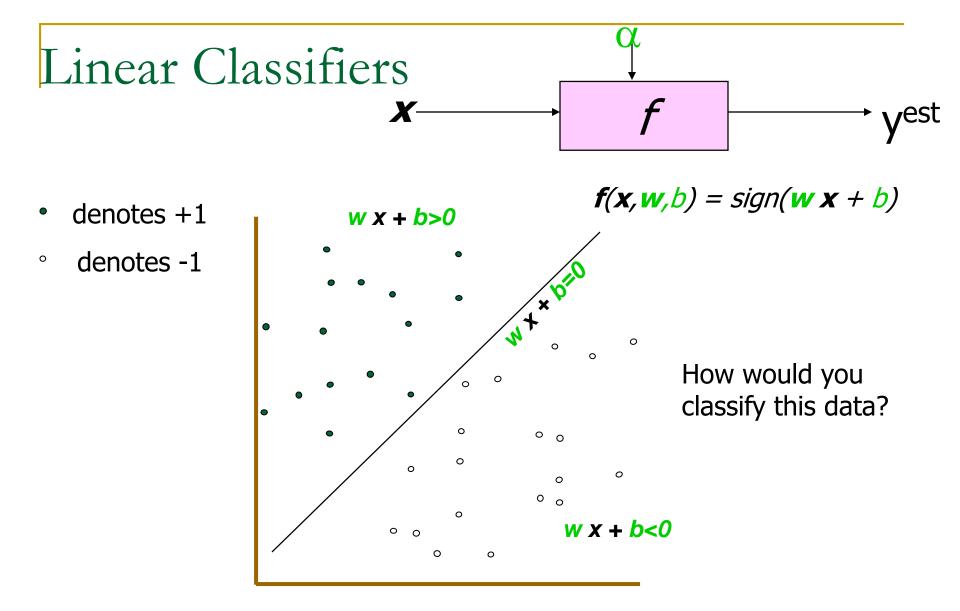
Support Vector Machines



How do we characterize "power"?

- Different machines have different amounts of "power".
- Tradeoff between:
 - More power: Can model more complex classifiers but might overfit.
 - Less power: Not going to overfit, but restricted in what it can model.
- How do we characterize the amount of power?

Some definitions

- Given some machine f
- And under the assumption that all training points (x_k, y_k) were drawn i.i.d from some distribution.
- And under the assumption that future test points will be drawn from the same distribution

Define

$$R(\alpha) = \text{TESTERR}(\alpha) = E\left[\frac{1}{2}|y - f(x, \alpha)|\right] = \frac{\text{Probability of}}{\text{Misclassification}}$$
Official terminology we'll use

Some definitions Given some machine f

- And under the assumption that all training points (x_k, y_k) were drawn i.i.d from some distribution.
- And under the assumption that future test points will be drawn from the same distribution
- Define

$$R(\alpha) = \text{TESTERR}(\alpha) = E\left[\frac{1}{2}|y - f(x,\alpha)|\right] = \frac{\text{Probability of}}{\text{Misclassification}}$$
Official terminology Terminology we'll use
$$R^{emp}(\alpha) = \text{TRAINERR}(\alpha) = \frac{1}{R}\sum_{k=1}^{R}\frac{1}{2}|y_k - f(x_k,\alpha)| = \frac{\text{Fraction Training}}{\text{Set misclassified}}$$

$$R = \#\text{training set data}$$

Vapnik-Chervonenkis dimension
TESTERR(
$$\alpha$$
) = $E\left[\frac{1}{2}|y-f(x,\alpha)|\right]$ TRAINERR(α) = $\frac{1}{R}\sum_{k=1}^{R}\frac{1}{2}|y_k-f(x_k,\alpha)|$

- Given some machine **f**, let *h* be its VC dimension.
- h is a measure of f's power (h does not depend on the choice of training set)
- Vapnik showed that with probability 1-η

TESTERR(
$$\alpha$$
) \leq TRAINERR(α) + $\sqrt{\frac{h(\log(2R/h) + 1) - \log(\eta/4)}{R}}$

This gives us a way to estimate the error on future data based only on the training error and the VC-dimension of f

What VC-dimension is used for TESTERR $(\alpha) = E \left| \frac{1}{2} |y - f(x, \alpha)| \right|$ TRAINERR $(\alpha) = \frac{1}{R} \sum_{k=1}^{K} \frac{1}{2} |y_k - f(x_k, \alpha)|$ Given some machine **f**, let h be its $//C_{/}$ But given machine f, how do we define and compute h? h is a measure of f's power. Vapnik showed ti $\log(\eta/4)$ TESIP stimate the error on عند من المنتخبي من المنتخبي stimate the error on at at ase a only on the training error and the VC-dimension of f

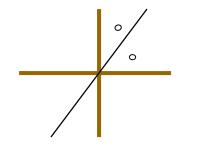
• Machine f can shatter a set of points x_1 , x_2 ... x_r if and only if...

For every possible training set of the form (x_1, y_1) , (x_2, y_2) , ..., (x_r, y_r)

...There exists some value of α that gets zero training error.

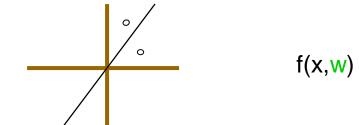
There are 2^r such training sets to consider, each with a different combination of +1's and –1's for the y's

- Machine f can *shatter* a set of points x₁, x₂...X_r if and only if...
 For every possible training set of the form (x₁,y₁), (x₂,y₂),... (x_r,y_r)
 ...There exists some value of α that gets zero training error.
- Question: Can the following f shatter the following points?



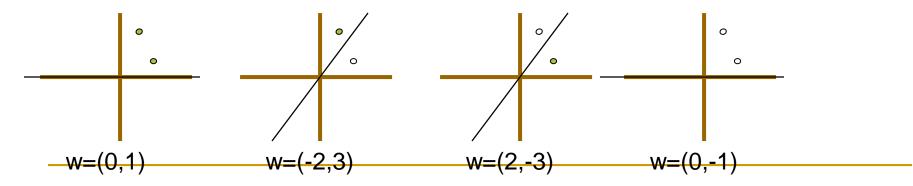
f(x, w) = sign(x.w)

- Machine f can *shatter* a set of points x₁, x₂...X_r if and only if...
 For every possible training set of the form (x₁,y₁), (x₂,y₂),... (x_r,y_r)
 ...There exists some value of α that gets zero training error.
- Question: Can the following f shatter the following points?

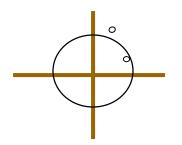


f(x,w) = sign(x.w)

• Answer: No problem. There are four training sets to consider

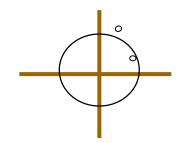


 Machine f can *shatter* a set of points x₁, x₂...X_r if and only if... For every possible training set of the form (x₁,y₁), (x₂,y₂),... (x_r,y_r) ...There exists some value of α that gets zero training error.
 Question: Can the following f shatter the following points?



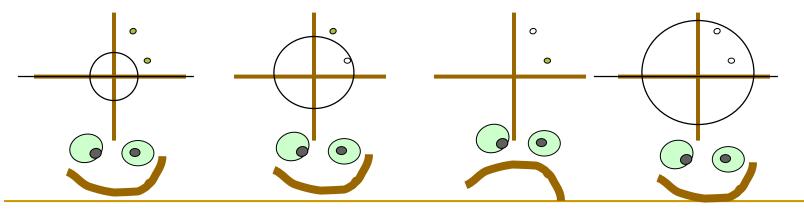
f(x,b) = sign(x.x-b)

- Machine f can *shatter* a set of points x₁, x₂...X_r if and only if...
 For every possible training set of the form (x₁,y₁), (x₂,y₂),... (x_r,y_r)
 ...There exists some value of α that gets zero training error.
- Question: Can the following f shatter the following points?



f(x,b) = sign(x.x-b)

• Answer: No way my friend.



Definition of VC dimension

Given machine *f*, the VC-dimension *h* is

The maximum number of points that can be arranged so that f shatter them.

Example: What's VC dimension of f(x,b) = sign(x.x-b)

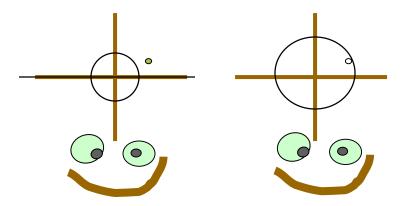
VC dim of trivial circle

Given machine *f*, the VC-dimension *h* is

The maximum number of points that can be arranged so that f shatter them.

Example: What's VC dimension of f(x,b) = sign(x.x-b)

Answer = 1: we can't even shatter two points! (but it's clear we can shatter 1)



Reformulated circle

Given machine *f*, the VC-dimension *h* is

The maximum number of points that can be arranged so that f shatter them.

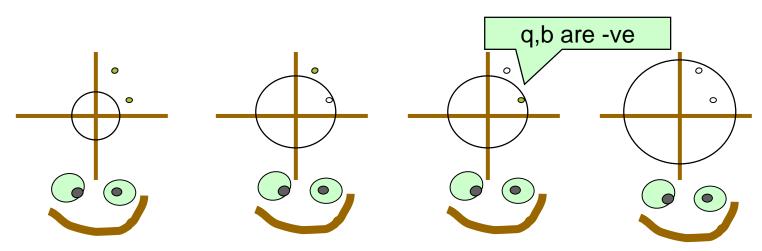
Example: For 2-d inputs, what's VC dimension of f(x,q,b) = sign(qx.x-b)

Reformulated circle Given machine *f*, the VC-dimension *h* is

The maximum number of points that can be arranged so that f shatter them.

Example: What's VC dimension of f(x,q,b) = sign(qx.x-b)

• Answer = 2



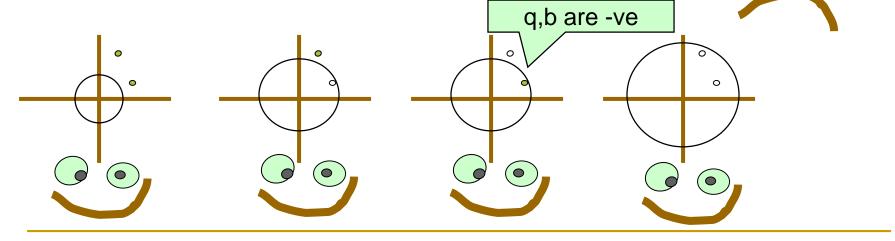
Reformulated circle Given machine *f*, the VC-dimension *h* is

The maximum number of points that can be arranged so that f shatter them.

Example: What's VC dimension of f(x,q,b) = sign(qx.x-b)

0





Vapnik-Chervonenkis dimension
TESTERR(
$$\alpha$$
) = $E\left[\frac{1}{2}|y-f(x,\alpha)|\right]$ TRAINERR(α) = $\frac{1}{R}\sum_{k=1}^{R}\frac{1}{2}|y_k-f(x_k,\alpha)|$

- Given some machine **f**, let *h* be its VC dimension.
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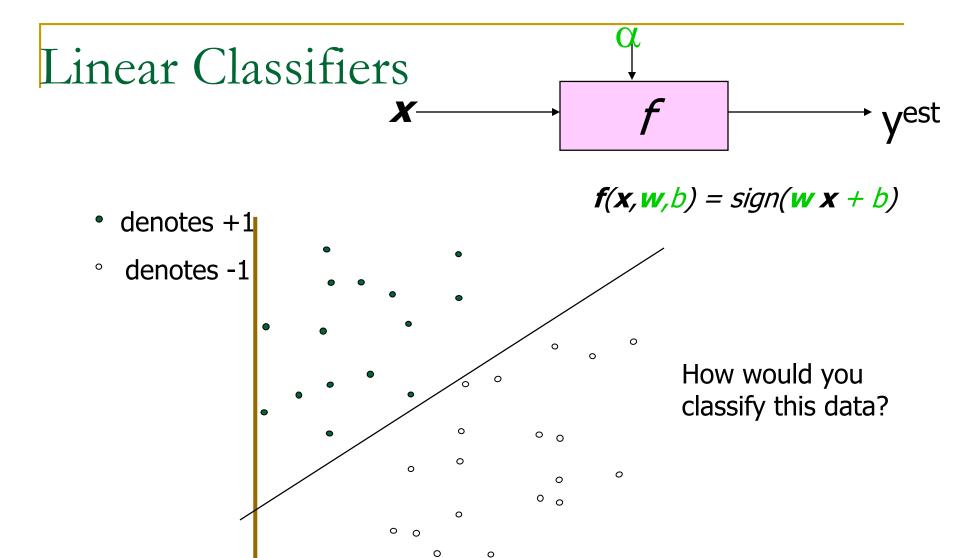
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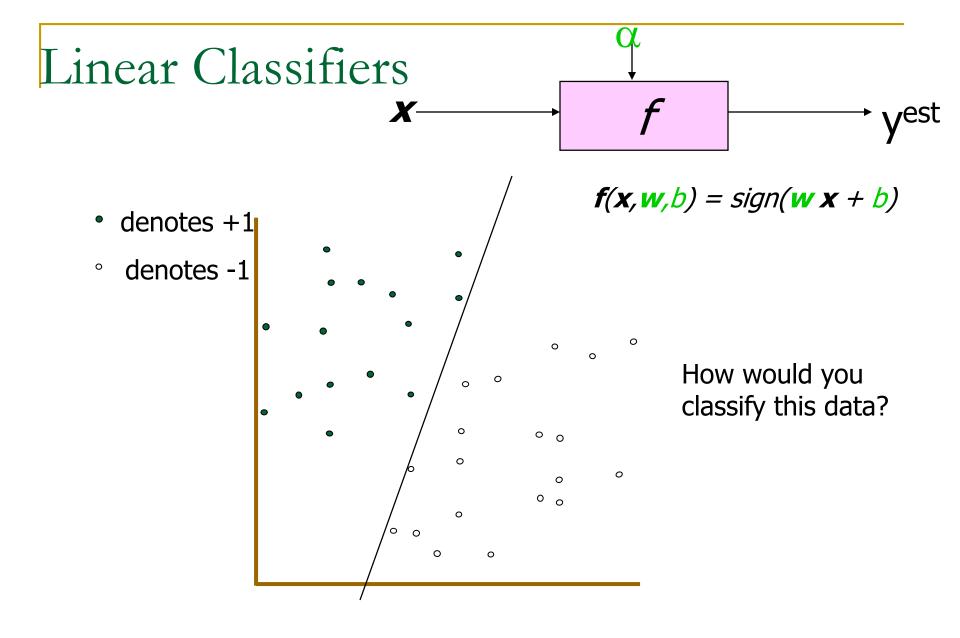
Definition of VC dimension

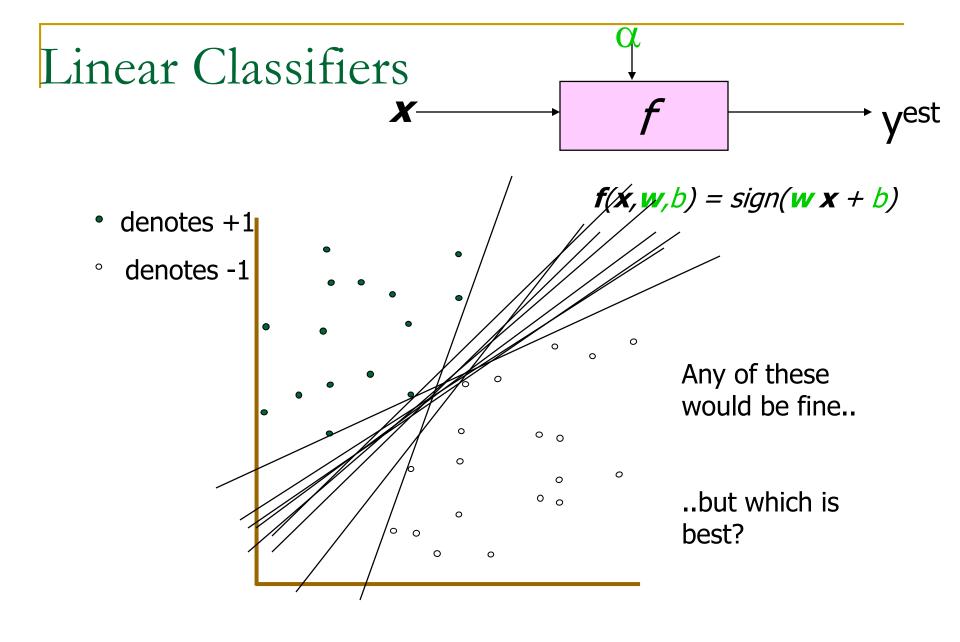
Given machine *f*, the VC-dimension *h* is

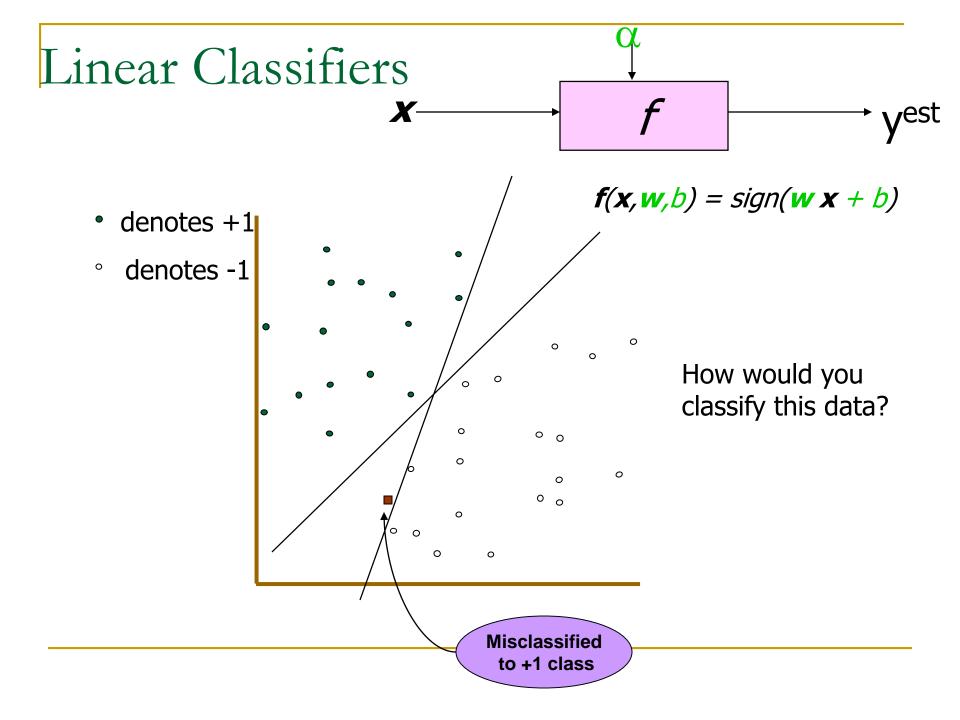
The maximum number of points that can be arranged so that f shatter them.

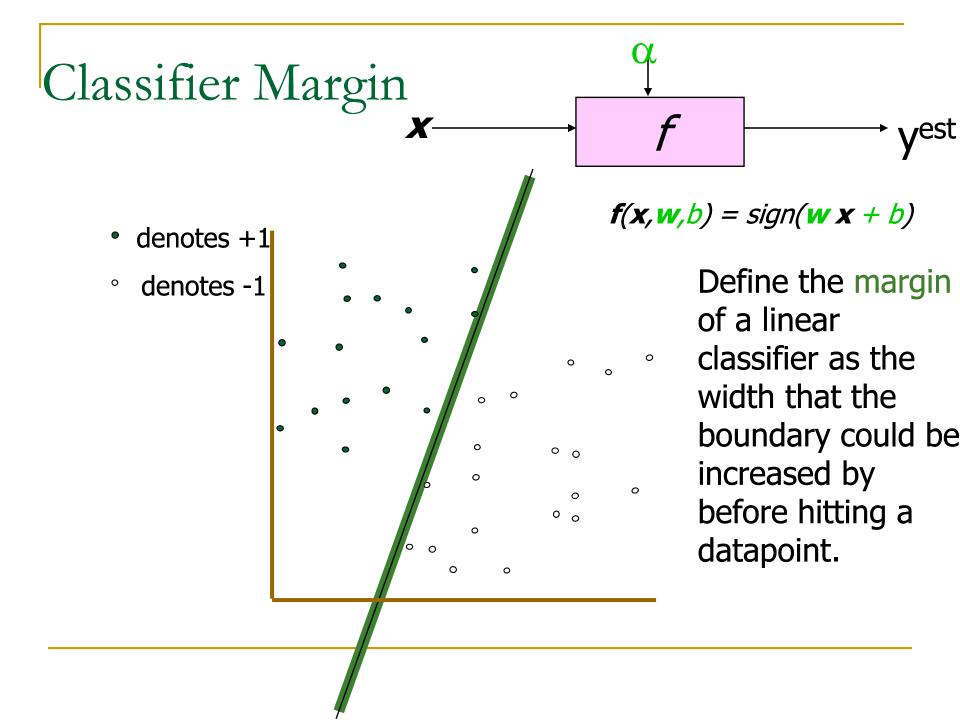
Example: What's VC dimension of f(x,b) = sign(x.x-b)

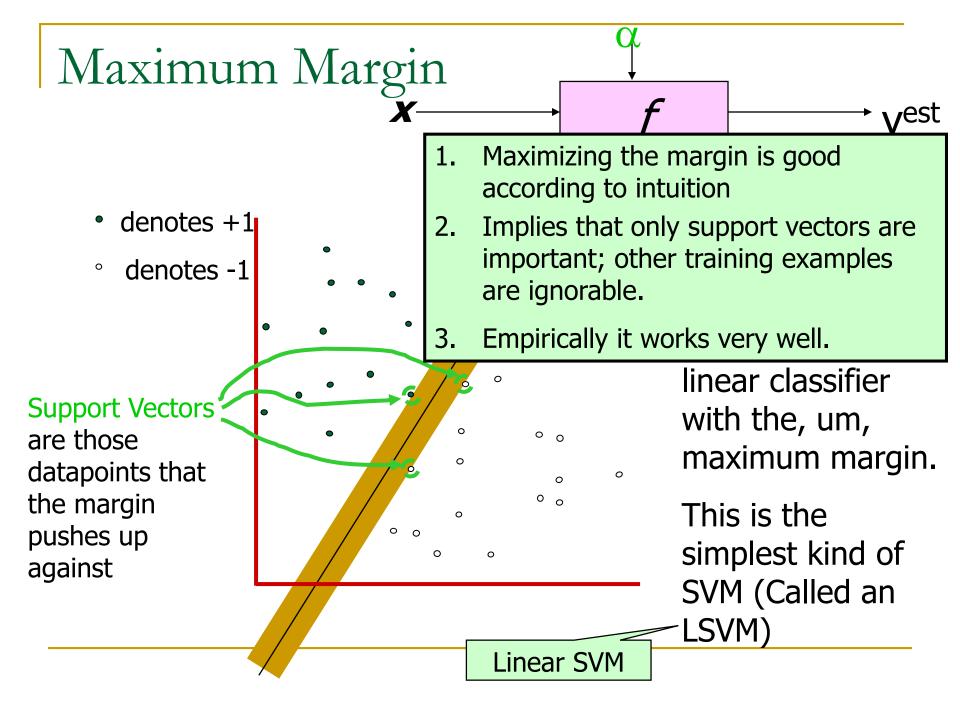


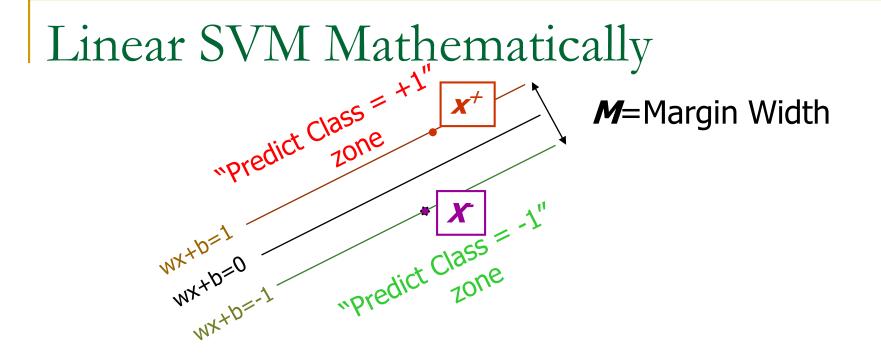












What we know:

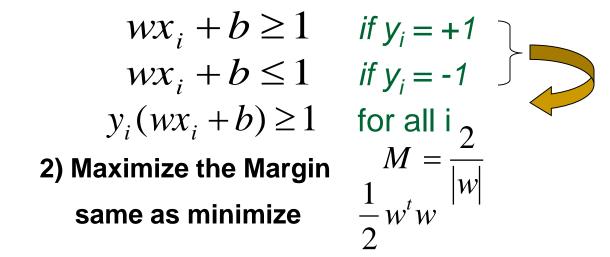
- **W**. **X**⁺ + b = +1
- **w**. **x** + b = -1

•
$$W \cdot (X^+ - X^-) = 2$$

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

Linear SVM Mathematically

Goal: 1) Correctly classify all training data



• We can formulate a Quadratic Optimization Problem and solve for w and b

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

subject to $y_i(wx_i + b) \ge 1 \quad \forall i$

Solving the Optimization Problem

Find w and b such that $\Phi(w) = \frac{1}{2} w^T w$ is minimized;

and for all $\{(\mathbf{x}_i, y_i)\}$: $y_i (\mathbf{w}^T \mathbf{x}_i + b) \ge 1$

- Need to optimize a *quadratic* function subject to *linear* constraints.
- Quadratic optimization problems are a well-known class of mathematical programming problems, and many (rather intricate) algorithms exist for solving them.
- The solution involves constructing a *dual problem* where a Lagrange multiplier α_i is associated with every constraint in the primary problem:

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

The Optimization Problem Solution

The solution has the form:

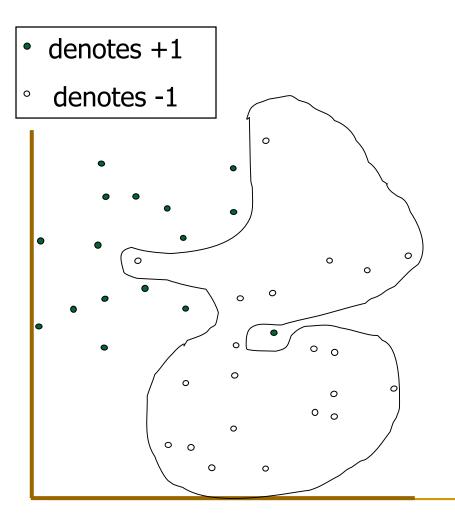
 $\mathbf{w} = \sum \alpha_i y_i \mathbf{x}_i$ $b = y_k - \mathbf{w}^T \mathbf{x}_k$ for any \mathbf{x}_k such that $\alpha_k \neq 0$

- Each non-zero α_i indicates that corresponding x_i is a support vector.
- Then the classifying function will have the form:

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

- Notice that it relies on an *inner product* between the test point x and the support vectors x_i.
- Also keep in mind that solving the optimization problem involved computing the inner products x_i^Tx_j between all pairs of training points.

Dataset with noise

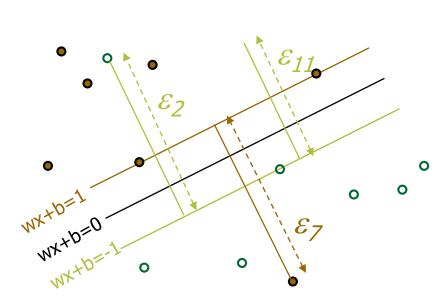


- Hard Margin: So far we require all data points be classified correctly
 - No training error
 - What if the training set is noisy?
 - Solution 1: use very powerful kernels

OVERFITTING!

Soft Margin Classification

Slack variables ξi can be added to allow misclassification of difficult or noisy examples.



What should our quadratic optimization criterion be? Minimize

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

Hard Margin v.s. Soft Margin

The old formulation:

Find w and b such that $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w}$ is minimized and for all $\{(\mathbf{x}_{i}, y_{i})\}$ $y_{i} (\mathbf{w}^{\mathrm{T}} \mathbf{x}_{i} + \mathbf{b}) \ge 1$

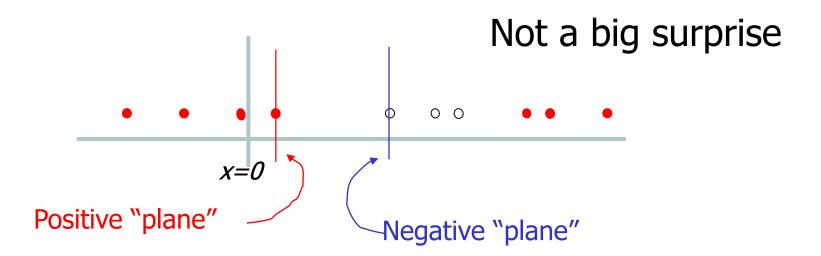
The new formulation incorporating slack variables:

Find w and b such that $\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^{\mathrm{T}} \mathbf{w} + C \Sigma \xi_{i} \text{ is minimized and for all } \{(\mathbf{x}_{i}, y_{i})\}$ $y_{i} (\mathbf{w}^{\mathrm{T}} \mathbf{x}_{i} + b) \ge 1 - \xi_{i} \text{ and } \xi_{i} \ge 0 \text{ for all } i$

Parameter C can be viewed as a way to control overfitting.

Hard 1-dimensional Dataset

What would SVMs do with this data?



Doesn't look like slack variables will save us this time...

Hard 1-dimensional Dataset Make up a new feature! Sort of... ... computed from original feature(s) $|\mathbf{Z}_k| = (x_k, x_k^2)$ Separable! MAGIC!

New features are sometimes called *basis functions*. Now drop this "augmented" data into our linear SVM.

Kernels and Linear Classifiers

Let $\vec{x} = [\vec{x}_1, \vec{x}_2] \in \mathbb{R}^2$ be a vectorial representation of object $x \in \mathcal{X}$

Let $\phi: \mathcal{X} \to \mathcal{K} \subset \mathbb{R}^3$ feature map be given by

$$\phi(\vec{x}) \doteq [\vec{x}_1, \vec{x}_2^2, \vec{x}_1 \vec{x}_2]^T \in \mathcal{K} \subset \mathbb{R}^3$$

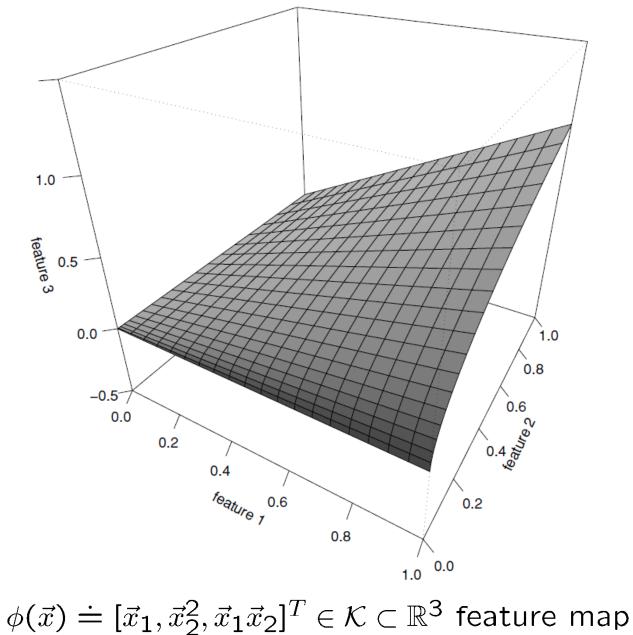
Def. Feature space: \mathcal{K}

We will use linear classifiers in this feature space.

In the original space \mathbb{R}^2 for a given $\mathbf{w}\in\mathbb{R}^3$ the decision surface is:

$$\tilde{X}_0(\mathbf{w}) = \{ \vec{x} \in \mathbb{R}^2 \mid w_1 \vec{x}_1 + w_2 \vec{x}_2^2 + w_3 \vec{x}_1 \vec{x}_2 = 0 \}$$

- This is nonlinear in $\vec{x} \in \mathbb{R}^2$
- This is linear in the feature space $\phi(\vec{x}) \in \mathcal{K} \subset \mathbb{R}^3$



Kernels and Linear Classifiers

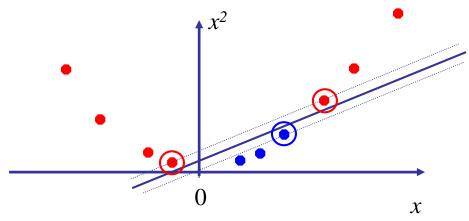
 $\phi(\vec{x}) \doteq [\phi_1(\vec{x}), \phi_2(\vec{x}), \phi_3(\vec{x})] \doteq [\vec{x}_1, \vec{x}_2^2, \vec{x}_1 \vec{x}_2]^T$

Feature functions

- We seek for a small set of basis vectors $\{\phi_i\}$ which allows perfect discrimination between the classes in \mathcal{X} (Feature selection)
- If we have too many features \Rightarrow overfitting can happen.

Non-linear SVMs

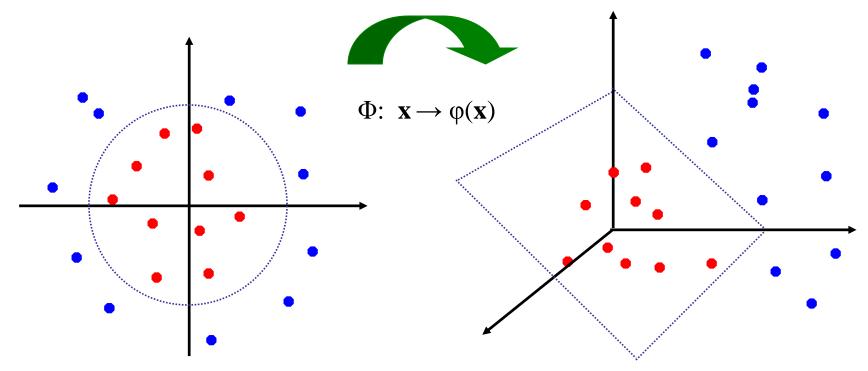
- Datasets that are linearly separable with some noise work out great:
- But what are we going to do if the dataset is just too hard?
- How about... mapping data to a higher-dimensional space:



х

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"

- To produce linear separability in Higher Dimension, the linear classifier relies on dot product between vectors $K(x_i,x_j)=x_i^Tx_j$
- If every data point is mapped into high-dimensional space via some transformation Φ : $x \rightarrow \phi(x)$, the dot product becomes:

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

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

2-dimensional vectors $\mathbf{x} = [x_1 \ x_2]$; let $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$, Need to show that $K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$: $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$, $= 1 + x_{iI}^2 x_{jI}^2 + 2 x_{iI} x_{jI} x_{i2} x_{j2} + x_{i2}^2 x_{j2}^2 + 2 x_{iI} x_{jI} + 2 x_{i2} x_{j2}$ $= [1 \ x_{iI}^2 \ \sqrt{2} \ x_{iI} x_{i2} \ x_{i2}^2 \ \sqrt{2} x_{iI} \ \sqrt{2} x_{i2}]^T [1 \ x_{jI}^2 \ \sqrt{2} \ x_{jI} x_{j2} \ x_{j2}^2 \ \sqrt{2} x_{jI} \ \sqrt{2} x_{j2}]$ $= \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$, where $\varphi(\mathbf{x}) = [1 \ x_{I}^2 \ \sqrt{2} \ x_{I} x_2 \ x_{2}^2 \ \sqrt{2} x_{I} \ \sqrt{2} x_{2}]$

What Functions are Kernels?

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

 $K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$ 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=	$K(\mathbf{x}_1,\mathbf{x}_1)$	$K(\mathbf{x_1},\mathbf{x_2})$	$K(\mathbf{x}_1,\mathbf{x}_3)$	•••	$K(\mathbf{x}_1,\mathbf{x}_N)$
	$K(\mathbf{x}_2,\mathbf{x}_1)$	$K(\mathbf{x}_2,\mathbf{x}_2)$	$K(\mathbf{x}_2,\mathbf{x}_3)$		$K(\mathbf{x}_2,\mathbf{x}_N)$
	•••	• • •	• • •	• • •	•••
	$K(\mathbf{x}_{N},\mathbf{x}_{1})$	$K(\mathbf{x}_{N},\mathbf{x}_{2})$	$K(\mathbf{x}_{N},\mathbf{x}_{3})$	•••	$K(\mathbf{x}_{N},\mathbf{x}_{N})$

Examples of Kernel Functions

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

• Polynomial of power *p*: $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$

Gaussian (radial-basis function network): $K(\mathbf{x_i}, \mathbf{x_j}) = \exp(-\frac{\|\mathbf{x_i} - \mathbf{x_j}\|^2}{2\sigma^2})$

Sigmoid: $K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1)$

Non-linear SVMs Mathematically

Dual problem formulation:

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

• The solution is:

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

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

Nonlinear SVM - Overview

- SVM locates a separating hyperplane in the feature space and classify points in that space
- It does not need to represent the space explicitly, simply by defining a kernel function
- The kernel function plays the role of the dot product in the feature space.

Properties of SVM

- Flexibility in choosing a similarity function
- Sparseness of solution when dealing with large data sets
 - only support vectors are used to specify the separating hyperplane
- Ability to handle large feature spaces
 - complexity does not depend on the dimensionality of the feature space
- Overfitting can be controlled by soft margin approach
- Nice math property: a simple convex optimization problem which is guaranteed to converge to a single global solution
- Feature Selection

SVM Applications

- SVM has been used successfully in many real-world problems
 - text (and hypertext) categorization
 - image classification
 - bioinformatics (Protein classification, Cancer classification)
 - hand-written character recognition

Weakness of SVM

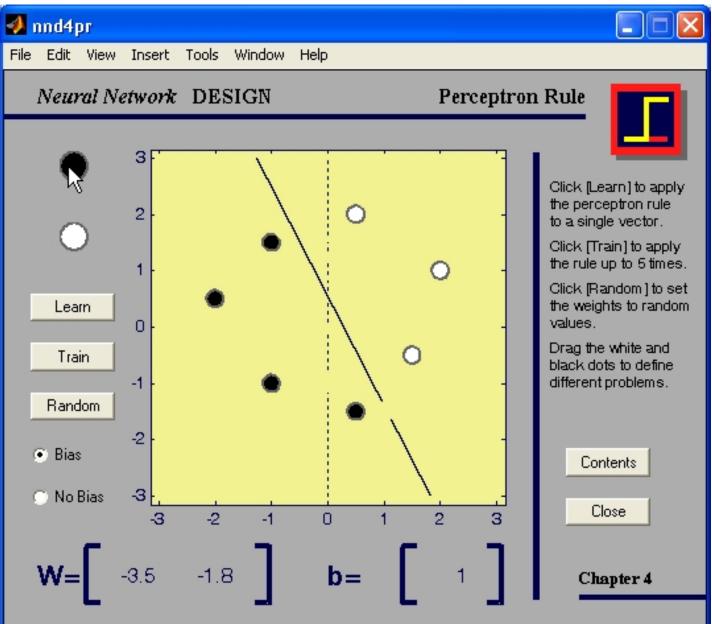
• It is sensitive to noise

- A relatively small number of mislabeled examples can dramatically decrease the performance

- It only considers two classes
 - how to do multi-class classification with SVM?
 - Answer:
 - 1) with output arity m, learn m SVM's
 - SVM 1 learns "Output==1" vs "Output != 1"
 - SVM 2 learns "Output==2" vs "Output != 2"
 - :
 - SVM m learns "Output==m" vs "Output != m"

2)To predict the output for a new input, just predict with each SVM and find out which one puts the prediction the furthest into the positive region.

Back to the Perceptron Example



The Perceptron

• The primal algorithm in the feature space

 $D = \{(x_i, y_i), i = 1, \dots, m\}$ training data set.

 $\mathbf{x}_i = \phi(x_i) \in \mathcal{K} \subset \mathbb{R}^n$ feature map.

1., $\mathbf{w} = 0 \in \mathbb{R}^n$ 2., $\forall (x_i, y_i), i = 1, ..., m$, evaluate $sign(y_i \langle \mathbf{x}_i, \mathbf{w} \rangle)$ 3., If x_i is misclassified $(sign(y_i \langle \mathbf{x}_i, \mathbf{w} \rangle) < 0)$ then $\mathbf{w} := \mathbf{w} + y_i \mathbf{x}_i$

4., If no mistakes occur \Rightarrow STOP

The primal algorithm in the feature space

Algorithm 1 Perceptron learning algorithm (in primal variables).

Require: A feature mapping $\boldsymbol{\phi} : \mathcal{X} \to \mathcal{K} \subseteq \ell_2^n$

Ensure: A linearly separable training sample $z = ((x_1, y_1), \dots, (x_m, y_m))$ $w_0 = 0; t = 0$

repeat for j = 1, ..., m **do if** $y_j \langle \phi(x_j), \mathbf{w} \rangle \leq 0$ **then** $\mathbf{w}_{t+1} = \mathbf{w}_t + y_j \phi(x_j)$ $t \leftarrow t+1$ **end if end for until** no mistakes have been made within the **for** loop **return** the final weight vector \mathbf{w}_t

The Perceptron

We start at $\mathbf{w}_0 = \mathbf{0} \in \mathcal{K} \subset \mathbb{R}^n$

m = num of training examples, $n = dim(\mathcal{K})$,

t = num of mistakes so far

$$\Rightarrow \mathbf{w}_t = \sum_{i=1}^m \alpha_i \phi(x_i) = \sum_{i=1}^m \alpha_i \mathbf{x}_i \in \mathbb{R}^n$$
 at time step t

Thus instead of tuning *n* variables $\mathbf{w} = (w_1, \dots, w_n)$ (**Primal variables**) in the large *n*-dimensional feautre space \mathcal{K} , it is enough to learn $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_m)$ values (**Dual variables**).

The Perceptron The Dual Algorithm in the feature space

 $D = \{(x_i, y_i), i = 1, \dots, m\} \text{ training data set.} \\ \mathbf{x}_i = \phi(x_i) \in \mathcal{K} \subset \mathbb{R}^n \text{ feaure map, } i = 1, \dots, m$

$$t = \text{num of mistakes so far} \\ \Rightarrow \mathbf{w}_t = \sum_{i=1}^m \alpha_i \phi(x_i) = \sum_{i=1}^m \alpha_i \mathbf{x}_i \in \mathbb{R}^n \text{ at time step } t$$

We update $oldsymbol{lpha}_{oldsymbol{t}} \in \mathbb{R}^m$ whenever a mistake occurs

1.,
$$\alpha_0 = 0 \in \mathbb{R}^m$$

2., $\forall j = 1, ..., m$ evaluate
 $y_j \langle \mathbf{x}_j, \mathbf{w}_t \rangle = y_j \langle \mathbf{x}_j, \sum_{i=1}^m \alpha_i \mathbf{x}_i \rangle = y_j \sum_{i=1}^m \alpha_i \langle \mathbf{x}_j, \mathbf{x}_i \rangle$
3., If x_j is misclassified $(y_j \langle \mathbf{x}_j, \mathbf{w}_t \rangle < 0)$ then update $\alpha_t \in k$
4., If no mistakes occur \Rightarrow STOP

The Dual Algorithm in the feature space

Algorithm 2 Perceptron learning algorithm (in dual variables).

Require: A feature mapping $\boldsymbol{\phi} : \mathcal{X} \to \mathcal{K} \subseteq \ell_2^n$

Ensure: A linearly separable training sample $z = ((x_1, y_1), \dots, (x_m, y_m))$ $\alpha = 0$

repeat

for
$$j = 1, ..., m$$
 do
if $y_j \sum_{i=1}^m \alpha_i \langle \boldsymbol{\phi}(x_i), \boldsymbol{\phi}(x_j) \rangle \leq 0$ then
 $\alpha_j \leftarrow \alpha_j + y_j$
end if
end for

until no mistakes have been made within the for loop return the vector α of expansion coefficients

The Dual Algorithm in the feature space

For the classification of a new object (x, y) we have to evaluate

$$y\sum_{i=1}^{m}\alpha_i \langle \mathbf{x}, \mathbf{x}_i \rangle$$

We don't have to know the actual values of $\mathbf{x} = \phi(x)!$

It is enough to know the inner products

$$\langle \mathbf{x}, \mathbf{x}_i \rangle \quad \forall i = 1, \dots, m$$

between the object and the training points

Kernels

Definition: (kernel)

We are given $\phi : \mathcal{X} \to \mathcal{K} \subset l_2^n$ feautre mapping.

The **kernel** $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is the corresponding inner product function:

$$k(x_i, x_j) \doteq \langle \underbrace{\phi(x_i)}_{\mathbf{x}_i}, \underbrace{\phi(x_j)}_{\mathbf{x}_j} \rangle_{\mathcal{K}} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle_{\mathcal{K}}$$

Kernels

Definition: (Gram matrix, kernel matrix)

Gram matrix $G \in \mathbb{R}^{m \times m}$ of kernel k at $\{x_1, \ldots, x_m\}$:

Given a kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and a training set $\{x_1, \dots, x_m\}$ $\} \Rightarrow G_{ij} \doteq k(x_i, x_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$

Definition: (Feature space, kernel space)

 $\mathcal{K} \doteq span\{\phi(x) \mid x \in \mathcal{X}\} \subset \mathbb{R}^n$

Kernel technique

Definition:

 $\begin{array}{l} \text{Matrix } G \in \mathbb{R}^{m \times m} \text{ is positive semidefinite (PSD)} \\ \Leftrightarrow G \text{ is symmetric, and } \mathsf{0} \leq \boldsymbol{\beta}^T G \boldsymbol{\beta} \ \forall \boldsymbol{\beta} \in \mathbb{R}^{m \times m} \end{array}$

Given a kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and a training set $\{x_1, \ldots, x_m\}$ $\} \Rightarrow G_{ij} \doteq k(x_i, x_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle_{\mathcal{K}}$

Lemma:

The Gram matrix is symmetric, PSD matrix.

Proof: $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_m] \in \mathbb{R}^{n \times m} \Rightarrow G = \mathbf{X}^T \mathbf{X} \in \mathbb{R}^{m \times m}$ $0 \le \langle \mathbf{X}\boldsymbol{\beta}, \mathbf{X}\boldsymbol{\beta} \rangle_{\mathcal{K}} = \boldsymbol{\beta}^T G \boldsymbol{\beta}$

Kernel technique

We already know that several algorithms use the **kernel values** only (...and NOT the **feature values**)!

Key idea:

Choose a nice kernel function
$$k$$

rather than an ugly feautre mapping
 $\phi: \mathcal{X} \to \mathbb{R}^n$

Kernel technique

We have seen so far how to build a kernel $k(\cdot, \cdot)$ from a given feature map $\phi : \mathcal{X} \to \mathbb{R}^n$

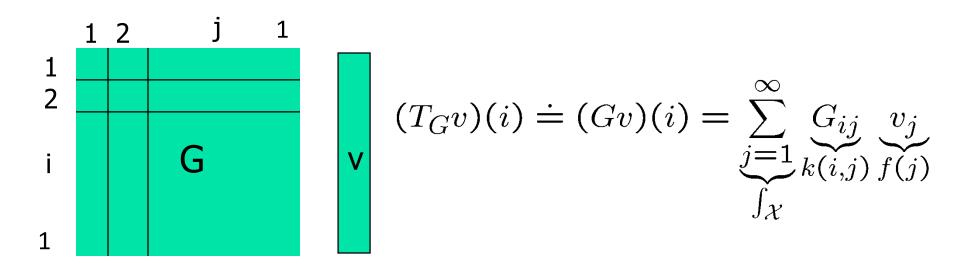
Now we want to do the opposite:

A function $k(\cdot, \cdot)$ is kernel \Leftrightarrow there exists a feature space \mathcal{K} and feature map $\phi : \mathcal{X} \to \mathcal{K}$, such that $k(x_1, x_2) = \langle \phi(x_1), \phi(x_2) \rangle_{\mathcal{K}}$



From Vector domain to Functions

- Observe that each vector v = (v[1], v[2], ..., v[n]) is a mapping from the integers {1,2,..., n} to <
- •We can generalize this easily to **INFINITE** domain w = (w[1], w[2], ..., w[n], ...) where w is mapping from {1,2,...} to <



From Vector domain to Functions

From integers we can further extend to

- < or
- <^m
- Strings
- Graphs
- Sets
- Whatever
- ...

Kernels

We don't need the $\mathcal{K} \subset l_2^n$ assumption. It is enough if \mathcal{K} is a complete inner product (Hilbert) space.

Definition: inner product, Hilbert spaces

 $\langle \cdot, \cdot \rangle : \mathcal{K} \times \mathcal{K} \to \mathbb{R}$ is an inner product in vector space \mathcal{K} , iff for all vectors $x, y, z \in \mathcal{K}$ and all scalars $a \in \mathbb{R}$:

* Symmetry:
$$\langle x, y \rangle = \langle y, x \rangle$$
.

* Linearity in the first argument: $\langle ax, y \rangle = a \langle x, y \rangle, \ \langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle.$

* Positive-definite: $\langle x, x \rangle \ge 0$ with equality only for x = 0.

This is more general than the inner product in $\mathbb{R}^n = l_2^n$ Examples:

- space of square integrable functions $L_2(\mathcal{X})$,
- space of square summable infinite series l_2

Integral operators, eigenfunctions

Definition: Eigenvalue, Eigenfunction

- λ is the eigenvalue,
- $\Psi \in L_2(\mathcal{X})$ is the eigenfunction of integral opreator $(T_k f)(\cdot) = \int k(\cdot, x) f(x) dx$

$$\Leftrightarrow \begin{cases} \int_{\mathcal{X}} k(x,\bar{x})\psi(\bar{x})d\bar{x} = \lambda\psi(x) \quad \forall x \in \mathcal{X} \\ \|\psi\|_{L_{2}}^{2} \doteq \int_{\mathcal{X}} \psi^{2}(x)dx = 1 \end{cases}$$

The previous $Gv = \lambda v$ is a special case of this, when $\mathcal{X} = \{x_1, \ldots, x_r\}$ is a finite set.

Positive (semi) definite operators

Definition: Positive Definite Operator

 $k(\cdot, \cdot)$ is symmetric kernel,

$$\Rightarrow (T_k f)(\cdot) \doteq \int_{\mathcal{X}} k(\cdot, x) f(x) dx$$

 $T_k: L_2(\mathcal{X}) \to L_2(\mathcal{X})$ operator is positive semi definit

$$\Leftrightarrow \int_{\mathcal{X}} \int_{\mathcal{X}} k(\tilde{x}, x) f(x) f(\tilde{x}) dx d\tilde{x} \ge 0 \quad \forall f \in L_2(\mathcal{X})$$

The previous $v^T G v \ge 0$ is a special case of this, when $\mathcal{X} = \{x_1, \dots, x_r\}$ is a finite set.

Mercer's theorem

 $\left\{ \begin{array}{l} k(\cdot, \cdot) \in L_2(\mathcal{X} \times \mathcal{X}), \\ k \text{ is symmetric: } k(x, \tilde{x}) = k(\tilde{x}, x) \\ (T_k f)(\cdot) = \int_{\mathcal{X}} k(\cdot, x) f(x) dx \text{ operator is pos. semi definit} \\ \psi_i, \ i = 1, 2, \dots \text{ are the eigenfunctions of } T_k \\ \text{with eigenvalues } \lambda_i \end{array} \right.$

$$\Rightarrow \begin{cases} (\lambda_{1}, \lambda_{2}, \ldots) \in l_{1}, \quad \lambda_{i} \geq 0 \quad \forall i \\ \psi_{i} \in L_{\infty}(\mathcal{X}), \quad \forall i = 1, 2, \ldots \\ k(x, \tilde{x}) = \sum_{i=1}^{\infty} \lambda_{i} \psi_{i}(x) \psi_{i}(\tilde{x}) \quad \forall x, \tilde{x} \\ 1 \quad \forall x_{i} \neq 0 \quad \forall x_{i} \neq x_{i} \neq 0 \quad$$

Mercer's theorem

We like the Mercer's theorem becuase of the expansion:

$$k(x,\tilde{x}) = \sum_{i=1}^{\infty} \lambda_i \psi_i(x) \psi_i(\tilde{x}) \quad \forall x, \tilde{x}$$

It shows the existence of the feature map $\phi : \mathcal{X} \to \mathcal{K} \subset l_2$

$$\begin{array}{l} \begin{array}{l} \begin{array}{l} \begin{array}{l} \begin{array}{l} \text{Let } \mathcal{K} \doteq l_2, \\ \text{and let } \phi(x) \doteq (\sqrt{\lambda_1}\psi_1(x), \sqrt{\lambda_2}\psi_2(x), \ldots)^T \end{array} \end{array} \end{array} \\ \\ \Rightarrow \langle \phi(x), \phi(\tilde{x}) \rangle_{l_2} \\ = (\sqrt{\lambda_1}\psi_1(x), \sqrt{\lambda_2}\psi_2(x), \ldots)^T (\sqrt{\lambda_1}\psi_1(x), \sqrt{\lambda_2}\psi_2(x), \ldots) \\ \\ = \sum\limits_{i=1}^{\infty} \lambda_i \psi_i(x) \psi_i(\tilde{x}) = k(x, \tilde{x}) \end{array} \end{array}$$

 $\psi(x) = (\psi_1(x), \psi_2(x), \ldots)$ is known as **Mercer map**

A nicer characterization

The (*) condition in the Mercer's theorem is a bit ugly, but we have a nicer form that characterizes when a function $k(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a kernel (i.e. scalar product in some inner product space)

Theorem: nicer kernel characterization

 $k(\cdot, \cdot)$ is a (Mercer) kernel

 $\Leftrightarrow (T_k f)(\cdot)$ is a pos. semi definite operator $\Leftrightarrow G = (k(x_i, x_j))_{ij}^r \in \mathbb{R}^{r \times r}$ Gram matrix is pos. semi definite $\forall r, \forall (x_1, \dots, x_r) \in \mathcal{X}^r$ **Vapnik-Chervonenkis dimension** TESTERR $(\alpha) = E\left[\frac{1}{2}|y - f(x, \alpha)|\right]$ TRAINERR $(\alpha) = \frac{1}{R}\sum_{k=1}^{R}\frac{1}{2}|y_k - f(x_k, \alpha)|$

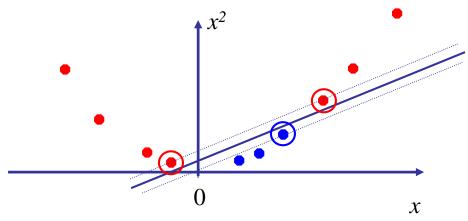
- Given some machine **f**, let *h* be its VC dimension.
- *h* is a measure of **f**'s power (*h* does not depend on the choice of training set)
- Vapnik showed that with probability $1-\eta$

TESTERR(
$$\alpha$$
) \leq TRAINERR(α) + $\sqrt{\frac{h(\log(2R/h) + 1) - \log(\eta/4)}{R}}$

This gives us a way to estimate the error on future data based only on the training error and the VC-dimension of *f*

Non-linear SVMs

- 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:



х

The "Kernel Trick"

- To produce linear separability in Higher Dimension, the linear classifier relies on dot product between vectors $K(x_i,x_j)=x_i^Tx_j$
- If every data point is mapped into high-dimensional space via some transformation Φ : $x \rightarrow \phi(x)$, the dot product becomes:

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

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

2-dimensional vectors $\mathbf{x} = [x_1 \ x_2]$; let $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$, Need to show that $K(\mathbf{x}_i, \mathbf{x}_j) = \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$: $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2$, $= 1 + x_{iI}^2 x_{jI}^2 + 2 x_{iI} x_{jI} x_{i2} x_{j2} + x_{i2}^2 x_{j2}^2 + 2 x_{iI} x_{jI} + 2 x_{i2} x_{j2}$ $= [1 \ x_{iI}^2 \ \sqrt{2} \ x_{iI} x_{i2} \ x_{i2}^2 \ \sqrt{2} x_{iI} \ \sqrt{2} x_{i2}]^T [1 \ x_{jI}^2 \ \sqrt{2} \ x_{jI} x_{j2} \ x_{j2}^2 \ \sqrt{2} x_{jI} \ \sqrt{2} x_{j2}]$ $= \varphi(\mathbf{x}_i)^T \varphi(\mathbf{x}_j)$, where $\varphi(\mathbf{x}) = [1 \ x_{I}^2 \ \sqrt{2} \ x_{I} x_2 \ x_{2}^2 \ \sqrt{2} x_{I} \ \sqrt{2} x_{2}]$

Examples of Kernel Functions

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

• Polynomial of power *p*: $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$

Gaussian (radial-basis function network): $K(\mathbf{x_i}, \mathbf{x_j}) = \exp(-\frac{\|\mathbf{x_i} - \mathbf{x_j}\|^2}{2\sigma^2})$

Sigmoid: $K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1)$

Mercer's theorem

 $\left\{ \begin{array}{l} k(\cdot, \cdot) \in L_2(\mathcal{X} \times \mathcal{X}), \\ k \text{ is symmetric: } k(x, \tilde{x}) = k(\tilde{x}, x) \\ (T_k f)(\cdot) = \int_{\mathcal{X}} k(\cdot, x) f(x) dx \text{ operator is pos. semi definit} \\ \psi_i, \ i = 1, 2, \dots \text{ are the eigenfunctions of } T_k \\ \text{with eigenvalues } \lambda_i \end{array} \right.$

$$\Rightarrow \begin{cases} (\lambda_{1}, \lambda_{2}, \ldots) \in l_{1}, \quad \lambda_{i} \geq 0 \quad \forall i \\ \psi_{i} \in L_{\infty}(\mathcal{X}), \quad \forall i = 1, 2, \ldots \\ k(x, \tilde{x}) = \sum_{i=1}^{\infty} \lambda_{i} \psi_{i}(x) \psi_{i}(\tilde{x}) \quad \forall x, \tilde{x} \\ \int 1 \quad \forall x_{i} = 1 \quad \forall x_{i} = 1 \end{cases}$$

For a given kernel $k(\cdot, \cdot)$ we already know how to define feature space \mathcal{K} , and $\phi : \mathcal{X} \to \mathcal{K}$ feature map (Mercer map):

$$\mathcal{K} = l_2$$
, and $\phi(x) \doteq (\sqrt{\lambda_1}\psi_1(x), \sqrt{\lambda_2}\psi_2(x), \ldots)^T$

Now, we show another way using RKHS

 $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ given kernel $\Rightarrow \mathcal{F}_0 \doteq \{k(x, \cdot) | x \in \mathcal{X}\}$ function space

We will add inner product to \mathcal{F}_0 function space \Rightarrow Pre-Hilbert space

Completing (closing) a pre-Hilbert space \rightarrow Hilbert space

 $k: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ given kernel $\Rightarrow \mathcal{F}_0 \doteq \{k(x, \cdot) | x \in \mathcal{X}\}$ function space

$$(x_1, \dots, x_r) \text{ given } \Rightarrow f(\cdot) \doteq \sum_{i=1}^r \alpha_i k(x_i, \cdot) \in \mathcal{F}_0$$
$$(\tilde{x}_1, \dots, \tilde{x}_s) \text{ given } \Rightarrow g(\cdot) \doteq \sum_{j=1}^s \beta_j k(\tilde{x}_j, \cdot) \in \mathcal{F}_0$$

The inner product:

Note:

While for calculating $\langle f,g \rangle_{\mathcal{F}_0}$ we use their representations: $\alpha \in \mathbb{R}^r, \beta \in \mathbb{R}^s, \{x_i\}_{i=1}^r, \{\tilde{x}_j\}_{j=1}^s$ the $\langle f,g \rangle_{\mathcal{F}_0}$ is independent of the representation of f,g

Proof:

If we change $\alpha \in \mathbb{R}^r$ or $x_i \Rightarrow \langle f, g \rangle_{\mathcal{F}_0}$ doesn't change (because of (*)) The same for $\beta \in \mathbb{R}^s$

$$\langle f,g \rangle_{\mathcal{F}_0} = \sum_{i_1}^r \alpha_i f(x_i) = \sum_{j=1}^s \beta_j f(\tilde{x}_j)$$
 (*)

Lemma:

 $\langle f,g\rangle$ is an inner product of \mathcal{F}_0

 $\Rightarrow \mathcal{F}_0$ is pre-Hilbert space

 $\mathcal{F} \doteq close(\mathcal{F}_0)$ is a Hilbert space

• **Pre-Hilbert** space:

Like the Euclidean space with rational scalars only

• Hilbert space:

Like the Euclidean space with *real* scalars

Proof:

1., $\langle f, g \rangle_{\mathcal{F}_0} = \langle g, f \rangle_{\mathcal{F}_0}$ 2., $\langle cf + dg, h \rangle_{\mathcal{F}_0} = c \langle f, h \rangle_{\mathcal{F}_0} + d \langle g, h \rangle_{\mathcal{F}_0}$, $\forall c, d \in \mathbb{R}, \forall f, g, h \in \mathcal{F}_0$ 3., $\langle f, f \rangle_{\mathcal{F}_0} \ge 0$ 4., $\langle f, f \rangle_{\mathcal{F}_0} = 0 \Leftrightarrow f = 0$

Reproducing Kernel Hilbert Spaces Lemma: (Reproducing property)

$$\langle f, k(x, \cdot) \rangle_{\mathcal{F}} = f(x)$$

Proof: definition of $\langle f,g\rangle_{\mathcal{F}}$

Lemma: The constructed features match to *k*

Huhh...

$$\langle \underbrace{k(x_i, \cdot)}_{\phi(x_i)}, \underbrace{k(x_j, \cdot)}_{\phi(x_j)} \rangle_{\mathcal{F}} = k(x_i, x_j)$$

Proof: reproducing property

Proof of property 4.,:

$$0 \leq (f(x))^2 = \langle f, k(x, \cdot) \rangle_{\mathcal{F}}^2, \forall x$$

$$|$$
rep. property

$$\langle f, k(x, \cdot) \rangle_{\mathcal{F}}^2 \leq \langle f, f \rangle_{\mathcal{F}} \langle k(x, \cdot), k(x, \cdot) \rangle_{\mathcal{F}} \quad \forall x$$

we need only that <0,0>=0!

Hence, if $\langle f, f \rangle_{\mathcal{F}} = 0 \Rightarrow (f(x))^2 = 0, \ \forall x \in \mathcal{X}$ $\Rightarrow f(x) = 0, \ \forall x \in \mathcal{X}$ $\Rightarrow f = 0$

The Representer Theorem

In the perceptron problem we could use the dual algorithm, because we had this representation:

$$f(x) \doteq \langle \phi(x), \mathbf{w} \rangle_{\mathcal{K}} = \sum_{i=1}^{m} \alpha_i k(x, x_i)$$

and thus we had to update $\alpha_1, \ldots, \alpha_m$ only, and not $\mathbf{w} \in \mathcal{K}!$

The **Representer theorem** provides us a big class of problems, where the solution can be represented by

$$f(\cdot) = \sum_{i=1}^{m} \alpha_i k(x_i, \cdot), \quad \alpha \in \mathbb{R}^m$$

The Representer Theorem

Theorem: $k(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, Mercer kernel on \mathcal{X}

 $oldsymbol{z} = (x_1, y_1), \ldots, (x_m, y_m) \in (\mathcal{X} imes \mathcal{Y})^m$ training sample

 $g_{emp}: (\mathcal{X} \times \mathcal{Y} \times \mathbb{R})^m \to \mathbb{R} \cup \{\infty\} \} \Rightarrow$

 $g_{reg}: \mathbb{R} \to [0,\infty)$ strictly increasing function

 \mathcal{F} : RKHS induced by $k(\cdot, \cdot)$

$$\Rightarrow f^* = \arg\min_{f \in \mathcal{F}} R_{reg}[f, z]$$

$$\doteq \arg\min_{f \in \mathcal{F}} \underbrace{g_{emp}[(x_i, y_i, f(x_i))_{i \in \{1...m\}}]}_{\checkmark} + \underbrace{g_{reg}(\|f\|)}_{\checkmark}$$

1st term, empirical loss 2nd term, regularization

admits the following representation:

$$f^*(\cdot) = \sum_{i=1}^m \alpha_i k(x_i, \cdot), \quad \alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{R}^m$$

The Representer Theorem

Message:

Optimizing in general function classes is difficult, but in RKHS it is only finite! (m) dimensional problem

Proof of Representer Theorem:

$$\phi(x) \doteq k(x, \cdot) = \phi(x)(\cdot)$$

 x_1, \ldots, x_m training samples are given

$$\begin{split} f \in \mathcal{F} \Rightarrow f(\cdot) &= \sum_{i=1}^{m} \alpha_{i} \phi(x_{i})(\cdot) + v(\cdot) \\ \text{where } \mathcal{F} \ni v \perp span\{\phi(x_{1}), \dots, \phi(x_{m})\}, \\ \text{thus } \langle v, \phi(x_{i}) \rangle_{\mathcal{F}} &= 0 \quad \forall i = 1, \dots, m \end{split}$$

Proof of the Representer Theorem

Proof of Representer Theorem

 $f^* = \arg\min_{f \in \mathcal{F}} R_{reg}[f, z] \doteq \arg\min_{f \in \mathcal{F}} g_{emp}[(x_i, y_i, f(x_i))_{i \in \{1...m\}}] + g_{reg}(||f||)$ $1^{st} \text{ term, empirical loss} \qquad 2^{nd} \text{ term, regularization}$ $\Rightarrow f(x_j) = \langle f, \underbrace{k(x_j, \cdot)}_{\phi(x_j)} \rangle_{\mathcal{F}} = \langle \sum_{i=1}^m \alpha_i \phi(x_i) + v, \phi(x_j) \rangle_{\mathcal{F}}$ $= \sum_{i=1}^m \alpha_i \langle \phi(x_i), \phi(x_j) \rangle_{\mathcal{F}} = \sum_{i=1}^m \alpha_i k(x_i, x_j)$

 $\Rightarrow f(x_j)$ depends only on $\alpha_1, \ldots, \alpha_m$, but independent from v! $\Rightarrow 1^{st}$ term depends only on $\alpha_1, \ldots, \alpha_m$, but not on v

Proof of the Representer Theorem $f^* = \arg\min_{f \in \mathcal{F}} R_{reg}[f, \mathbf{z}] \doteq \arg\min_{f \in \mathcal{F}} g_{emp}[(x_i, y_i, f(x_i))_{i \in \{1...m\}}] + g_{reg}(||f||)$ 1st term, empirical loss 2nd term, regularization Let us examine the 2^{nd} term. $g_{reg}(||f||) = g_{reg}(||\sum_{i=1}^{m} \alpha_i \phi(x_i) + v||)$ $= g_{reg}(\sqrt{\left\|\sum_{i=1}^{m} \alpha_i \phi(x_i)\right\|_{\mathcal{F}}^2 + \|v\|_{\mathcal{F}}^2}$ since $\mathcal{F} \ni v \perp span\{\phi(x_1), \ldots, \phi(x_m)\}$ $\geq g_{reg}(\|\sum_{i=1}^{m} \alpha_i \phi(x_i)\|_{\mathcal{F}})$ with equality only if v = 0!

$$\Rightarrow \text{ any minimizer } f^* \text{ must have } v = 0$$

$$\Rightarrow f^*(\cdot) = \sum_{i=1}^m \alpha_i k(x_i, \cdot)$$