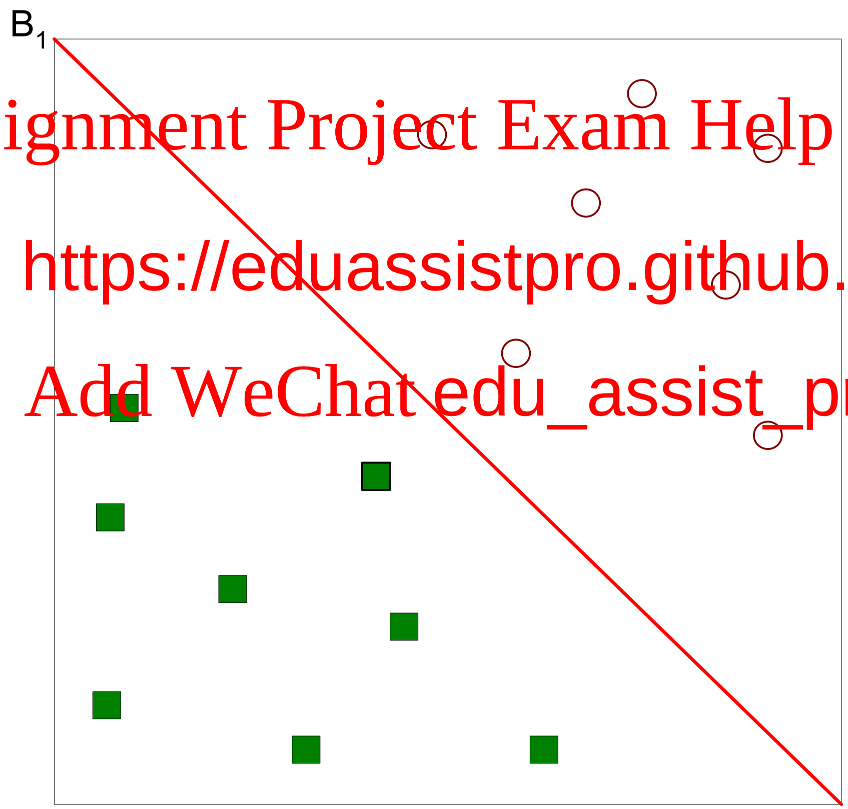
Support Vector Machines: Intuition

- Assuming the data is linearly separable
- Aim: find a linear hyperplane (decision boundary) that will separate the data

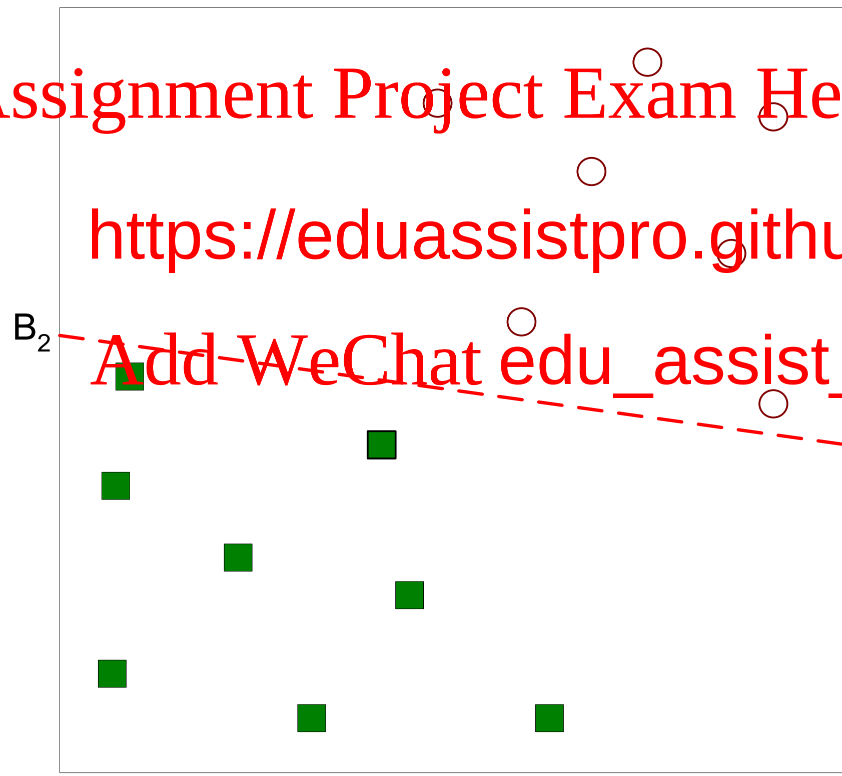
Support Vector Machines: Intuition

- One Possible Solution



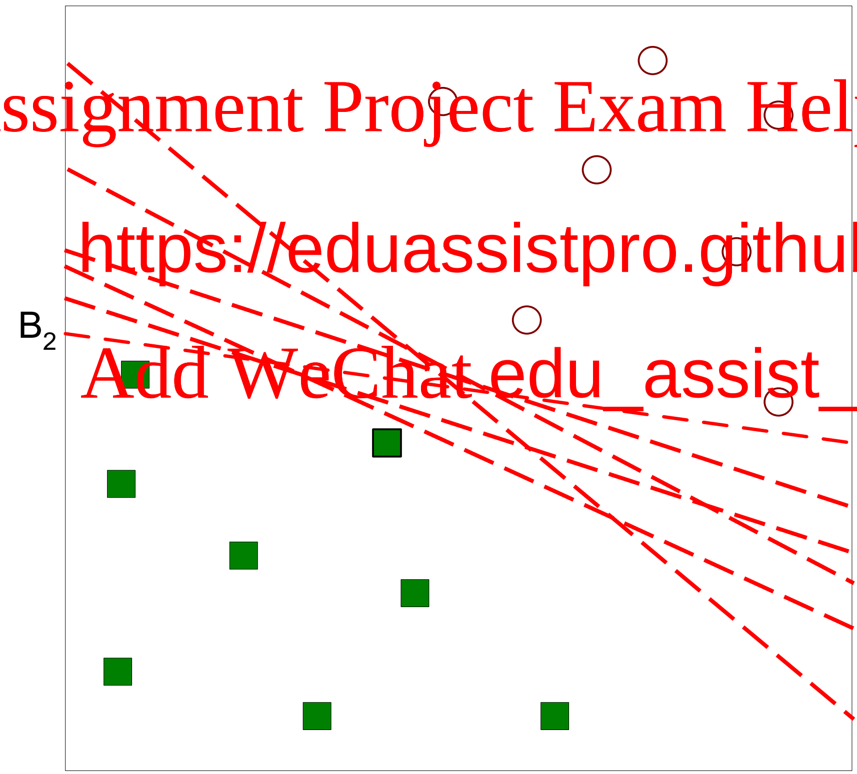
Support Vector Machines: Intuition

- Another Possible Solution



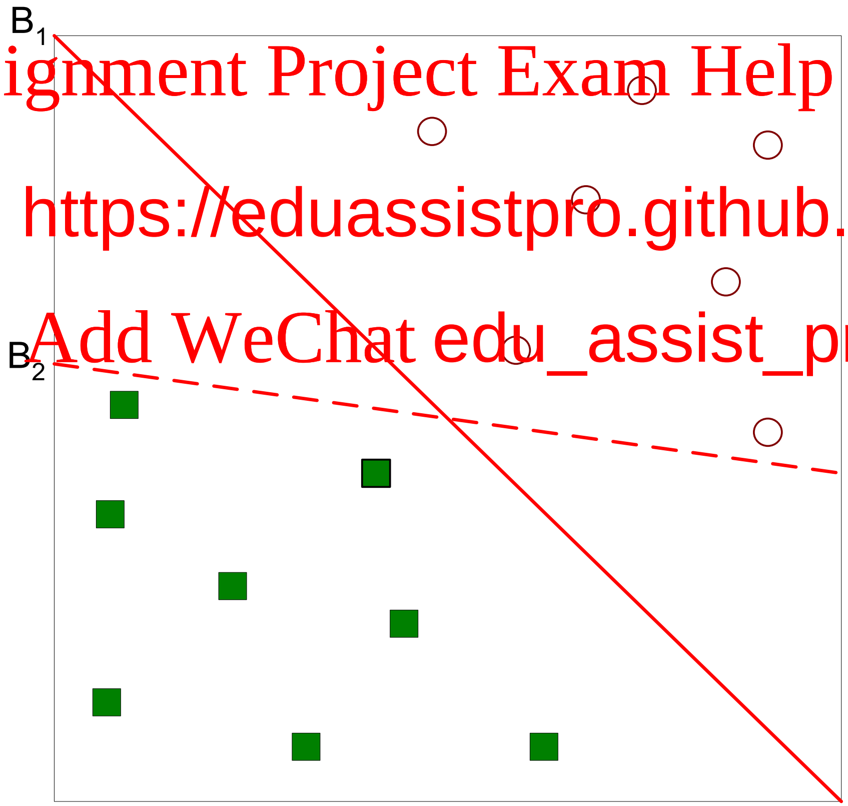
Support Vector Machines: Intuition

- Other Possible Solutions



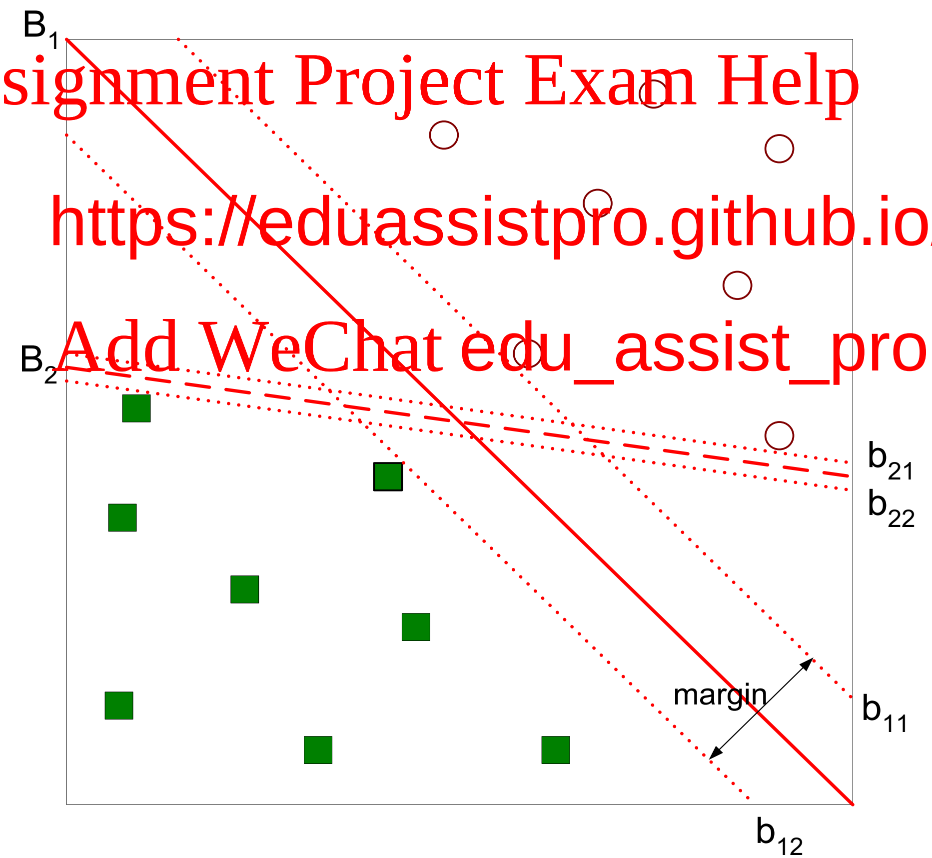
Support Vector Machines: Intuition

- Which one is better? B1 or B2?
- How do you define better?

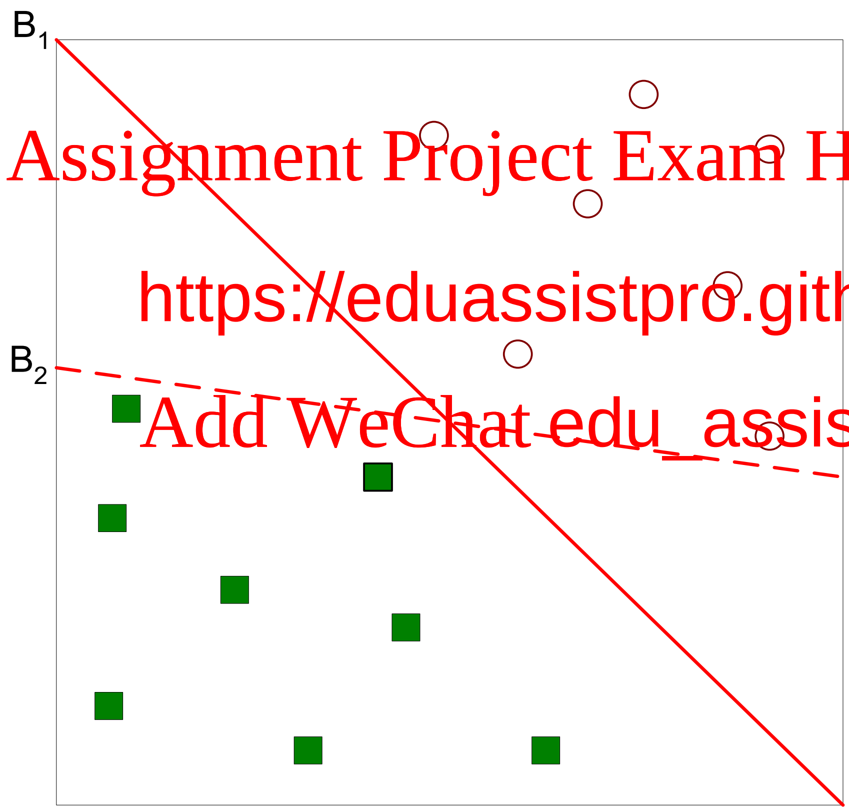


Support Vector Machines: Large Margin Classifiers

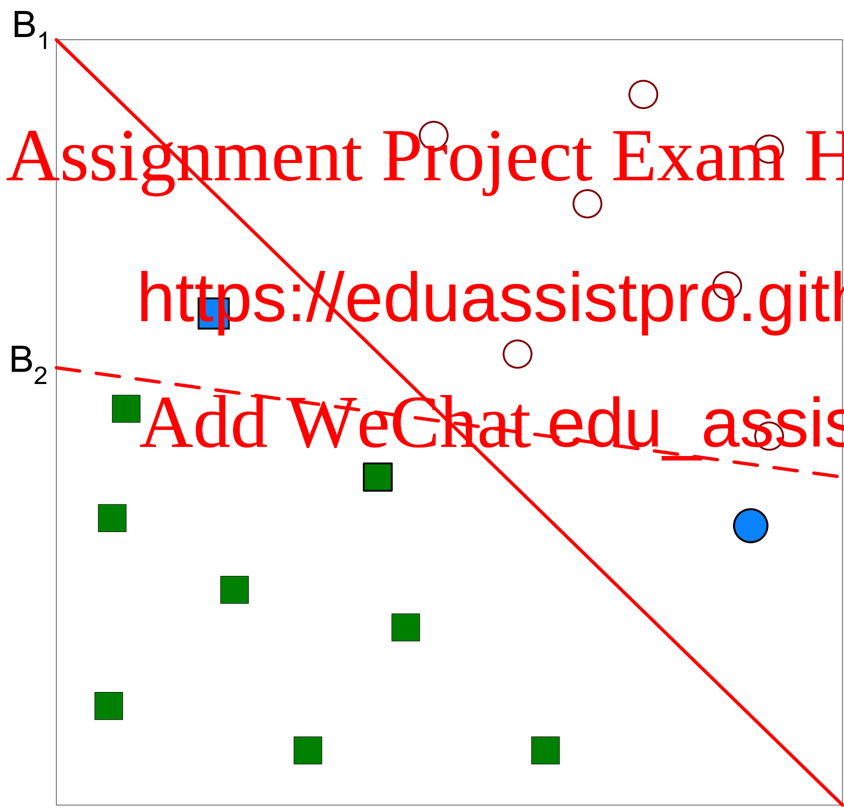
- Find hyperplane maximises the margin => B1 is better than B2
- Margin: sum of shortest distances from the planes to the positive/negative samples



Why Large Margin?



Why Large Margin?



Why Large Margin?

- Small margin separating planes:
  - are more fragile to noise
  - may over-fit the data

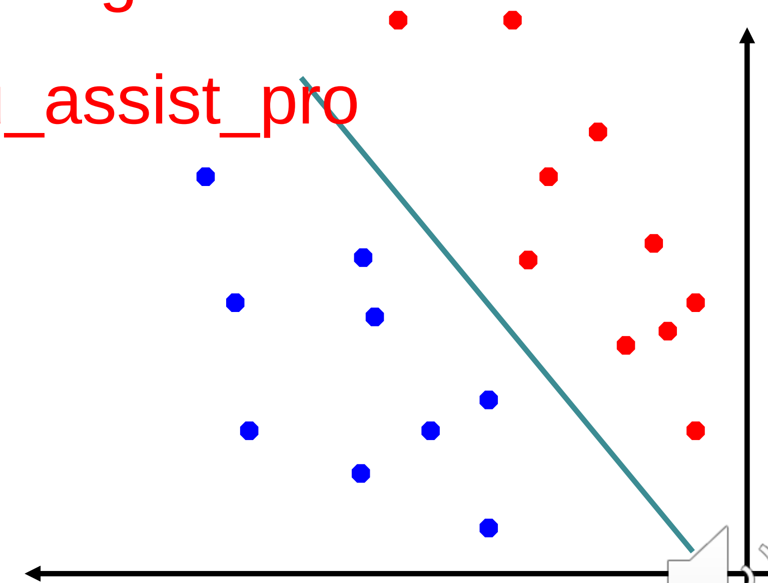
- Large margin separating planes:
  - are more robust to n
  - From statistical lear nes generalises better to unseen data

Linear Classifiers Formulation

$\{\mathbf{x}_i, y_i\}$ where $i = 1 \ldots L, y_i \in \{-1, 1\}, \mathbf{x}_i \in \mathbb{R}^D$

This hyperplane can be described by $\mathbf{x} \cdot \mathbf{w} + b = 0$ where:

- $\mathbf{w}$ is normal to the hyperplane.
- $\frac{b}{\|\mathbf{w}\|}$ is the perpendicular distance from the hyperplane to the origin.



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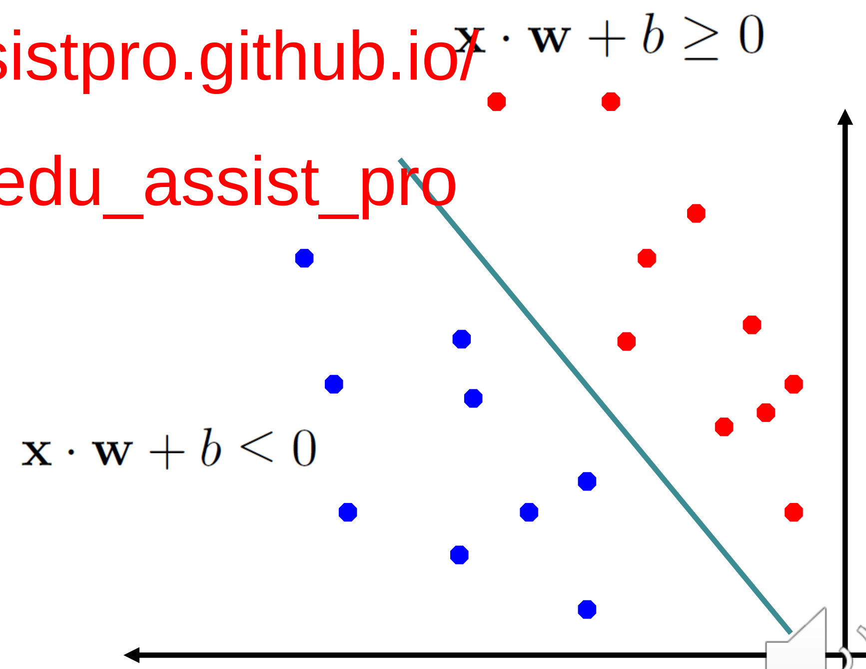


Classification rule

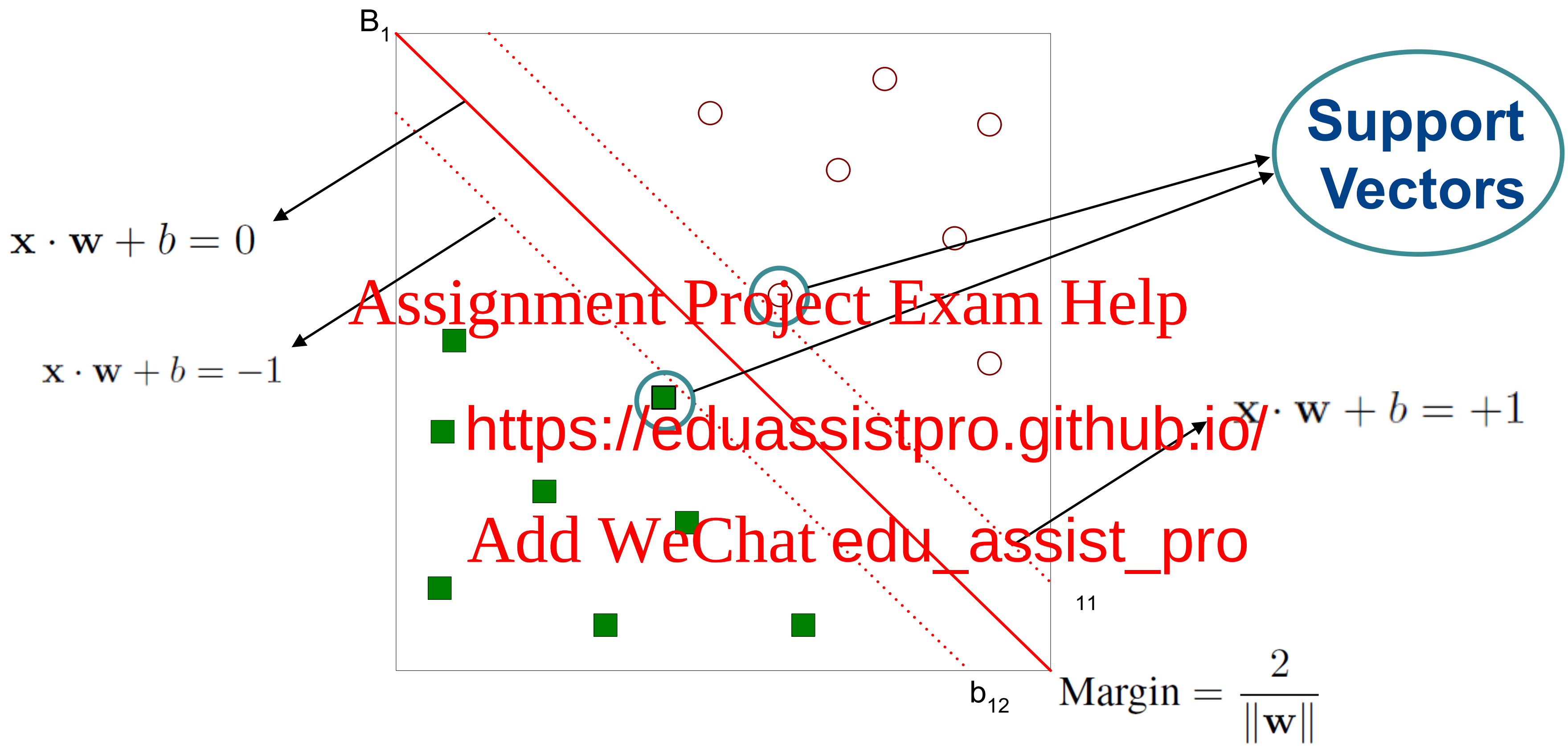
$$f(\mathbf{x}) = \mathrm{sign}(\mathbf{x} \cdot \mathbf{w} + b) = \begin{cases} +1 \text{ if } \mathbf{x} \cdot \mathbf{w} + b \geq 0 \\ -1 \text{ if } \mathbf{x} \cdot \mathbf{w} + b < 0 \end{cases}$$

Find $\mathbf{w}$ and b such that:

$$\mathbf{x}_i \cdot \mathbf{w} + b \geq 0 \text{ for } y_i = +1$$
$$\mathbf{x}_i \cdot \mathbf{w} + b < 0 \text{ for } y_i = -1$$
$$\text{for all } i = 1 \ldots L$$

Training objective

Linear Support Vector Machines: Need to Consider Margin



Requirement for margin:

$$\mathbf{x}_i \cdot \mathbf{w} + b \geq +1 \quad \text{for } y_i = +1$$
$$\mathbf{x}_i \cdot \mathbf{w} + b \leq -1 \quad \text{for } y_i = -1$$

Linear Support Vector Machines Formulation

Margin

Note that:

$$\mathbf{x}_i \cdot \mathbf{w} + b \geq +1 \quad \text{for } y_i = +1$$
$$\mathbf{x}_i \cdot \mathbf{w} + b \leq -1 \quad \text{for } y_i = -1$$

These equations can be combined into:

$$y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \geq 0 \ \forall_i$$

Linear Support Vector Machines Equivalent Formulations

(1) $$\max \frac{2}{\|\mathbf{w}\|} \quad \text{s.t.} \quad y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \geq 0 \quad \forall i$$

(2)

(3)

Linear SVM Feasibility

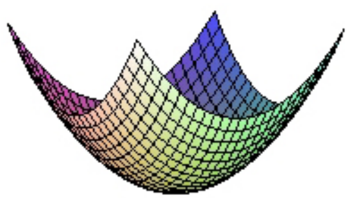
$$\min \frac{1}{2}\|\mathbf{w}\|^2 \qquad \text{s.t.} \qquad y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \geq 0 \quad \forall_i$$

- For linearly separable data: a max-margin solution is **guaranteed** to exist
- For non- linearly separable data: a solution does not exist

Solving the Optimization Problem

$$\min \frac{1}{2} \|\mathbf{w}\|^2 \qquad \text{s.t.} \qquad y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \geq 0 \;\; \forall_i$$

- Need to optimize a *quadratic* function subject to *linear* constraints.
- Convex quadratic optimization problem
- Convex objective: any l [illegible] al minimum



Convex **Non Convex**

Solving the Optimization Problem: Duality Formulation

***Primal problem**: solve for **w** and b*

$$\min \frac{1}{2}\|\mathbf{w}\|^2 \qquad \text{s.t.} \qquad y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \geq 0 \;\; \forall_i$$

Solving the Optimization Problem: Duality Formulation

***Primal problem**: solve for **w** and b*

$$\min \frac{1}{2}\|\mathbf{w}\|^2 \qquad \text{s.t.} \qquad y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 \geq 0 \ \ \forall_i$$

Equivalent **dual problem** *formulation: solve for* $\alpha_1 \ldots \alpha_L$: Lagrange multipliers for each data point

More convenient to solve

See Ref. [1] for derivation

Solution: Dual to Primal

- Given a solution $\alpha_1 \ldots \alpha_L$ 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 fun ... ed **w** explicitly):

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

tion

- 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.

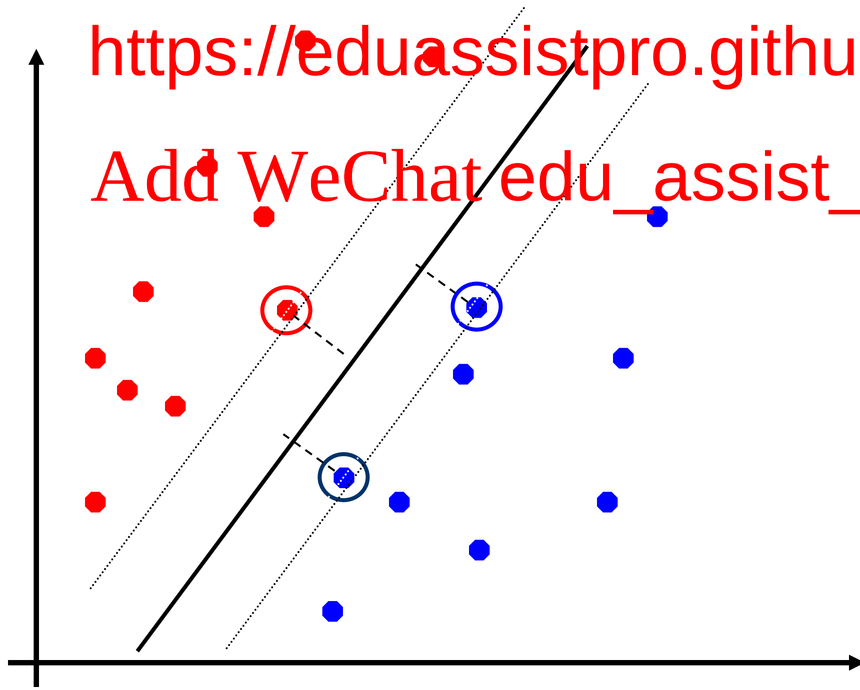
Solution: Support Vectors

- Classification function:

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

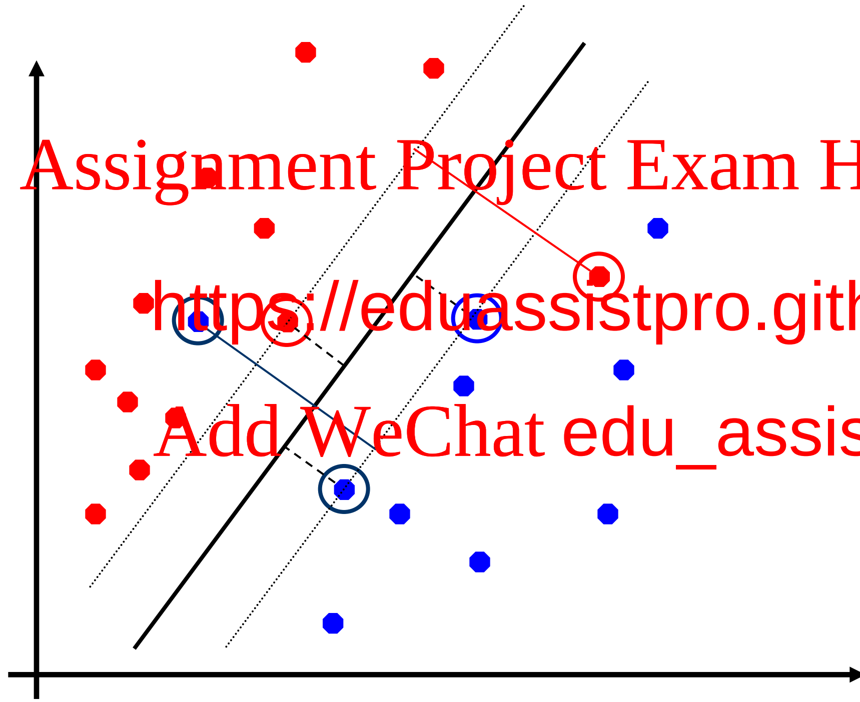
Linear SVM

- Only support vectors matter; other training examples are ignorable.



Soft Margin Classification

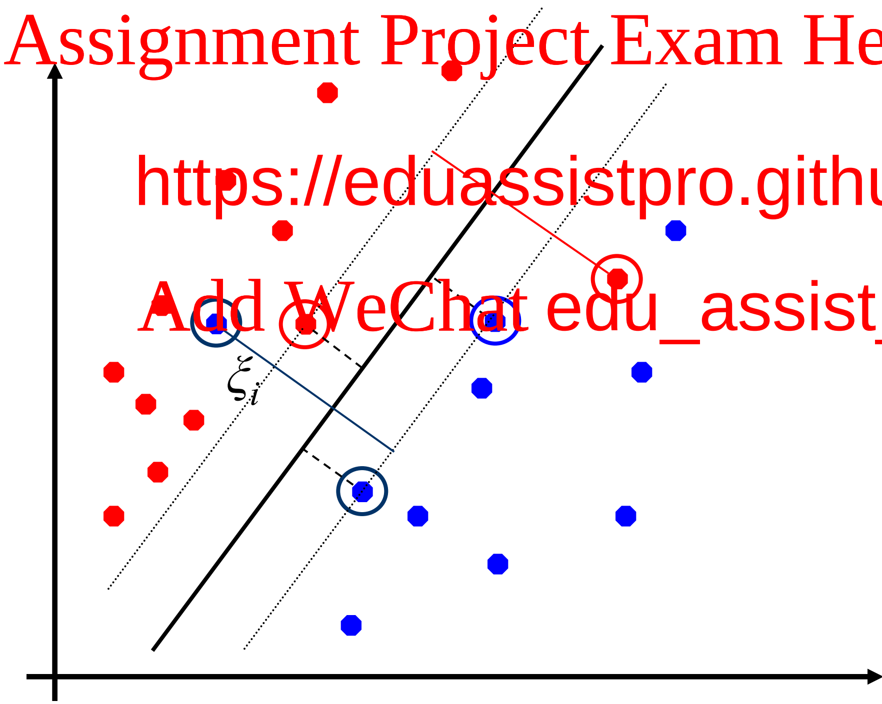
- What if the training set is mostly, but not exactly, linearly separable?



*The (hard) linear SVM problem is **infeasible** here.*

Soft Margin Classification

- ***Slack variables*** ξ_i can be added to allow misclassification of difficult or noisy examples, resulting margin called *soft*.



Soft Margin Classification Mathematically

- The old formulation (hard SVM):

Find **w** and b such that
$\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{w}$ is minimized
and for all $(\mathbf{x}_i, y_i)$, i=1..L : $y_i\,(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b) \geq 1$

- Modified formulation inc oft SVM):

Find **w** and b such that

$\mathbf{\Phi}(\mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{w} + C\Sigma\xi_i$ is minimized
and for all $(\mathbf{x}_i, y_i)$, i=1..L : $y_i\,(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i + b) \geq 1 - \xi_i$, $\xi_i \geq 0$

- **Parameter *C*** can be viewed as a way to control overfitting: it "trades off" the relative importance of maximizing the margin and fitting the training data.

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Soft Margin Classification – Solution

- Dual problem is identical to separable case:

Find $\alpha_1 \ldots \alpha_L$ such that

$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j$ is maximized and

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

(2) $0 \le \alpha_i \le$

- Again, $\mathbf{x}_i$ with non-zero α_i will be support vector
- Solution to the primal problem is:

$$\mathbf{w} = \Sigma\alpha_i y_i \mathbf{x}_i$$

$$b = y_k(1 - \xi_k) - \Sigma\alpha_i y_i \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_k \quad \text{for any } k \text{ s.t. } \alpha_k > 0$$

- Again, we don't need to compute **w** explicitly for classification:

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

Linear SVMs: Review

- The classifier is a *separating hyperplane*
- Most "important" training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non α_i.

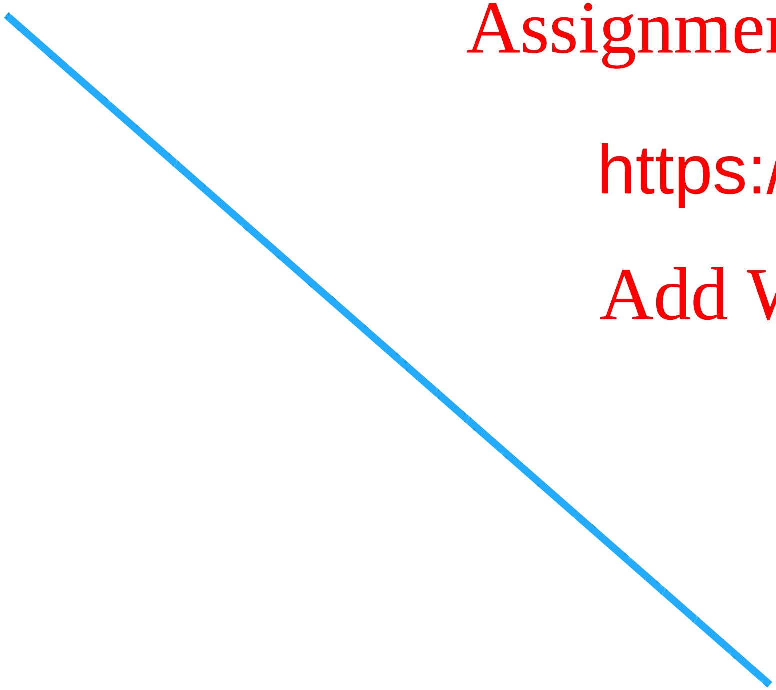
- Model complexity depends on #support v

- Both in the dual formulation of the problem and in the solution, training points appear only inside inner products:

Find $\alpha_1 \ldots \alpha_L$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \boxed{\mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

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

Overfitting - Underfitting



Underfitting: model not expressive enough to capture patterns in the data

Overfitting: model too complicated; capture noise the data

st right: model res essential ns in the data

Non-Linear SVM Motivation

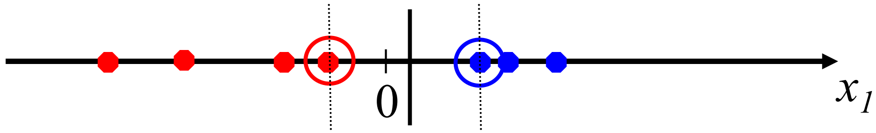
Linear model underfitting: model not expressive enough to capture patterns in the data

t-Margin (linear) SVM cater for a small ber of training errors

But is still a linear model

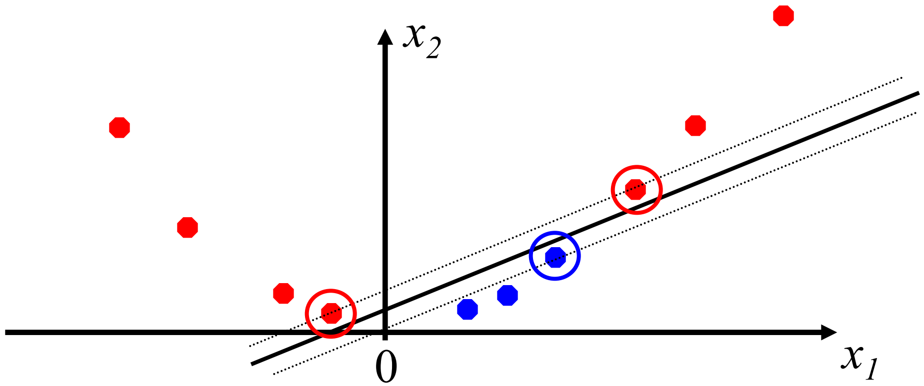
Non-Linear SVM Motivation–

- Datasets that are linearly separable with some noise work out great:



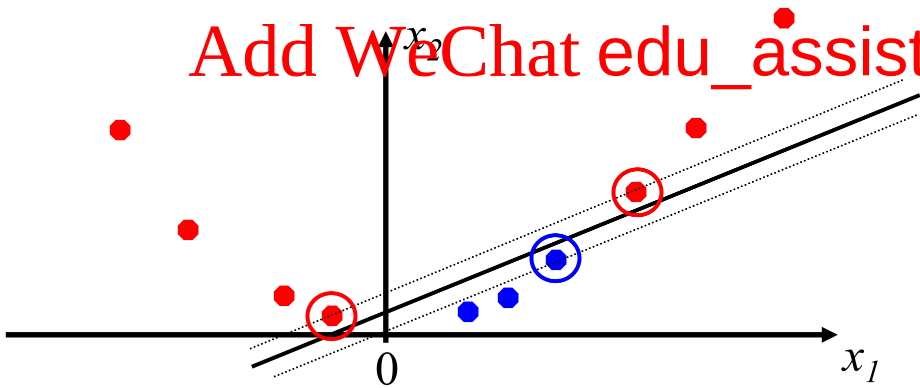
- But what are we going to do if the dataset is just too hard?

- How about… mapping data to a higher-dimensional space:



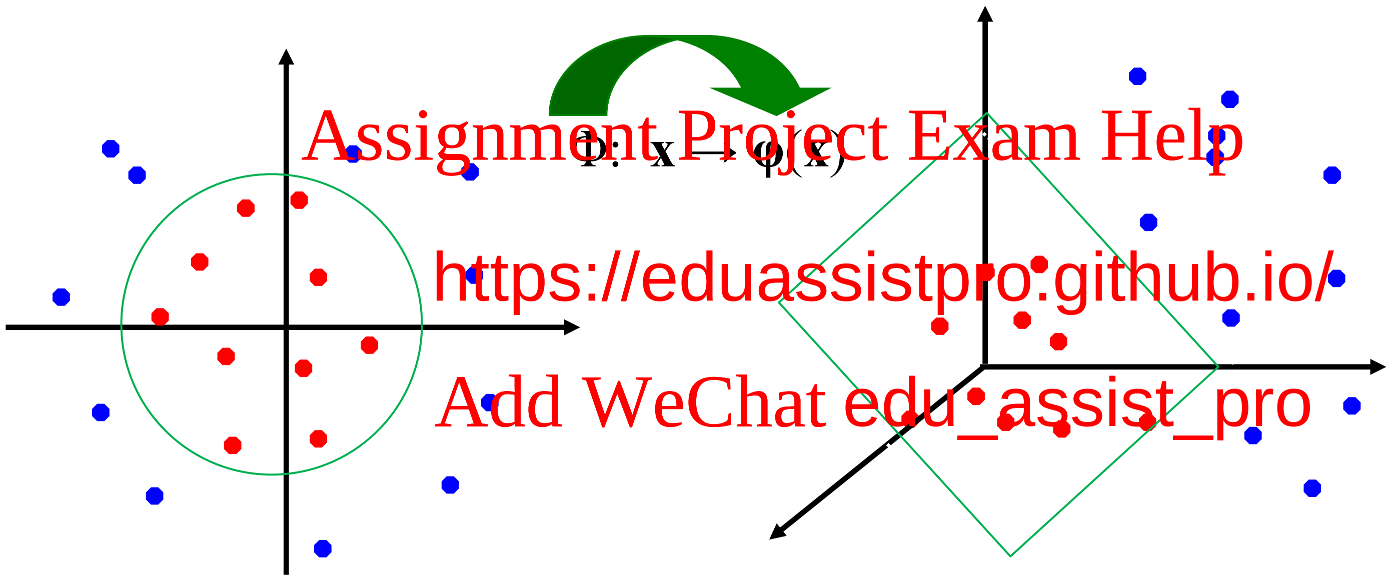
Non-linear SVMs Overview

- Turn linear SVM into a non-linear model
- By mapping the original data into a high dimensional space where the data is hopefully linearly separable



Non-linear SVMs Overview

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



- Higher-dimensional space still has *intrinsic* dimensionality *d*, but linear separators in it correspond to *non-linear* separators in original space.

Turning Linear SVM into Non-linear SVM

Find $\alpha_1 \ldots \alpha_L$ such that

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

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

(2) $0 \leq \alpha_i \leq C$ for all α_i

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

- The linear SVM classifi ween vectors $\mathbf{x}_i^{\mathbf{T}}\mathbf{x}_j$ *(pair-wise dot products b*

- If every data point is mapped into high-di ace via some transformation Φ : $\mathbf{x} \rightarrow \varphi(\mathbf{x})$, the inner product becomes:

$$\boldsymbol{\varphi}(\mathbf{x}_i)^{\mathbf{T}}\boldsymbol{\varphi}(\mathbf{x}_j)$$

Turning Linear SVM into Non-linear SVM

- Explicit mapping & Plug

$$\boldsymbol{\varphi}(\mathbf{x}_i)^T\boldsymbol{\varphi}(\mathbf{x}_j)$$

In place of

$$\mathbf{x}_i^T\mathbf{x}_j$$

Find $\alpha_1 \dots \alpha_L$ such that

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

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

(2) $0 \leq \alpha_i \leq C$ for all α_i

$\alpha_i y_i \boxed{\varphi(\boldsymbol{x}_i)^T \varphi(\boldsymbol{x}_j)} + b$

What if we can by-pass this explicit mapping step?

The "Kernel Trick": The Dot Product

- SVM does not need direct access to the original feature space, i.e., original data representation **x**
- It only requires access to the dot products $\mathbf{x}_i^T\mathbf{x}_j$
- The inner products

$$K(\mathbf{x}_i,\mathbf{x}_j) = \mathbf{x}_i^T\mathbf{x}_j$$

Can be regarded as a measure of simil data points (think cosine similarity)

Find $\alpha_1 \ldots \alpha_L$ such that

$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\sigma\alpha_i\alpha_j y_i y_j \boxed{K(\mathbf{x}_i,\mathbf{x}_j)}$ is maximized and

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

(2) $0 \leq \alpha_i \leq C$ for all α_i

$$f(\mathbf{x}) = \Sigma\alpha_i y_i \boxed{K(\mathbf{x}_i,\mathbf{x})} + b$$

The “Kernel Trick”: Implicit Mapping

- What if we have a function that compute the inner product $K(\mathbf{x}_i,\mathbf{x}_j)$ directly without explicitly performing the mapping Φ: $\mathbf{x} \rightarrow \varphi(\mathbf{x})$

Find $\alpha_1 \ldots \alpha_L$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\sigma\alpha_i\alpha_j y_i y_j$ $\boxed{\phantom{K(\mathbf{x}_i,\mathbf{x}_j)}}$
maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

$$= \Sigma\alpha_i y_i \boxed{K(\mathbf{x}_i, \mathbf{x})} + b$$

Kernel Functions

- A *kernel function* is a function that is equivalent to an inner product in some feature space.
- Thus, a kernel function *implicitly* maps data to a high-dimensional space (without the need to compute each $\boldsymbol{\varphi}(\mathbf{x})$ explicitly).
- Why implicit mapping?
  - Save computation
  - The target space nality

Kernel Example

- 2-dimensional vectors $\mathbf{x}=[x_1 \;\; x_2]$
- Let: $K(\mathbf{x}_i,\mathbf{x}_j) = (1 + \mathbf{x}_i^{\mathsf{T}}\mathbf{x}_j)^2$
- What mapping is this?
- Need to show that $K(\mathbf{x}_i,\mathbf{x}_j) = \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathsf{T}}\boldsymbol{\varphi}(\mathbf{x}_j)$ for some $\boldsymbol{\varphi}$

$$
\begin{aligned}
K(\mathbf{x}_i,\mathbf{x}_j) &= (1 + \mathbf{x}_i^{\mathsf{T}}\mathbf{x}_j)^2 = 1 + x_{i1}^2 x_{j1}^2 + 2\, x_{i1} x_{j1} x_{i2} x_{j2} + x_{i2}^2 x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2} \\
&= [1 \;\; x_{i1}^2 \;\; \sqrt{2}\, x_{i1}x_{i2} \;\; x_{i2}^2 \;\; \sqrt{2}x_{i1} \;\; \sqrt{2}x_{i2}]^{\mathsf{T}} [1 \;\; x_{j1}^2 \;\; \sqrt{2}\, x_{j1}x_{j2} \;\; x_{j2}^2 \;\; \sqrt{2}x_{j1} \;\; \sqrt{2}x_{j2}] \\
&= \boldsymbol{\varphi}(\mathbf{x}_i)^{\mathsf{T}}\boldsymbol{\varphi}(\mathbf{x}_j),
\end{aligned}
$$

where $\boldsymbol{\varphi}(\mathbf{x}) = [1 \;\; x_1^2 \;\; \sqrt{2}\, x_1x_2 \;\; x_2^2 \;\; \sqrt{2}x_1 \;\; \sqrt{2}x_2]$

Kernel Functions

- Not all 'similarity' measures are proper kernels

$$K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2$$

$$K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^3 \; ??$$

- For some functions K … $\varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_j)$ can be cumbersome.

What Functions are Kernels?

- Mercer's theorem:

  Every positive semi-definite symmetric function is a kernel

- Positive semi-definite symmetric functions correspond to a positive semi-definite symmetric Gram matrix:

K=

$K(\mathbf{x}_1,\mathbf{x}_1)$	$K(\mathbf{x}_1,\mathbf{x}_2)$	$K(\mathbf{x}_1,\mathbf{x}_3)$		$K(\mathbf{x}_1,\mathbf{x}_n)$
$K(\mathbf{x}_2,\mathbf{x}_1)$	$K(\mathbf{x}_2,\mathbf{x}_2)$	$K(\mathbf{x}_2,\mathbf{x}_3)$		$K(\mathbf{x}_2,\mathbf{x}_n)$
…	…	…	…	…
$K(\mathbf{x}_n,\mathbf{x}_1)$	$K(\mathbf{x}_n,\mathbf{x}_2)$	$K(\mathbf{x}_n,\mathbf{x}_3)$	…	$K(\mathbf{x}_n,\mathbf{x}_n)$

Non examinable

Examples of Kernel Functions

- Linear:

$$K(\mathbf{x}_i,\mathbf{x}_j)= \mathbf{x}_i^T\mathbf{x}_j$$

  – Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}(\mathbf{x})$ is $\mathbf{x}$ itself

- Polynomial of power

i j

  – Mapping Φ: $\mathbf{x} \rightarrow \boldsymbol{\varphi}(\mathbf{x})$, where $\boldsymbol{\varphi}$ $\left(p \right)$ dimensions

Examples of Kernel Functions

- Gaussian (Radial-Basis Function (RBF)):

$$K(\mathbf{x}_i,\mathbf{x}_j) = e^{\frac{-\|x_i - x_j\|^2}{2\sigma^2}}$$

  – Mapping Φ: **x** -*dimensional*: every point is mapped to *a f*

Non-linear SVMs Mathematically

- Dual problem formulation:

Find $\alpha_1 \dots \alpha_L$ such that

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

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

(2) $C \geq \alpha_i \geq 0$

- The classifier function is:

$$f(\mathbf{x}) = \Sigma\alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + b$$

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

In Practice

- Are we guaranteed that the kernel trick will make the data linearly separable?
  - No
  - But usually work

- How to find the suitabl meters?
  - Method: Using M- te

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Multi-class Extension

- SVM is inherently a binary classifier
- Extension to multiclass:
  - One-versus-all: build M classifiers for M classes. Choose class with largest margin for test data
  - One-versus-one: one classifier per pair of classes (M(M-1)/2 classifiers in total ost classifiers

SVM Applications

- SVMs were originally proposed by Boser, Guyon and Vapnik in 1992 and gained increasing popularity in late 1990s.
- SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
- SVMs can be applied to complex data types beyond feature vectors (e.g. graphs, sequences, relational data) by designing kernel functions for such data.

- SVM techniques hav r of tasks such as regression [Vapnik *et al.* '97], principal nalysis [Schölkopf *et al.* '99], etc.
- Most popular optimization algorithms for SVMs use *decomposition* to hill-climb over a subset of α_i's at a time, e.g. SMO [Platt '99] and [Joachims '99]
- Tuning SVMs remains a black art: selecting a specific kernel and parameters is usually done in a try-and-see manner.

References

- [1]https://static1.squarespace.com/static/58851af9ebbd1a30e98fb283/t/58902fbae4fcb5398aeb7505/1485844411772/SVM+Explained.pdf
- [2] A Tutorial on Support Vector Machines for Pattern Recognition
- [3] Demo: http://cs.stanford.edu/people/karpathy/svmjs/demo/
  - (Note: C is the i
- [4] Demo: http://ww VMDemo.zip

Summary

- What is the intuition of Support Vector Machines (SVMs)?
- How to formulate and solve SVM?
- What is linear and non-linear SVM?