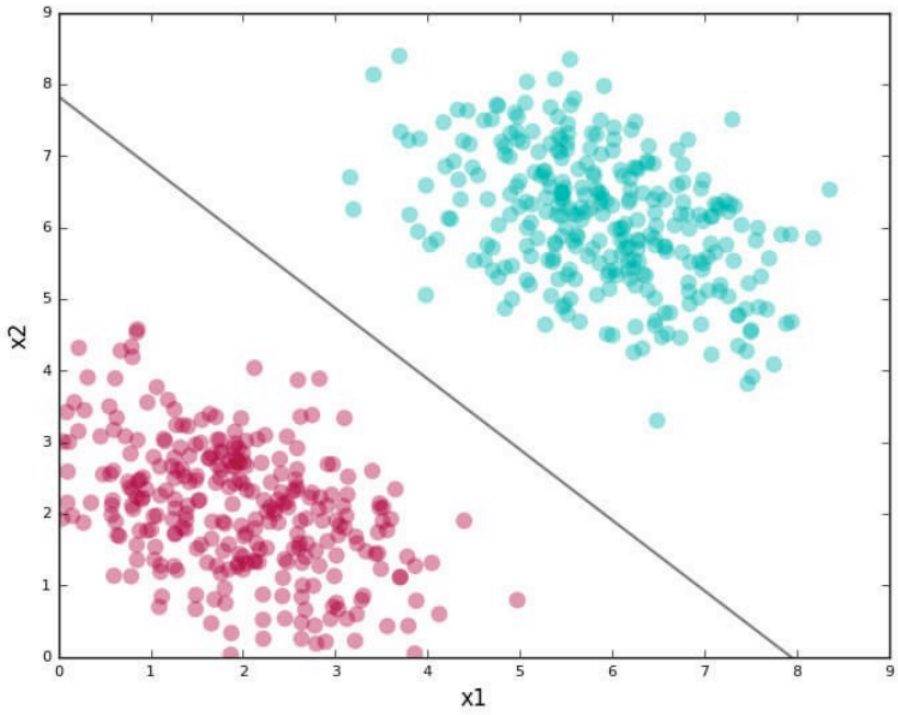
Good vs Bad Classifiers

Q: Both lines separate the red and green clusters. Is there a good reason to choose one over another?





Good vs Bad Classifiers

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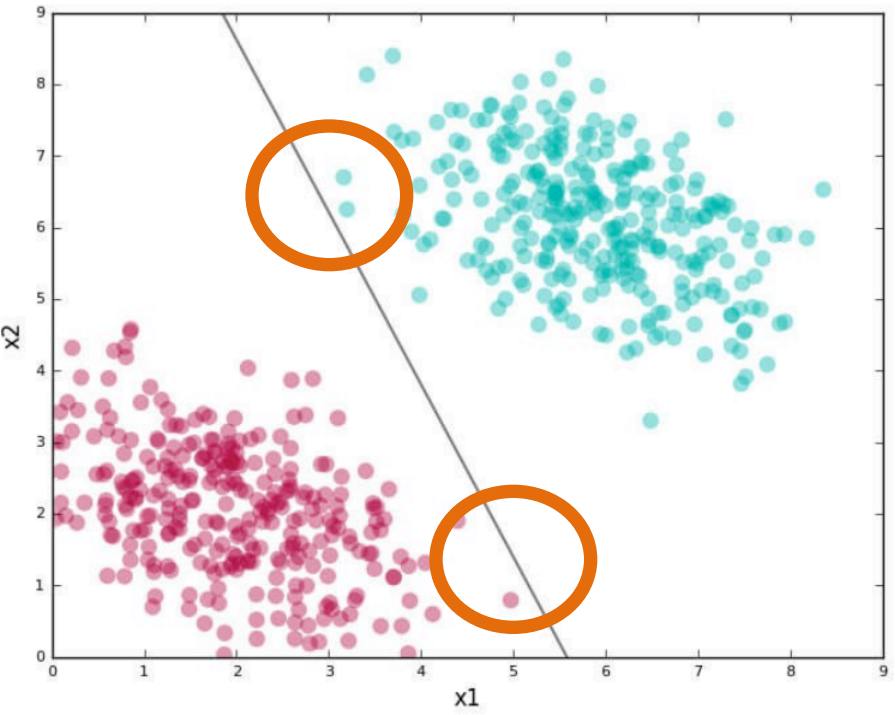
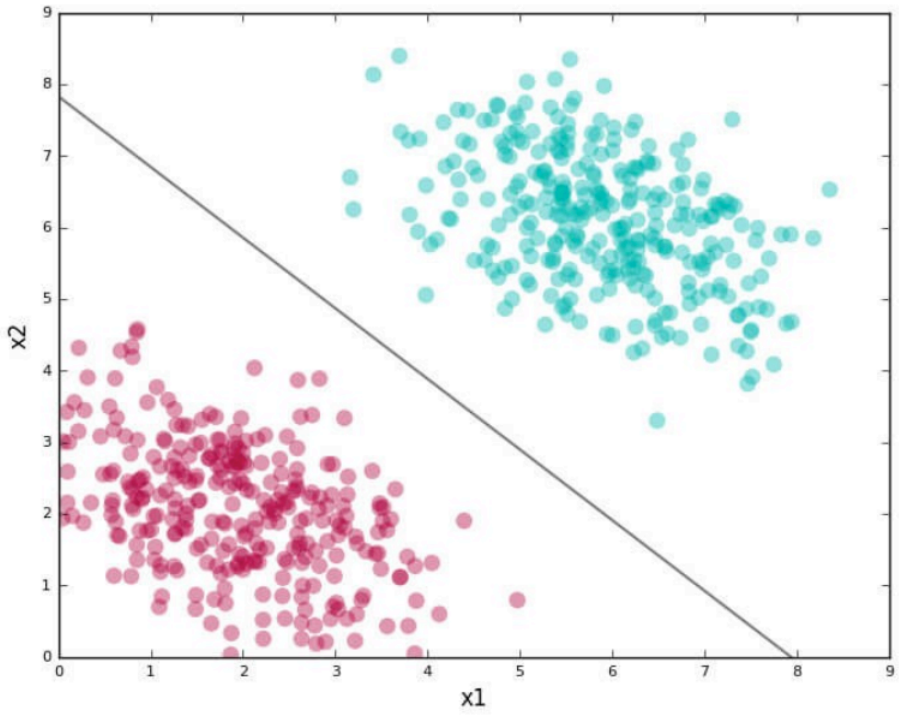
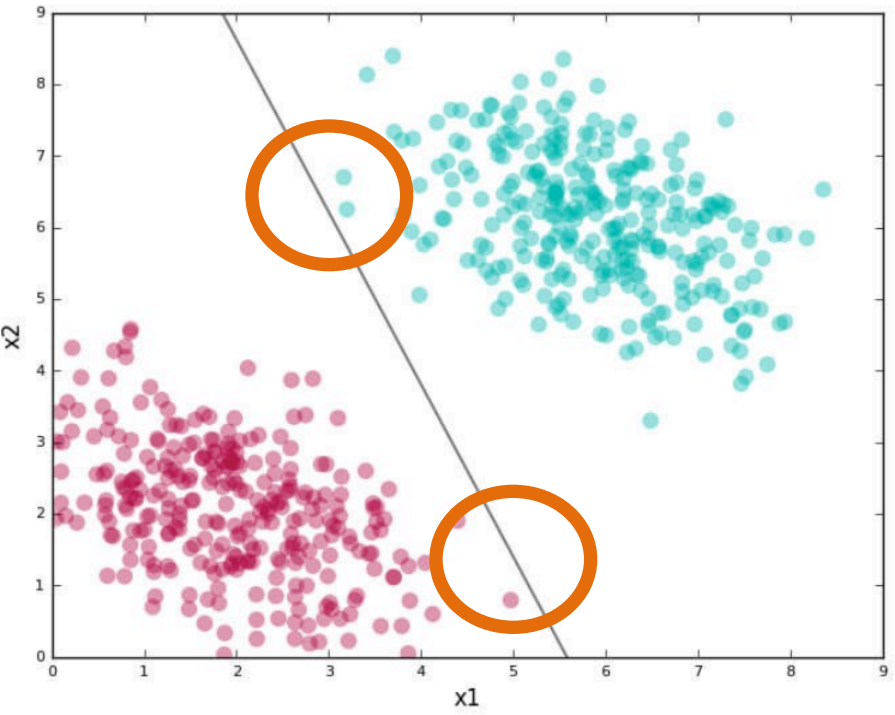


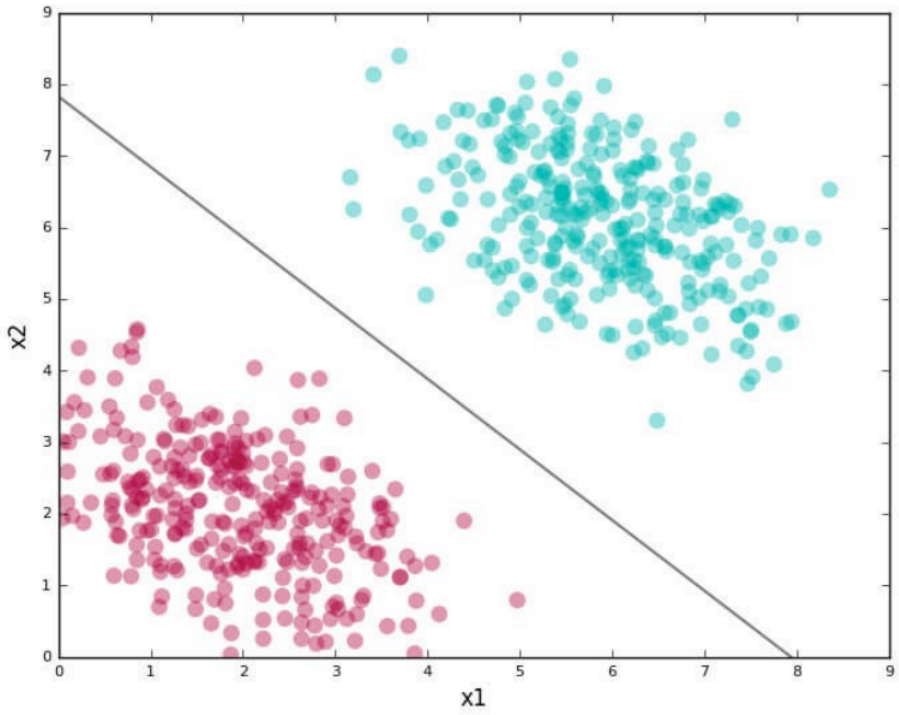


Good vs Bad Classifiers

A: We try to find the second kind of line.

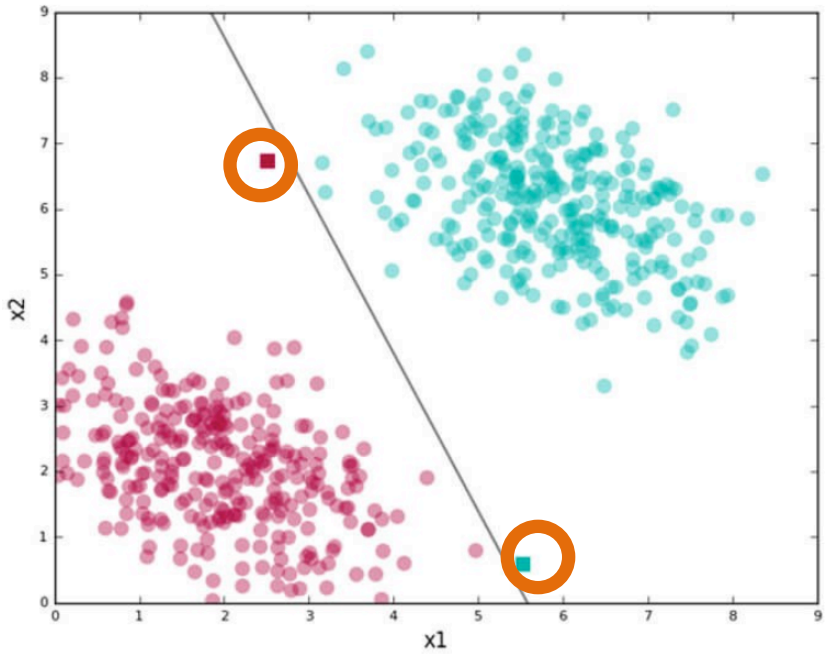
Q': Define ***underlying philosophy*** in the general case.

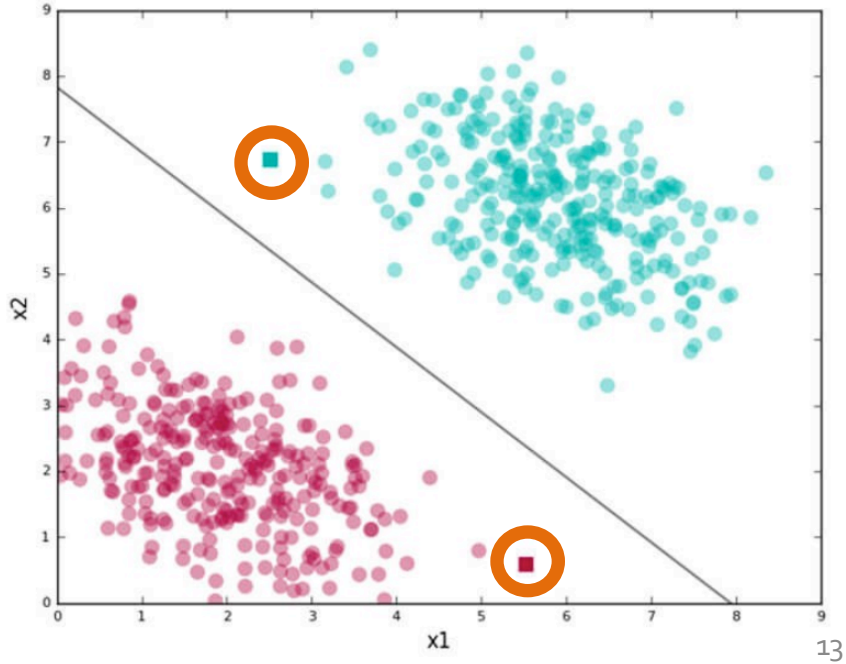




Good vs Bad Classifiers

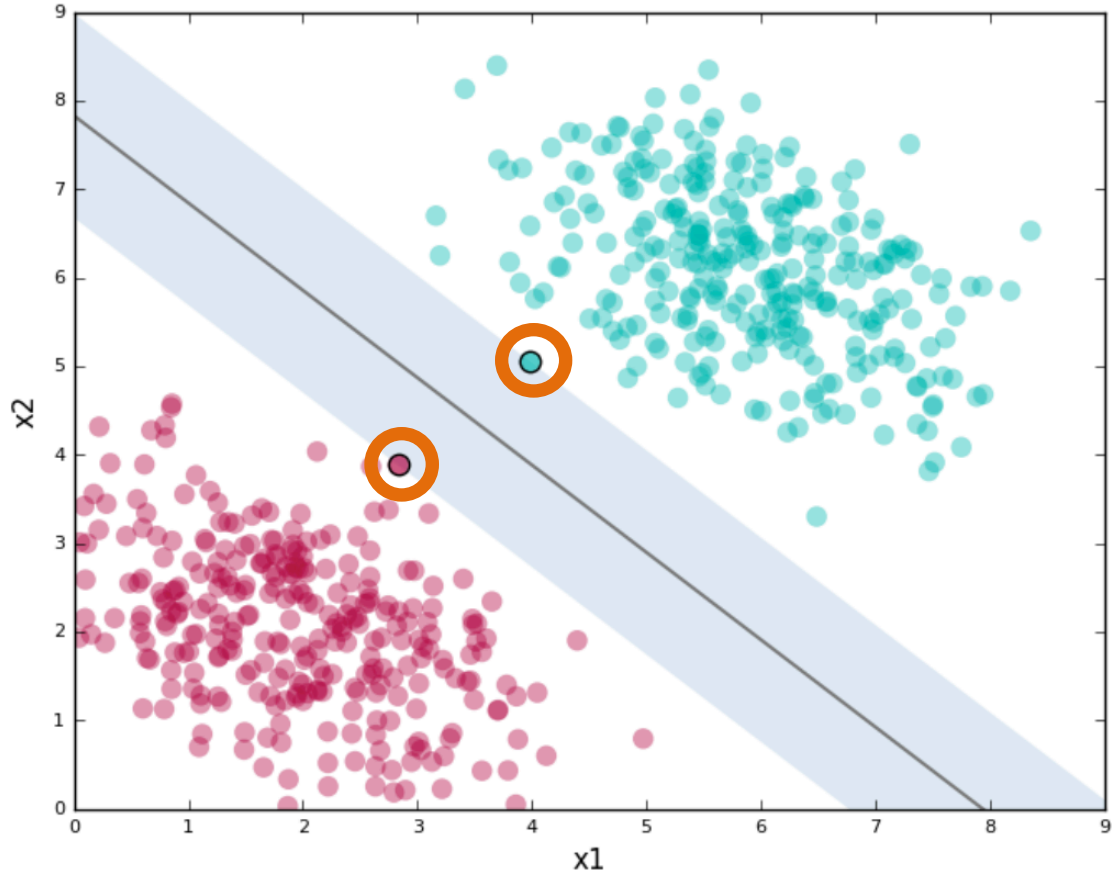
- Philosophy
  - Find lines that *correctly* classify the training data
  - Among all such lines, pick the one that has the *greatest distance* to the points closest to it





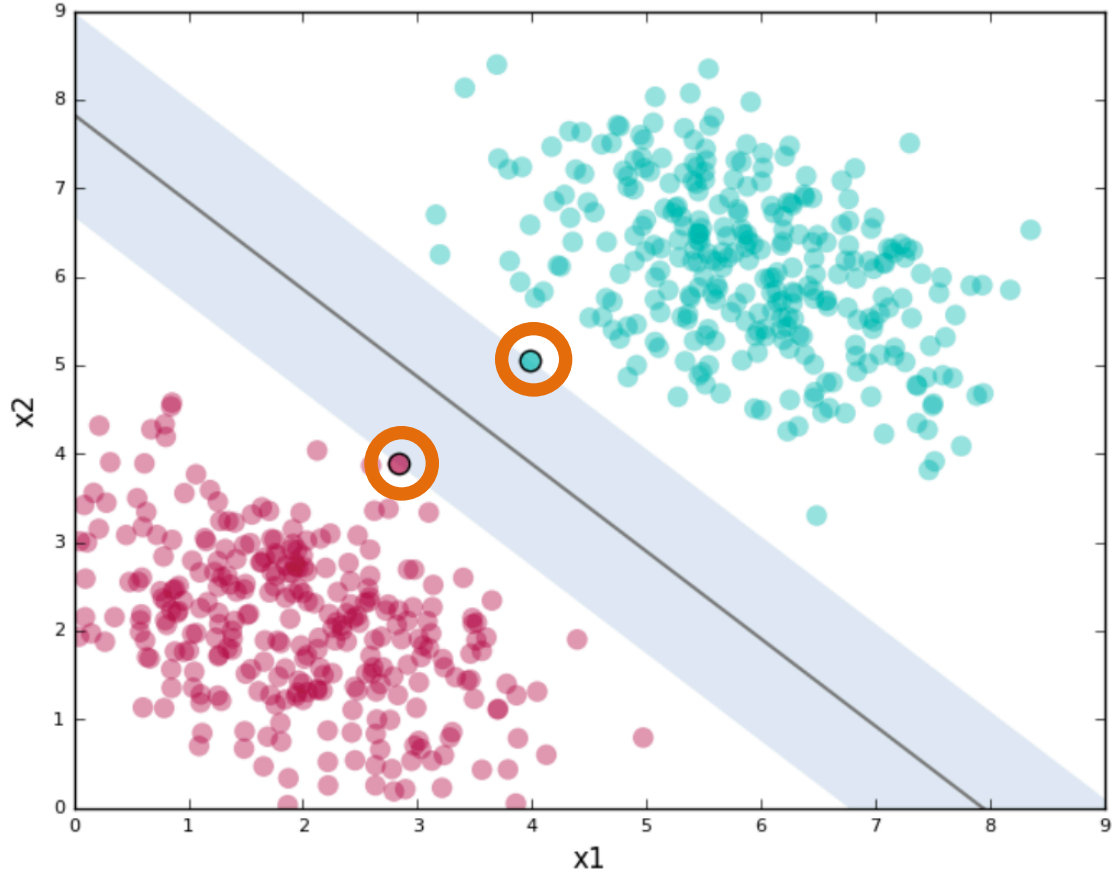
Concept 2: Support Vector

- The *closest points* that identify this line are known as ***support vectors***.

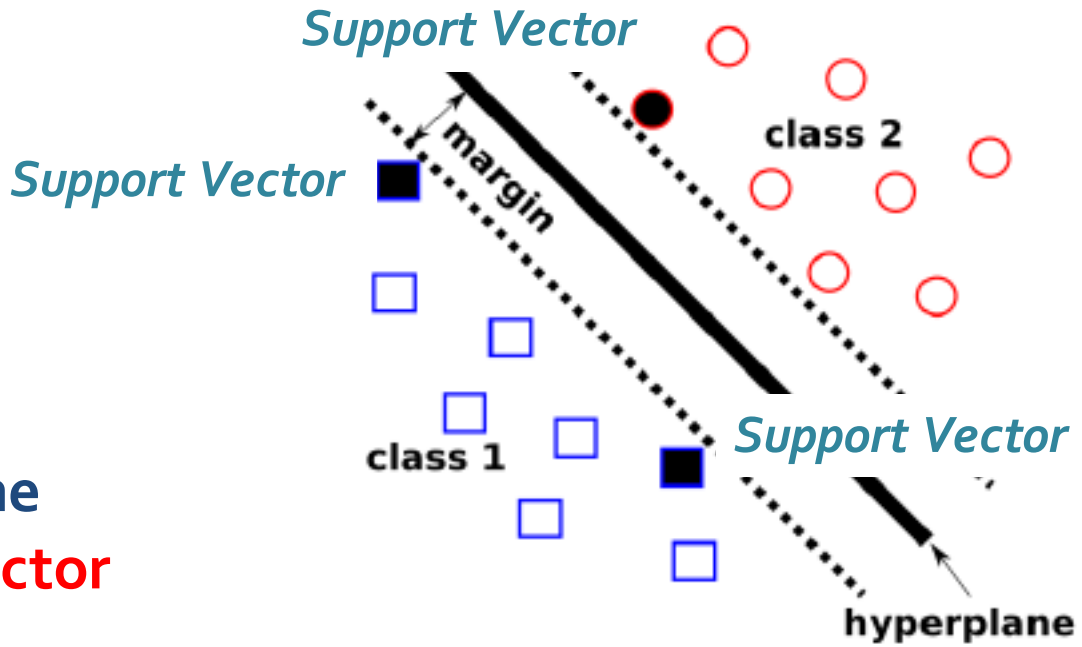


Concept 3: Margin

- The *(shaded) region* support vectors define around the line is known as the ***margin***.



Concepts



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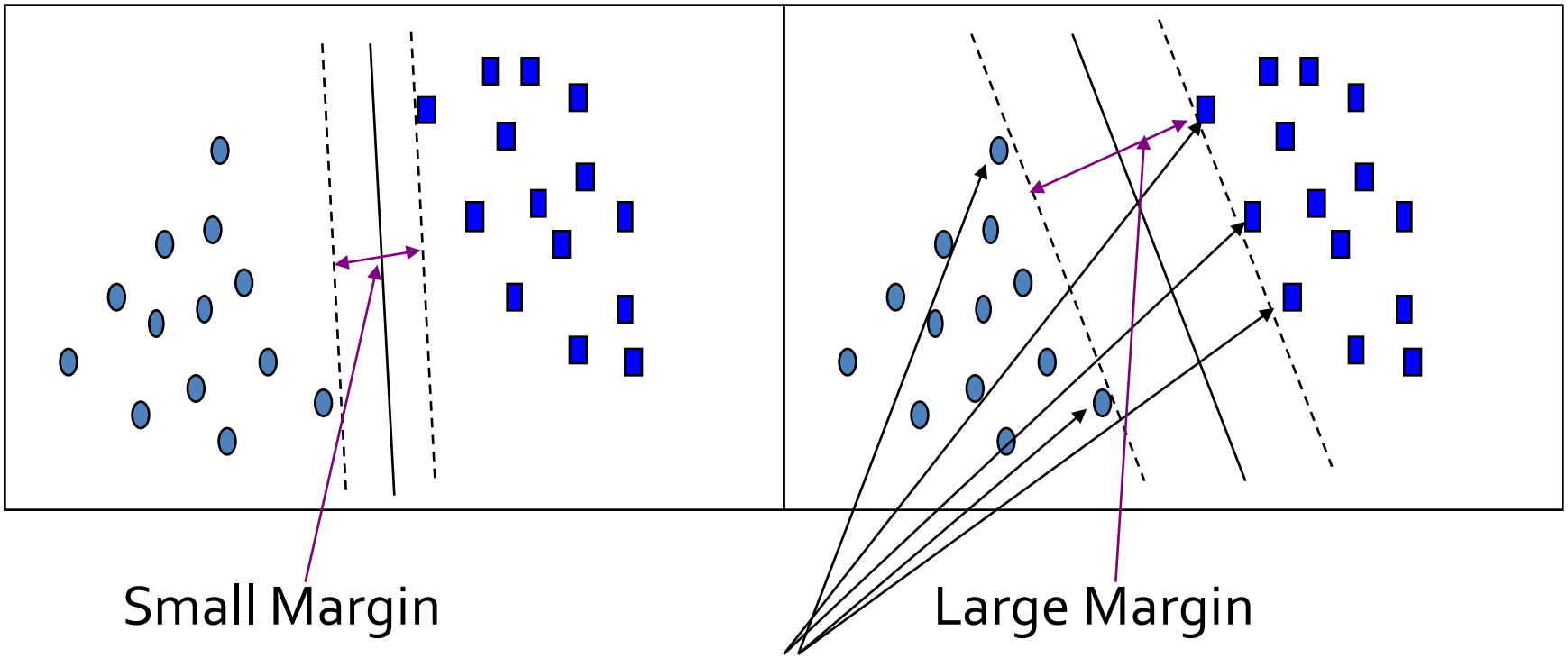
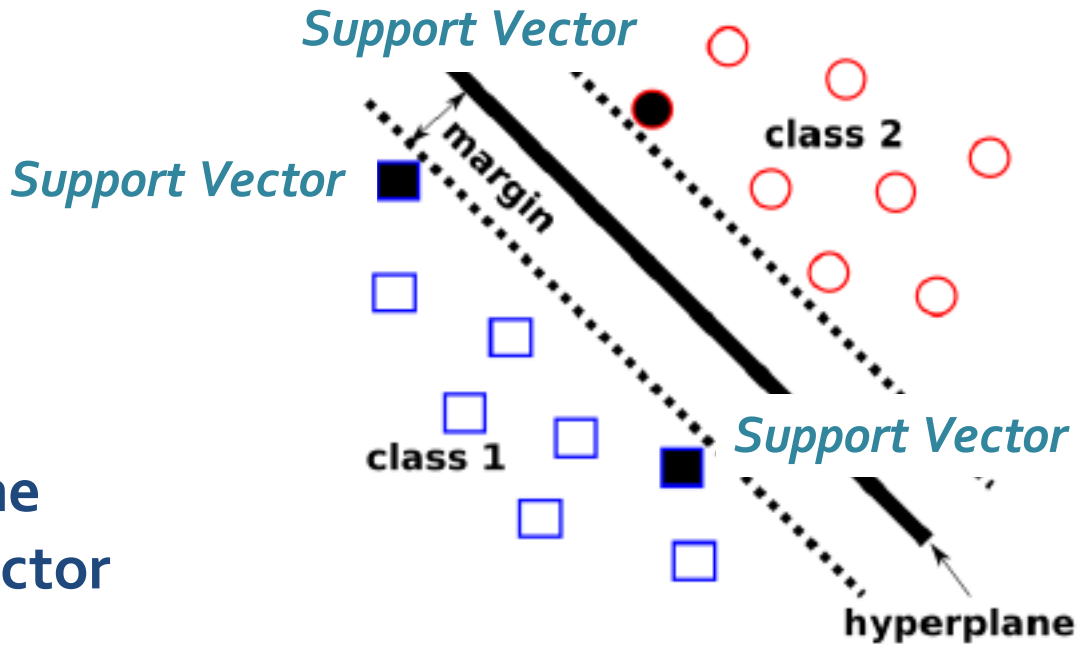
Support Vector Machines

- Definition (Wikipedia)
  - A SVM is a discriminative classifier formally defined by a *separating hyperplane*. In other words, given *labeled training data*, the algorithm outputs an *optimal hyperplane* which categorizes ***new examples***.
  - A *data point* is viewed as a *p*-dimensional vector, and we want to know whether we can separate such points with a *(p-1)*-dimensional hyperplane.
- Use
  - SVMs give you a way to *pick between many possible classifiers* in a way that guarantees a higher chance of correctly labeling your ***test data***.

SVM's General Philosophy: Largest Margin



Concepts



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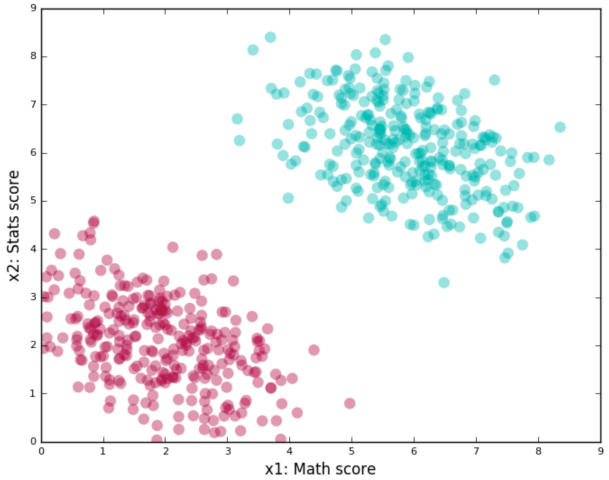
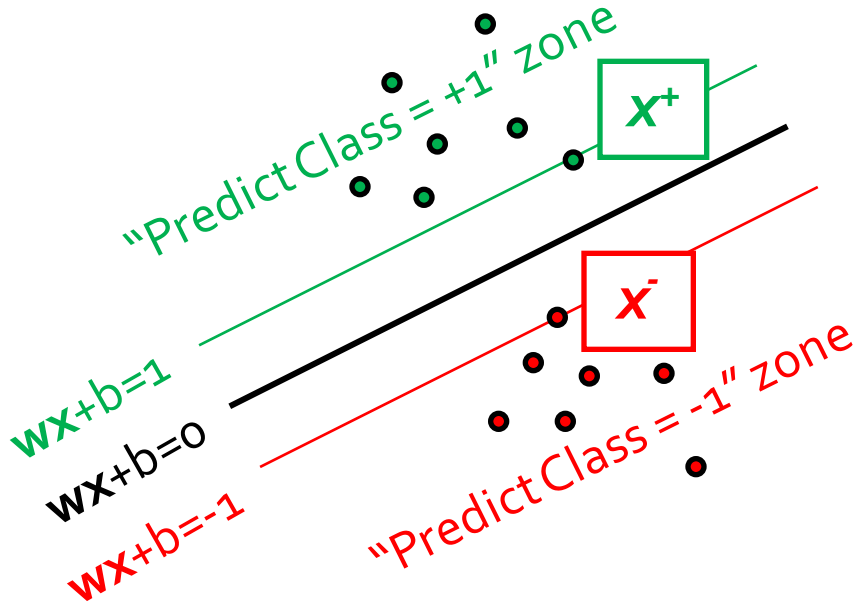
Formally Define the Problem

- Binary Classification
  - E.g., course performance classification
    - $x_i = (x_1, x_2, x_3, \ldots)$: Subject scores
    - $y_i = +1$ or -1: "Good" or "Bad"
    - x_1 : score of subject Math
    - x_2 : score of subject Stats



- Mathematically, $x \in \Re^n$, $y \in \{+1, -1\}$,
  - We want to derive a function **f: X → Y**

Optimization



Support vectors: x^+ x^-

Hyperplane: $\mathbf{wx}+b=0$

What we know:

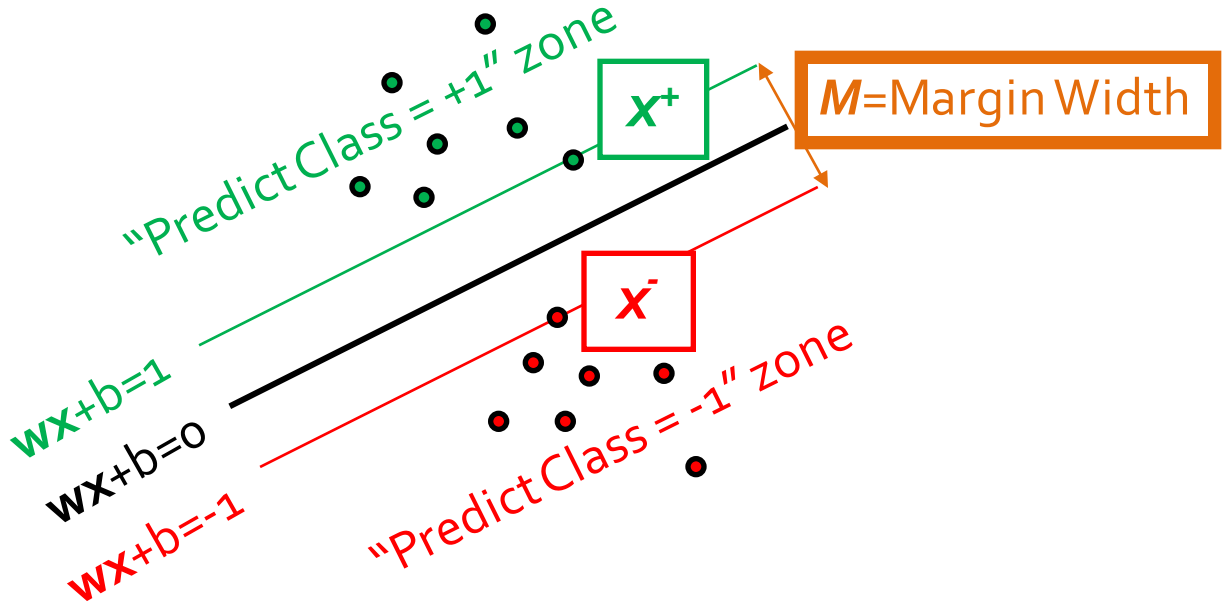
- $\boldsymbol{w} \cdot \boldsymbol{x}^+ + b = +1$
- $\boldsymbol{w} \cdot \boldsymbol{x}^- + b = -1$

A separating hyperplane can be written as

$$\mathbf{w} \cdot \mathbf{x} + b = 0,$$

where $\mathbf{w}=\{w_1, w_2, \ldots, w_n\}$ is a weight vector and b a scalar (bias).

Optimization



Support vectors: x^+ x^-

Hyperplane: $wx+b=0$

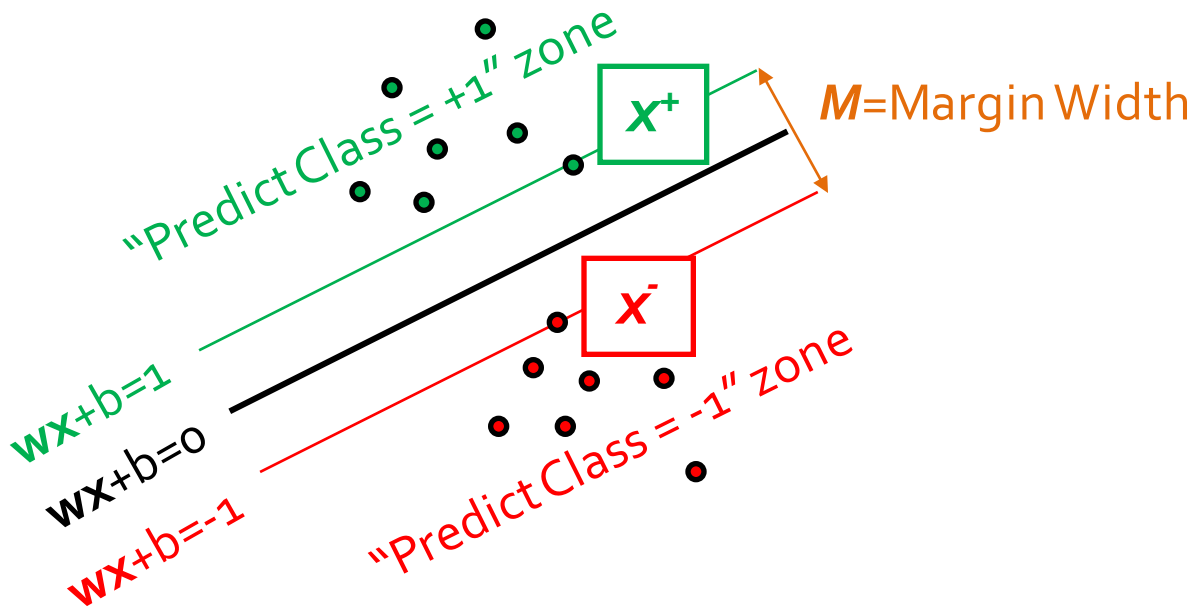
What we know:

- $w \cdot x^+ + b = +1$
- $w \cdot x^- + b = -1$

How to calculate the Margin Width?

Distance between two parallel lines.

Optimization: Maximize Margin Width



Support vectors: x^+ x^-

Hyperplane: **wx**+b=0

What we know:

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

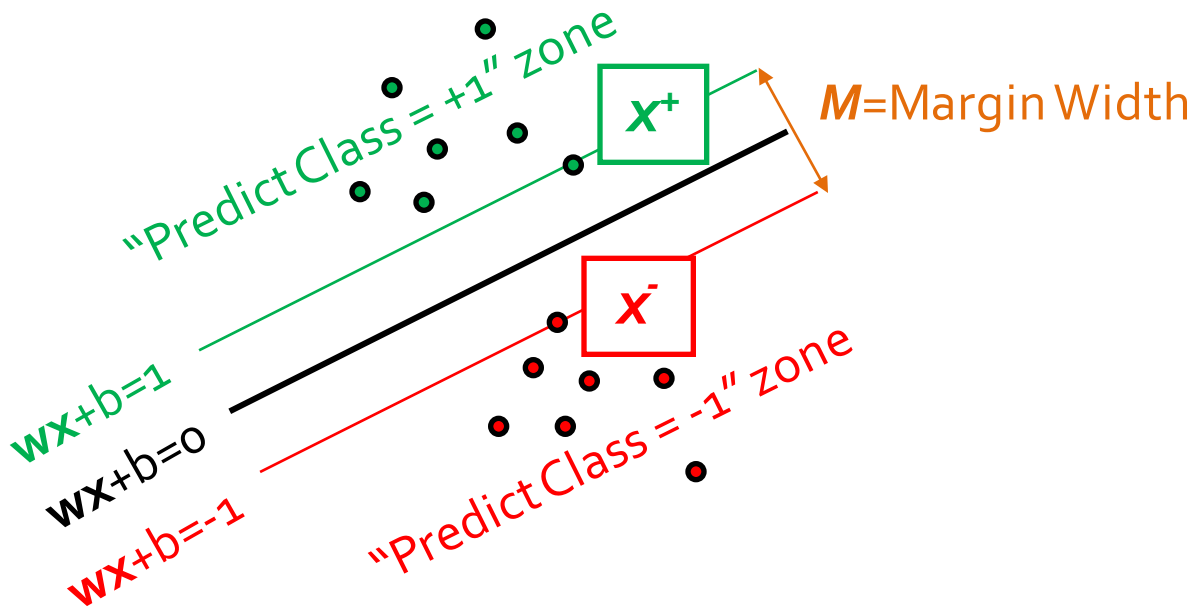
max $M = \dfrac{(x^+ - x^-) \cdot w}{|w|} = \dfrac{2}{|w|}$

same as *min* $\dfrac{1}{2} w^t w$

Any constraints?

Correctly categorize…

Optimization: Maximize Margin Width



Support vectors: x^+ x^-

Hyperplane: **wx**+b=0

What we know:

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

$$\textit{max} \quad M = \frac{(x^+ - x^-) \cdot w}{|w|} = \frac{2}{|w|}$$

same as *min* $\frac{1}{2} w^t w$

H_1: $\mathbf{wx_i} + b \geq 1$ for $y_i = +1$

H_2: $\mathbf{wx_i} + b \leq -1$ for $y_i = -1$

→ y_i $(\mathbf{wx_i} + b) \geq 1$ for all i

The MMW Problem

$$\min \ \Phi(w) = \frac{1}{2} w^t w$$

$$\text{s.t.} \ \ y_i(wx_i + b) \geq 1 \ \text{ for all i}$$

It's a Constrained (Convex) Quadratic Optimization Problem!

Quadratic optimization problems are a well-known class of mathematical programming problems, and many (rather intricate) algorithms exist for solving them.

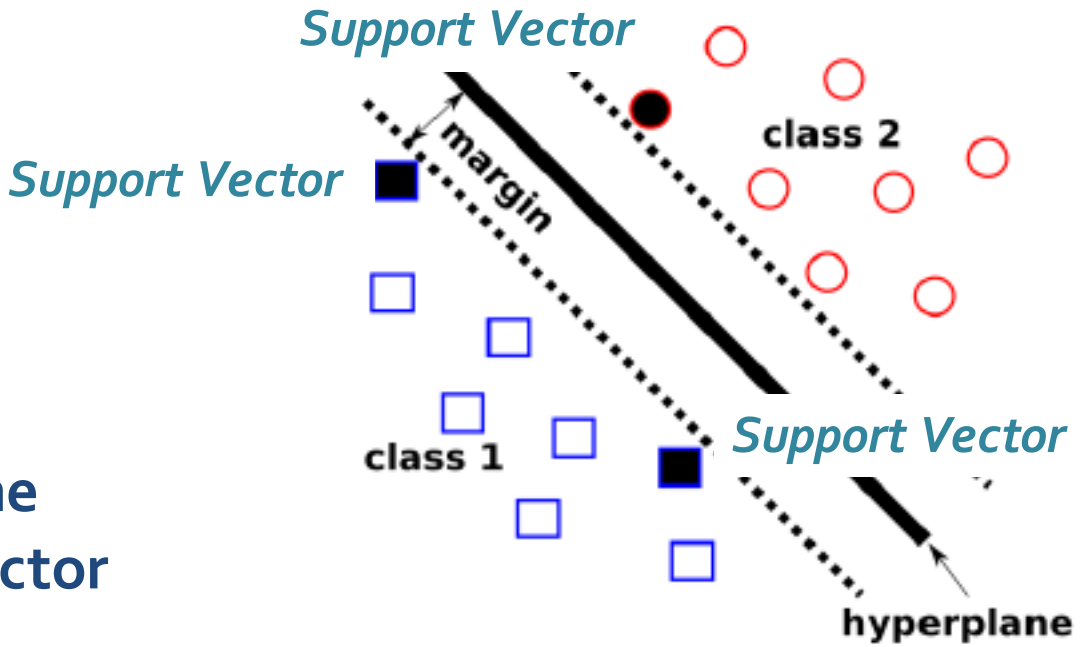
Solving the MMW Problem

- Need to optimize a quadratic function subject to linear constraints.
- Quadratic objective function and linear constraints → *Quadratic Programming (QP)* → Lagrangian multipliers
- The solution involves constructing a dual problem where a **Lagrange multiplier α_i** is associated with every constraint in the primary problem:

Find $\mathbf{w}$ and b such that
$\Phi(\mathbf{w}) = \frac{1}{2}\,\mathbf{w}^T\mathbf{w}$ is minimized;
and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i\,(\mathbf{w}^T\mathbf{x_i} + b) \geq 1$

Find $\alpha_1 \ldots \alpha_N$ such that
$Q(\boldsymbol{\alpha}) = \sum\alpha_i - \frac{1}{2}\sum\sum\alpha_i\alpha_j y_i y_j \mathbf{x_i}^T\mathbf{x_j}$
is maximized and
(1) $\sum\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

Concepts



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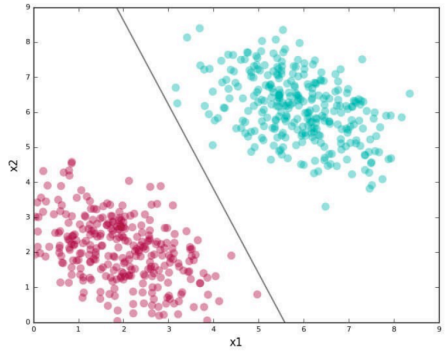
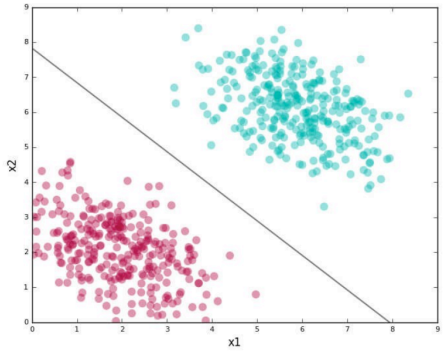
Why is SVM Effective on High Dimensional Data?

- The complexity of trained classifier is characterized by the *# of support vectors* rather than the *dimensionality of the data*.
- The *support vectors* are the *essential or critical* training examples — they lie closest to the decision boundary.
- If all other training examples are removed and the training is repeated, the ***same*** *separating hyperplane* would be found.

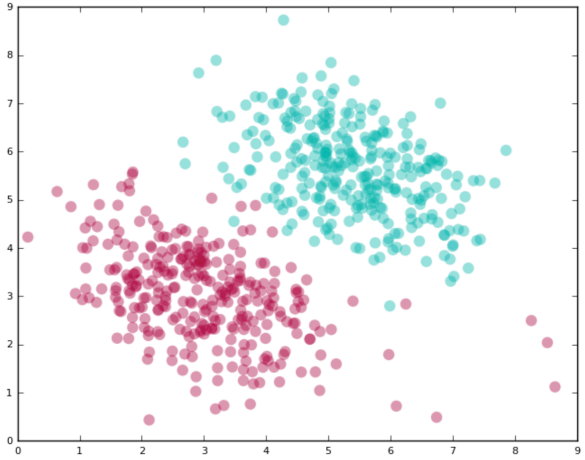
Allowing for Errors

- This is an easy case of perfectly linearly separable data.



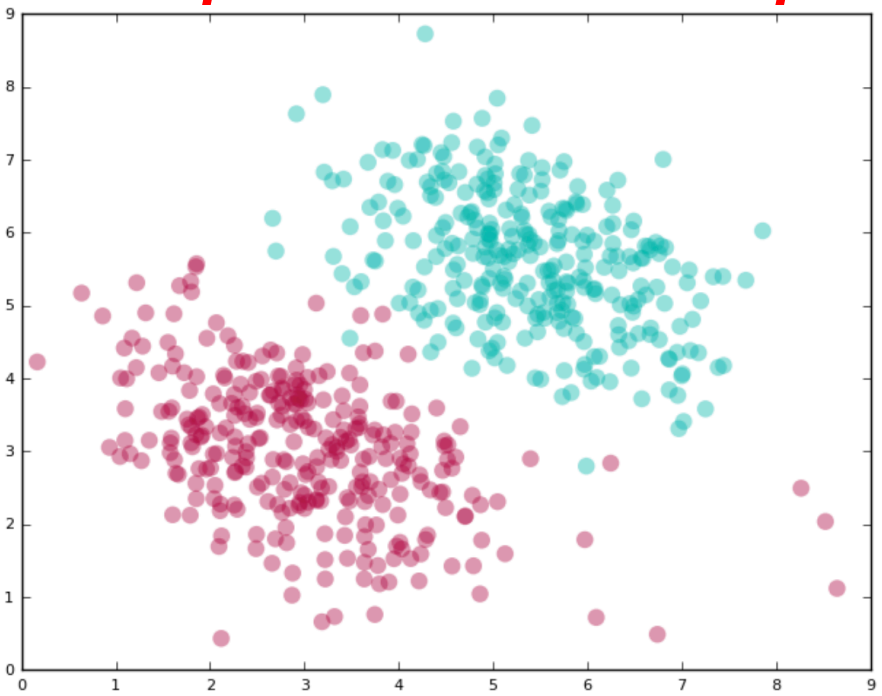


- Real-world data is, however, typically **messy**. You will almost always have a few instances that a linear classifier can't get right.



Allow for Errors (cont.)

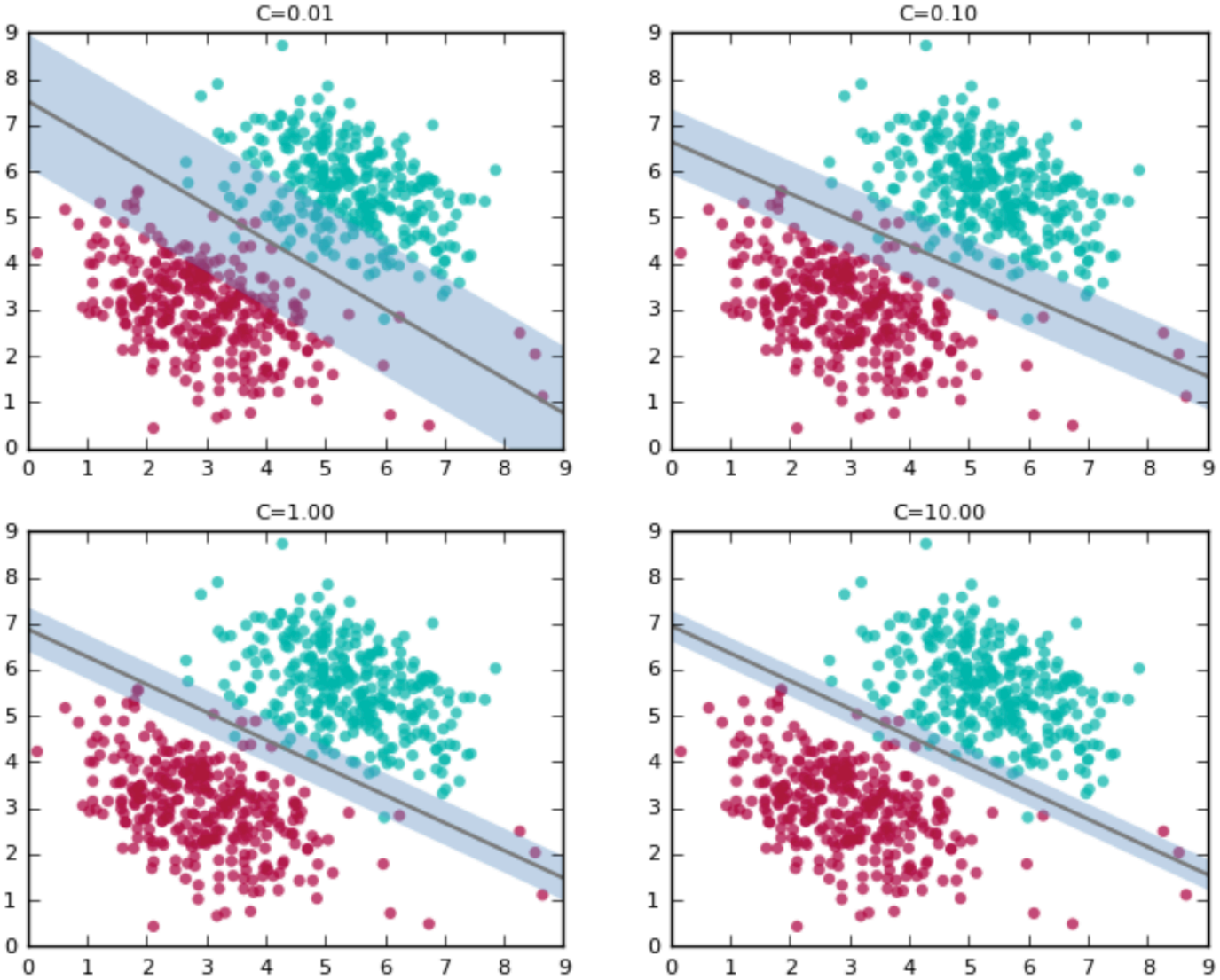
- If we are using a linear classifier, we are ***never*** going to be able to perfectly separate the labels.
- But a linear classifier does seem like ***a good fit*** for the problem ***except*** for a few ***errant points***.



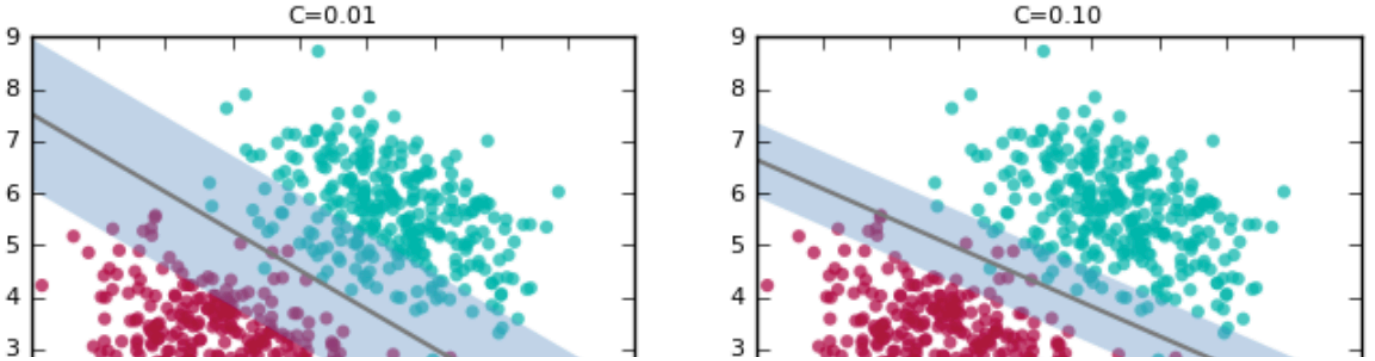
Allow for Errors (cont.)

- Solution: Provide a parameter called "C" to your SVM that allows you to dictate the tradeoff between:
  - Having a wide margin.
  - Correctly classifying training data.
- A ***higher*** value of C implies you want ***lesser errors*** on the training data.
  - C = 0.01 (allowing many errors) → Wide margin
  - C = 0.1
  - C = 1.0
  - C = 10.0 (allowing very few errors) → Narrow margin

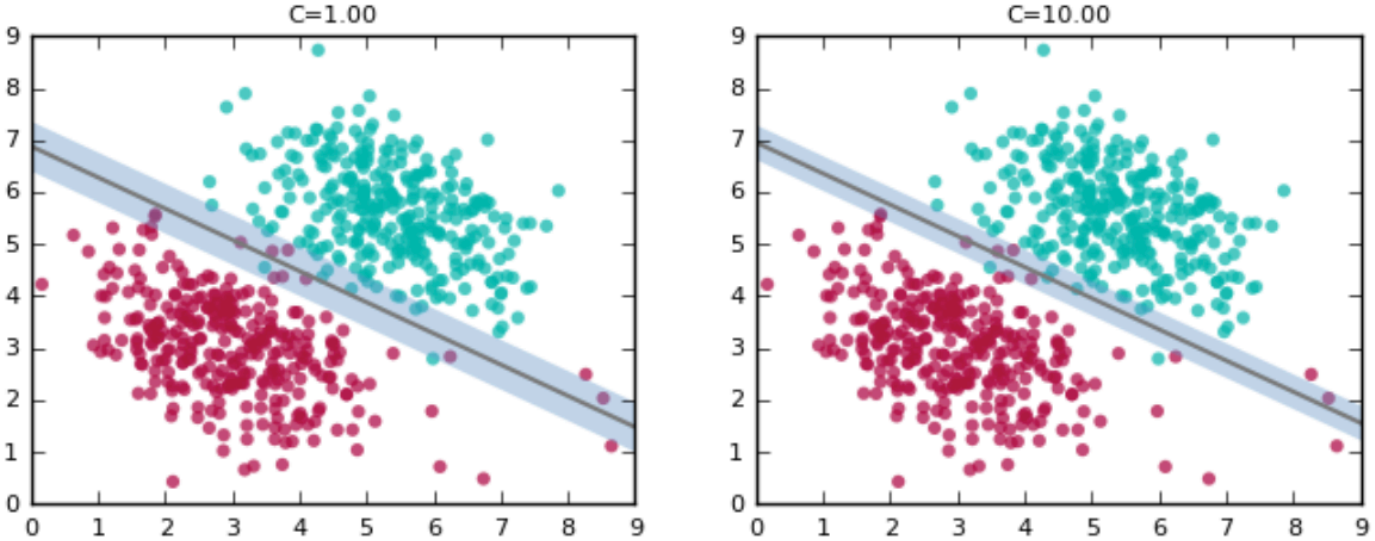
Allow for Errors (cont.)



Allow for Errors (cont.)



Note how the line "tilts" and how the width of the margin shrinks as we increase the value of C.



LinearSVM: Summary

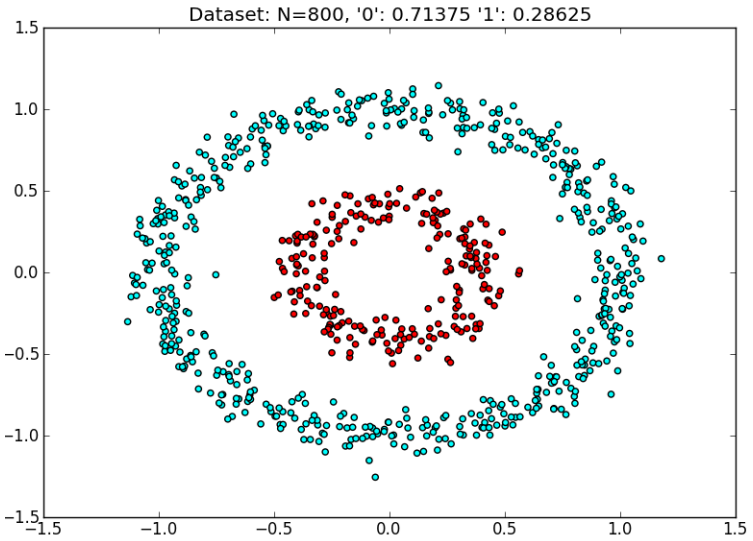
- The classifier is a separating hyperplane.
  - Linearly separable data points except for a few errant points.
- Most "important" training points are support vectors; they define the hyperplane.

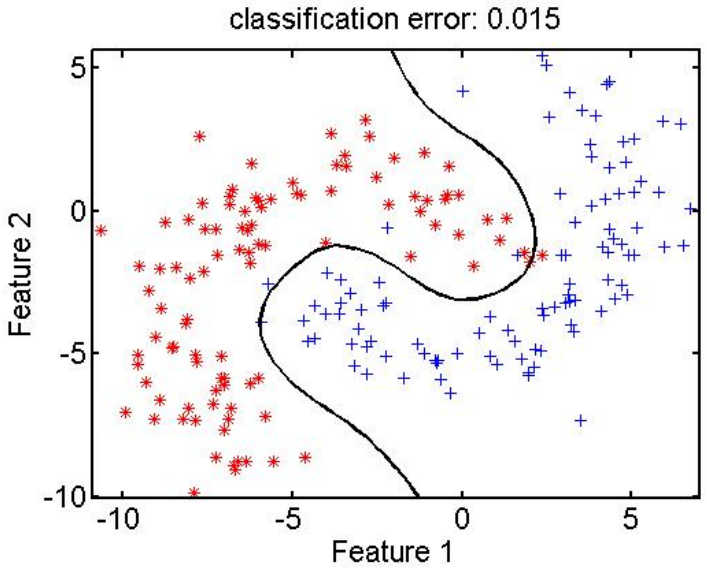
maximum marginal hyperplane

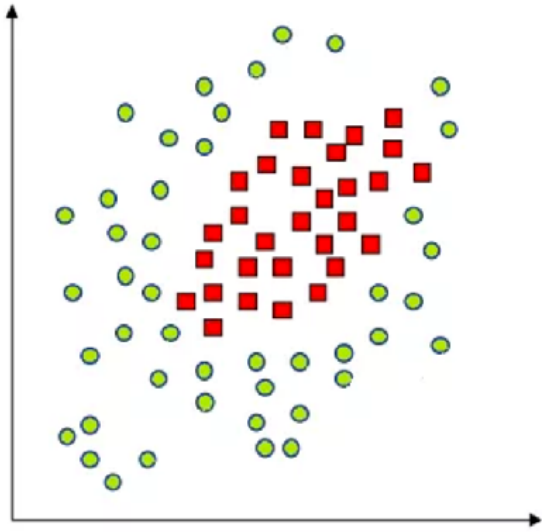
- Quadratic optimization algorithms can identify which training points x_i are support vectors with non-zero Lagrangian multipliers α_i.

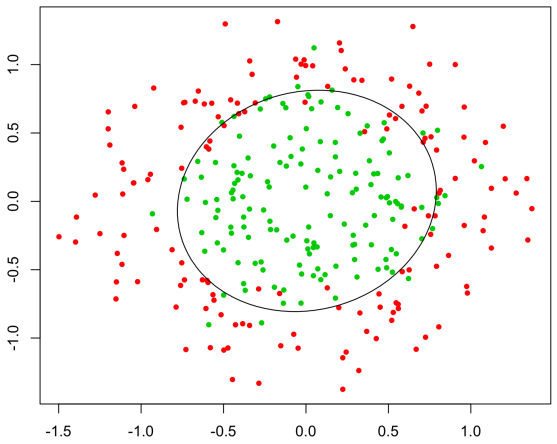
Find $\alpha_1 \ldots \alpha_N$ such that
$Q(\alpha) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j x_i^T x_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \le \alpha_i \le C$ for all α_i

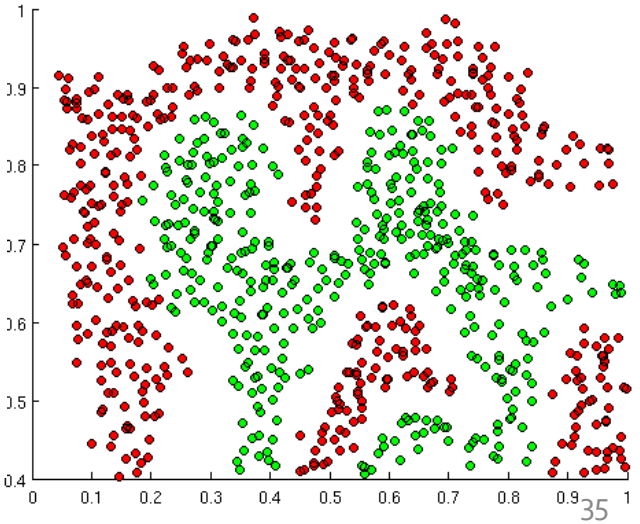
Non-Linear Data Points





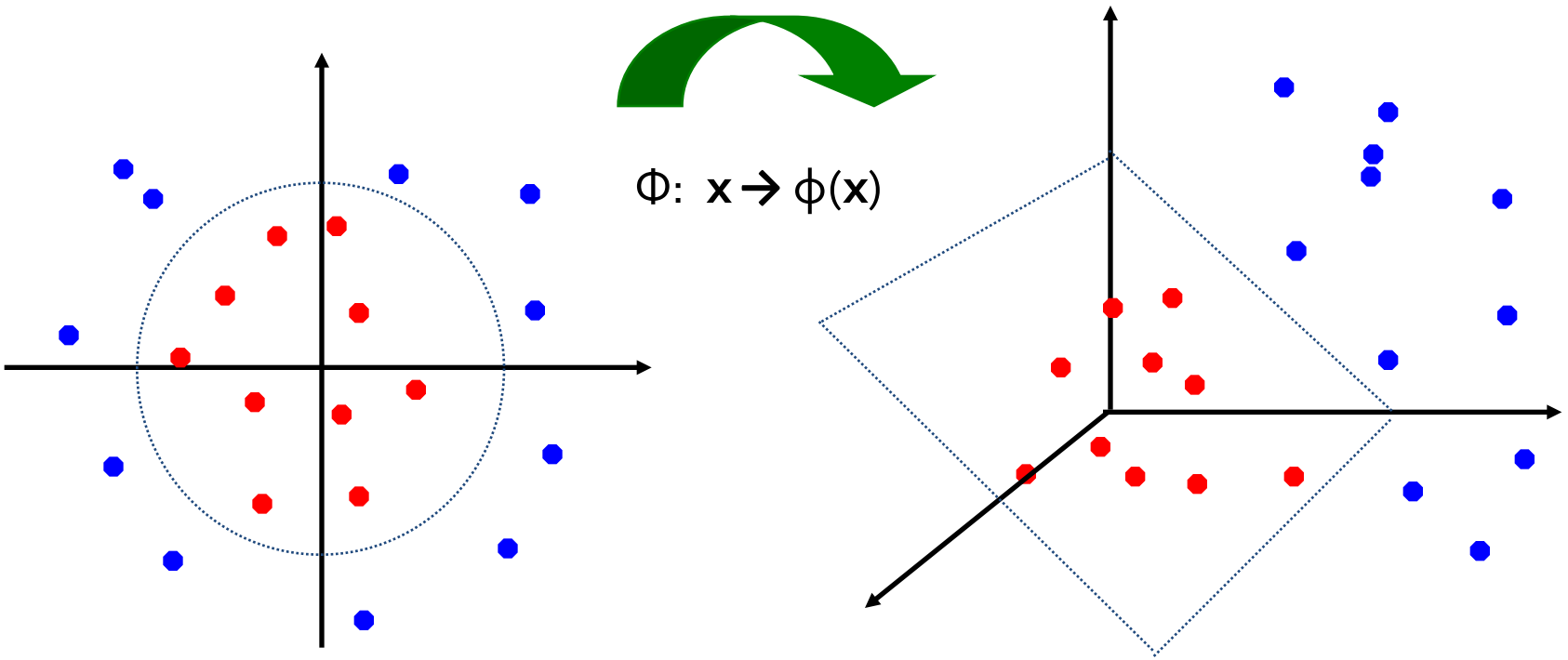






Non-linear SVMs: Feature Spaces

- General idea: The original input space can always be mapped to some higher-dimensional feature space where the training set is separable:



The "Kernel Trick"

- The classifier relies on dot product between vectors

$$K(x_i, x_j) = x_i^T x_j$$

- If every data point is mapped into high-dimensional space via some transformation Φ: $x \rightarrow \phi(x)$, the dot product becomes:

$$K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$$

- A *kernel function* is some function that corresponds to an inner product in some expanded feature space.

What Functions are Kernels?

- For some functions $K(x_i,x_j)$ checking that

  $K(x_i,x_j)= \phi(x_i)^T\phi(x_j)$ can be cumbersome.
- Mercer's theorem:

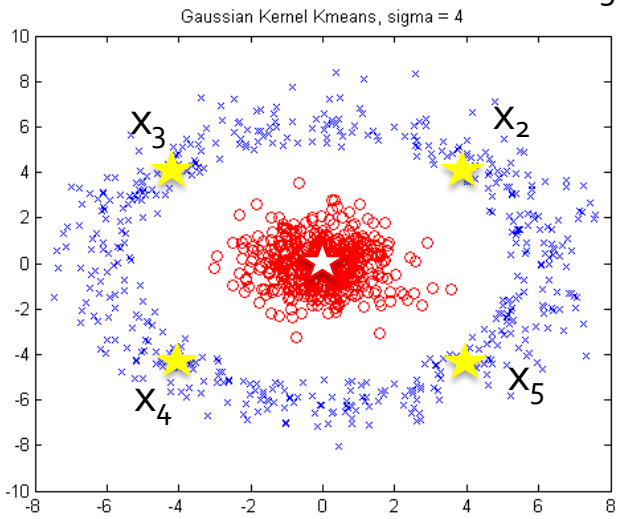
  Every semi-positive definite symmetric function is a kernel
- Semi-positive definite symmetric functions correspond to a semi-positive definite symmetric Gram matrix:

K =

$K(\mathbf{x_1},\mathbf{x_1})$	$K(\mathbf{x_1},\mathbf{x_2})$	$K(\mathbf{x_1},\mathbf{x_3})$	…	$K(\mathbf{x_1},\mathbf{x_N})$
$K(\mathbf{x_2},\mathbf{x_1})$	$K(\mathbf{x_2},\mathbf{x_2})$	$K(\mathbf{x_2},\mathbf{x_3})$		$K(\mathbf{x_2},\mathbf{x_N})$
…	…	…	…	…
$K(\mathbf{x_N},\mathbf{x_1})$	$K(\mathbf{x_N},\mathbf{x_2})$	$K(\mathbf{x_N},\mathbf{x_3})$	…	$K(\mathbf{x_N},\mathbf{x_N})$

Example: A Kernel Function

- Polynomial kernel of degree h=2: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = \boldsymbol{X}_i \cdot \boldsymbol{X}_j{}^2 \rightarrow \phi(x, y) = (x^2, \sqrt{2}xy, y^2)$
- Suppose there are 5 original 2-dimensional points:
  - $x_1(0, 0)$, $x_2(4, 4)$, $x_3(-4, 4)$, $x_4(-4, -4)$, $x_5(4, -4)$



	x	y	$\Phi 1 = x^2$	$\Phi 2 = xy$	$\phi 3 = y^2$
x_1	0	0	0	0	0
x_2	4	4	16	$16\sqrt{2}$	16
x_3	-4	4	16	$-16\sqrt{2}$	16
x_4	-4	-4	16	$16\sqrt{2}$	16
x_5	4	-4	16	$-16\sqrt{2}$	16

Example: A Kernel Function

- Polynomial kernel of degree h=2: $K(\boldsymbol{X}_i, \boldsymbol{X}_j) = \boldsymbol{X}_i \cdot \boldsymbol{X}_j{}^2 \rightarrow \phi(x, y) = (x^2, \sqrt{2}xy, y^2)$
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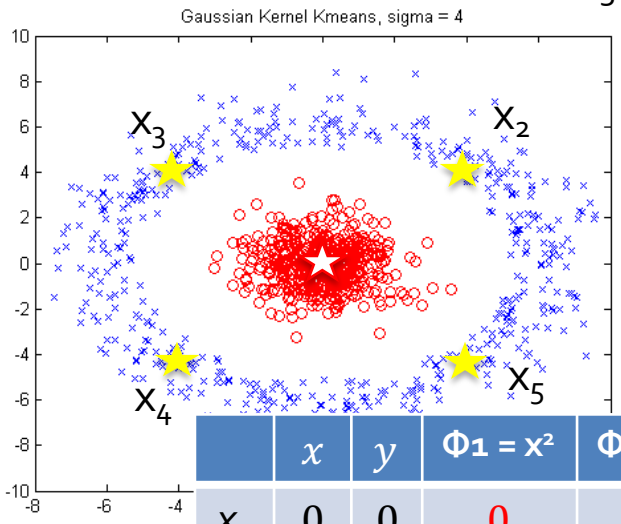
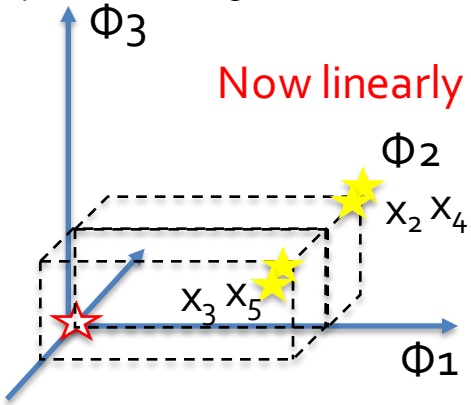




Now linearly separable!!!

	x	y	Φ1 = x²	Φ2 = xy	ϕ3 = y²	$K(x_i,x_1)$	$K(x_i,x_2)$	$K(x_i,x_3)$	$K(x_i,x_4)$	$K(x_i,x_5)$
x_1	0	0	0	0	0	0	0	0	0	0
x_2	4	4	16	$16\sqrt{2}$	16	0	32^2	0	32^2	0
x_3	-4	4	16	$-16\sqrt{2}$	16	0	0	32^2	0	32^2
x_4	-4	-4	16	$16\sqrt{2}$	16	0	32^2	0	32^2	0
x_5	4	-4	16	$-16\sqrt{2}$	16	0	0	32^2	0	32^2

Kernel Functions for Nonlinear Classification

- Instead of computing the dot product on the transformed data, it is mathematically equivalent to applying a kernel function $K(\mathbf{X}_i, \mathbf{X}_j)$ to the original data, i.e., $K(\mathbf{X}_i, \mathbf{X}_j) = \Phi(\mathbf{X}_i)\,\Phi(\mathbf{X}_j)$.
- Typical Kernel Functions

$$\textbf{Polynomial kernel of degree } h: \quad K(\boldsymbol{X}_i, \boldsymbol{X}_j) = (\boldsymbol{X}_i \cdot \boldsymbol{X}_j + 1)^h$$

$$\textbf{Gaussian radial basis function kernel}: \quad K(\boldsymbol{X}_i, \boldsymbol{X}_j) = e^{-\|\boldsymbol{X}_i - \boldsymbol{X}_j\|^2/2\sigma^2}$$

$$\textbf{Sigmoid kernel}: \quad K(\boldsymbol{X}_i, \boldsymbol{X}_j) = \tanh(\kappa \boldsymbol{X}_i \cdot \boldsymbol{X}_j - \delta)$$

Non-linear SVMs: Optimization

- Dual problem formulation:

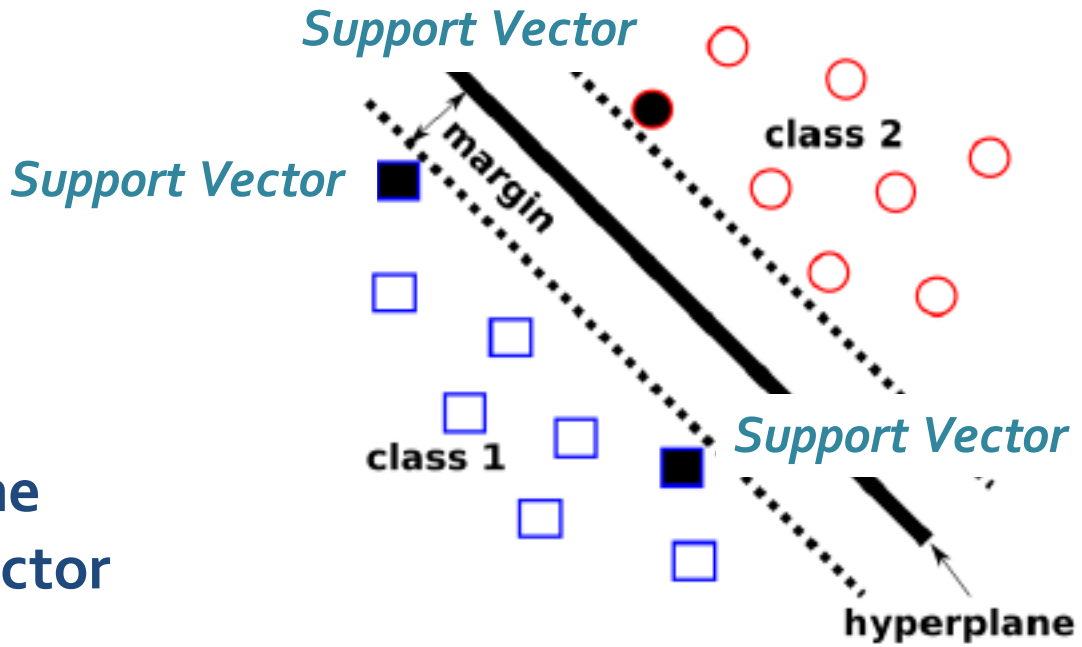
Find $\alpha_1 \ldots \alpha_N$ such that
$Q(\alpha) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j K(x_i, x_j)$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

- The solution is:

$$f(x) = \Sigma\alpha_i y_i K(x_i, x_j) + b$$

- Optimization techniques for finding α_i's remain the same!

Concepts



Quick start:

1. Hyperplane
2. Supper Vector
3. Margin
4. SVMs
5. Maximize Margin Width
6. Non-linear SVMs: Kernel Function

SVM: History and Applications

- Vapnik and colleagues (**1992**)—groundwork from Vapnik & Chervonenkis' *statistical learning theory* in **1960s**
- Features: **training can be slow but accuracy is high** owing to their ability to model **complex nonlinear decision boundaries** (margin maximization)
- Applications:
  - Text categorization
  - Image classification
  - Hand-written digit/character recognition
  - Object recognition
  - Bioinformatics (Protein classification, Cancer classification…)

SVM Related Links

- SVM Website: http://www.kernel-machines.org/
- Representative implementations
  - **LIBSVM**: an efficient implementation of SVM, multi-class classifications, nu-SVM, one-class SVM, including also various interfaces with java, python, etc.
  - **SVM-light**: simpler but performance is not better than LIBSVM, support only binary classification and only in C
  - **SVM-torch**: another recent implementation also written in C
  - http://www.meng-jiang.com/teaching/SVMDemo.zip

References

- C. M. Bishop, Neural Networks for Pattern Recognition. Oxford University Press, 1995
- L. Breiman, J. Friedman, R. Olshen, and C. Stone. Classification and Regression Trees. Wadsworth International Group, 1984
- C. J. C. Burges. A Tutorial on Support Vector Machines for Pattern Recognition. Data Mining and Knowledge Discovery, 2(2): 121-168, 1998
- N. Cristianini and J. Shawe-Taylor, Introduction to Support Vector Machines and Other Kernel-Based Learning Methods, Cambridge University Press, 2000
- H. Yu, J. Yang, and J. Han. Classifying large data sets using SVM with hierarchical clusters. KDD'03
- A. J. Dobson. An Introduction to Generalized Linear Models. Chapman & Hall, 1990
- R. O. Duda, P. E. Hart, and D. G. Stork. Pattern Classification, 2ed. John Wiley, 2001
- T. Hastie, R. Tibshirani, and J. Friedman. The Elements of Statistical Learning: Data Mining, Inference, and Prediction. Springer-Verlag, 2001
- S. Haykin, Neural Networks and Learning Machines, Prentice Hall, 2008
- D. Heckerman, D. Geiger, and D. M. Chickering. Learning Bayesian networks: The combination of knowledge and statistical data. Machine Learning, 1995
- H. Cheng, X. Yan, J. Han & C.-W. Hsu, Discriminative Frequent Pattern Analysis for Effective Classification, ICDE'07
- W. Cohen. Fast effective rule induction. ICML'95

References (cont.)

- H. Cheng, X. Yan, J. Han & P. S. Yu, Direct Discriminative Pattern Mining for Effective Classification, ICDE'08
- G. Cong, K. Tan, A. Tung & X. Xu. Mining Top-k Covering Rule Groups for Gene Expression Data, SIGMOD'05
- M. Deshpande, M. Kuramochi, N. Wale & G. Karypis. Frequent Substructure-based Approaches for Classifying Chemical Compounds, TKDE'05
- G. Dong & J. Li. Efficient Mining of Emerging Patterns: Discovering Trends and Differences, KDD'99
- W. Fan, K. Zhang, H. Cheng, J. Gao, X. Yan, J. Han, P. S. Yu & O. Verscheure. Direct Mining of Discriminative and Essential Graphical and Itemset Features via Model-based Search Tree, KDD'08
- W. Li, J. Han & J. Pei. CMAR: Accurate and Efficient Classification based on Multiple Class-association Rules, ICDM'01
- B. Liu, W. Hsu & Y. Ma. Integrating Classification and Association Rule Mining, KDD'98
- J. R. Quinlan and R. M. Cameron-Jones. FOIL: A midterm report. ECML'93
- Jingbo Shang, Wenzhu Tong, Jian Peng, and Jiawei Han, "DPClass: An Effective but Concise Discriminative Patterns-Based Classification Framework", SDM'16
- J. Wang and G. Karypis. HARMONY: Efficiently Mining the Best Rules for Classification, SDM'05
- X. Yin & J. Han. CPAR: Classification Based on Predictive Association Rules, SDM'03