Kernels Methods in Machine Learning

Kernelized Perceptron

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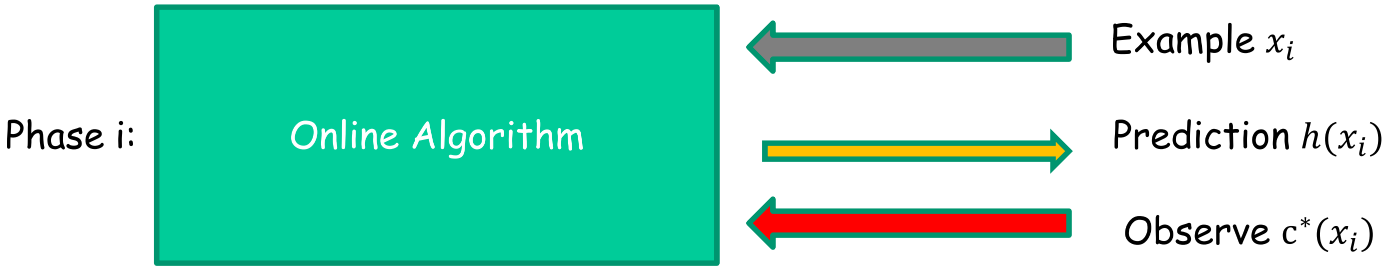
Quick Recap about Perceptron and Margins

The Online Learning Model

- Example arrive sequentially.
- We need to make a prediction.

  Afterwards observe the outcome.

For i=1, 2, ..., :



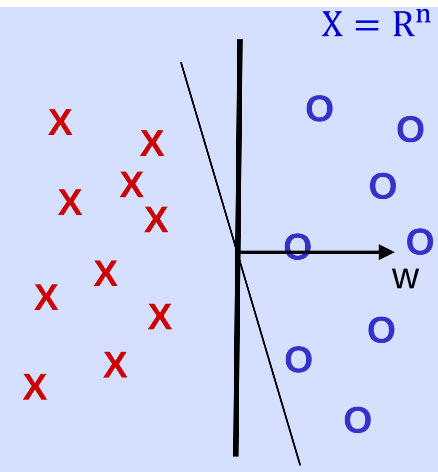
Mistake bound model

- Analysis wise, make no distributional assumptions.
- **Goal**: Minimize the number of mistakes.

Perceptron Algorithm in Online Model

WLOG homogeneous linear separators

- Set t=1, start with the all zero vector w_1.
- Given example x, predict + iff $w_t \cdot x \geq 0$
- On a mistake, update as follows:
  - Mistake on positive, $w_{t+1} \leftarrow w_t + x$
  - Mistake on negative, $w_{t+1} \leftarrow w_t - x$



Note 1: $\mathrm{w_t}$ is weighted sum of incorrectly classified examples

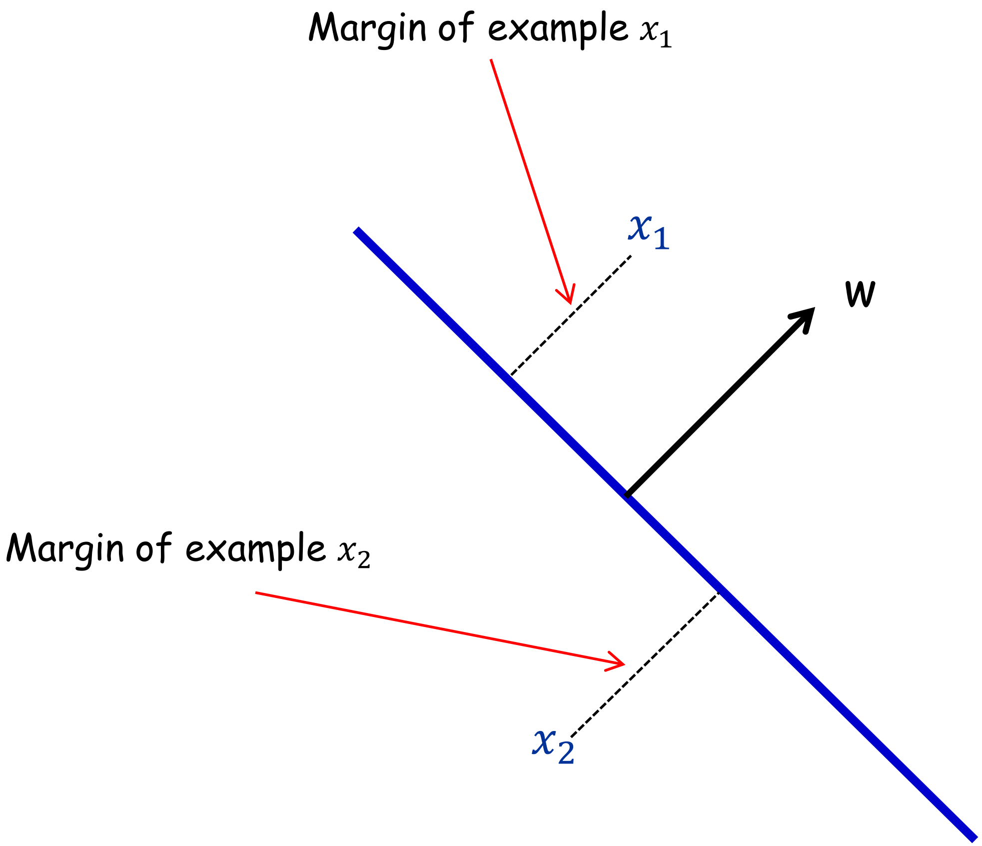
$w_t = a_{i_1} x_{i_1} + \cdots + a_{i_k} x_{i_k}$ So, $w_t \cdot x = a_{i_1} x_{i_1} \cdot x + \cdots + a_{i_k} x_{i_k} \cdot x$

Note 2: Number of mistakes ever made depends only on the geometric margin (amount of wiggle room) of examples seen.

- No matter how long the sequence is or how high dimension n is!

Geometric Margin

Definition: The margin of example x w.r.t. a linear sep. w is the distance from x to the plane $w \cdot x = 0$.



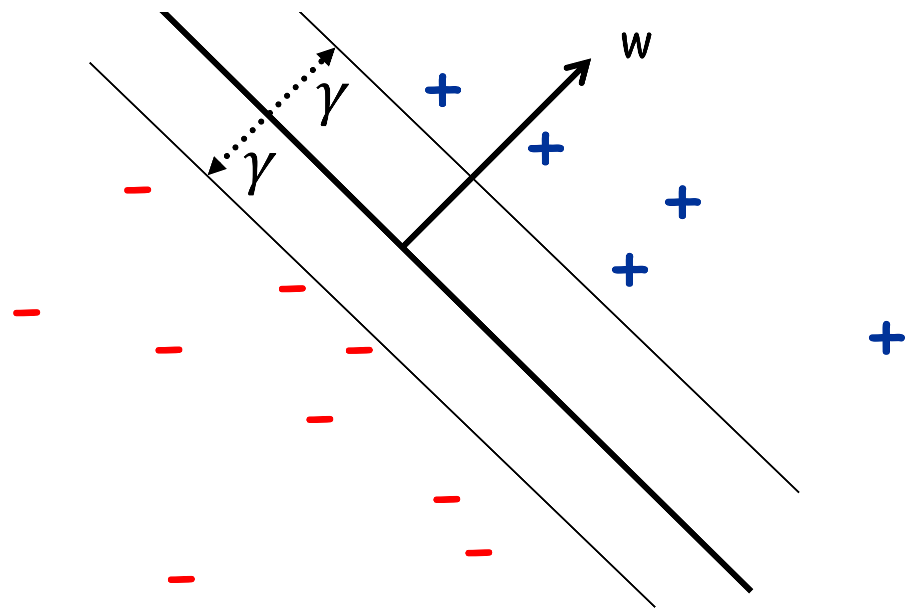
If $||w|| = 1$, margin of x w.r.t. w is $|x \cdot w|$.

Geometric Margin

Definition: The margin of example x w.r.t. a linear sep. w is the distance from x to the plane $w \cdot x = 0$.

Definition: The margin γ_w of a set of examples S wrt a linear separator w is the smallest margin over points $x \in S$.

Definition: The margin γ of a set of examples S is the maximum γ_w over all linear separators w.

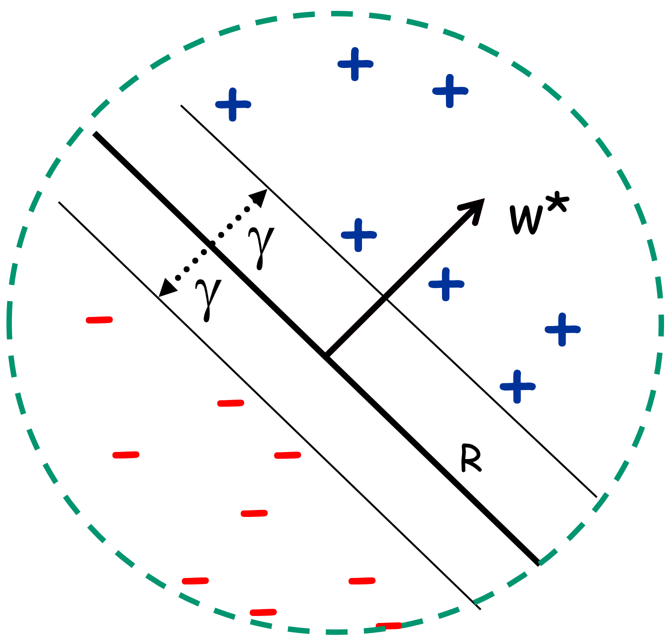


Poll time

Perceptron: Mistake Bound

Theorem: If data linearly separable by margin γ and points inside a ball of radius R, then Perceptron makes $\leq (R/\gamma)^2$ mistakes.

- No matter how long the sequence is how high dimension n is!



Margin: the amount of wiggle-room available for a solution.

(Normalized margin: multiplying all points by 100, or dividing all points by 100, doesn't change the number of mistakes; algo is invariant to scaling.)

So far, talked about margins in the context of (nearly) linearly separable datasets

What if Not Linearly Separable

Problem: data not linearly separable in the most natural feature representation.

Example:  vs 

No good linear separator in pixel representation.

Solutions:

- "Learn a more complex class of functions"
    - (e.g., decision trees, neural networks, boosting).
- "Use a Kernel" (a neat solution that attracted a lot of attention)
- "Use a Deep Network"
- "Combine Kernels and Deep Networks"

Overview of Kernel Methods

What is a Kernel?

A kernel K is a legal def of dot-product: i.e. there exists an implicit mapping Φ s.t. K( , ) = Φ()$\cdot$ Φ()

E.g., $K(x,y) = (x \cdot y + 1)^d$

ϕ: (n-dimensional space) $\rightarrow$ n^d-dimensional space

Why Kernels matter?

- Many algorithms interact with data only via dot-products.
- So, if replace $x \cdot z$ with $K(x,z)$ they act implicitly as if data was in the higher-dimensional Φ-space.
- If data is linearly separable by large margin in the Φ-space, then good sample complexity.

Kernels

Definition

$K(\cdot,\cdot)$ is a kernel if it can be viewed as a legal definition of inner product:

- $\exists\ \phi: X \to R^N$ s.t. $K(x,z) = \phi(x) \cdot \phi(z)$
  - Range of ϕ is called the Φ-space.
  - N can be very large.

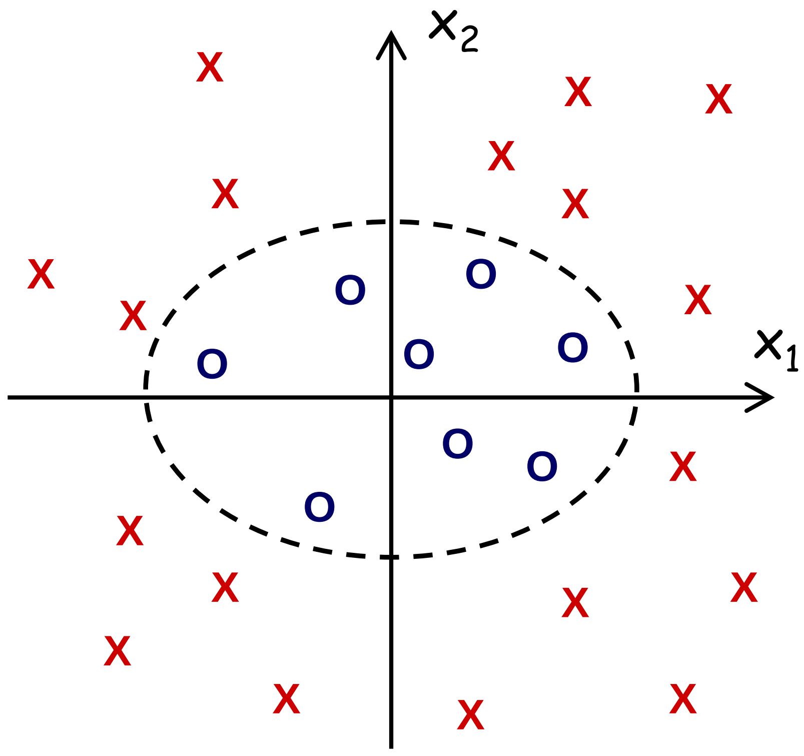
- But think of ϕ as implicit, not explicit!!!!

Example

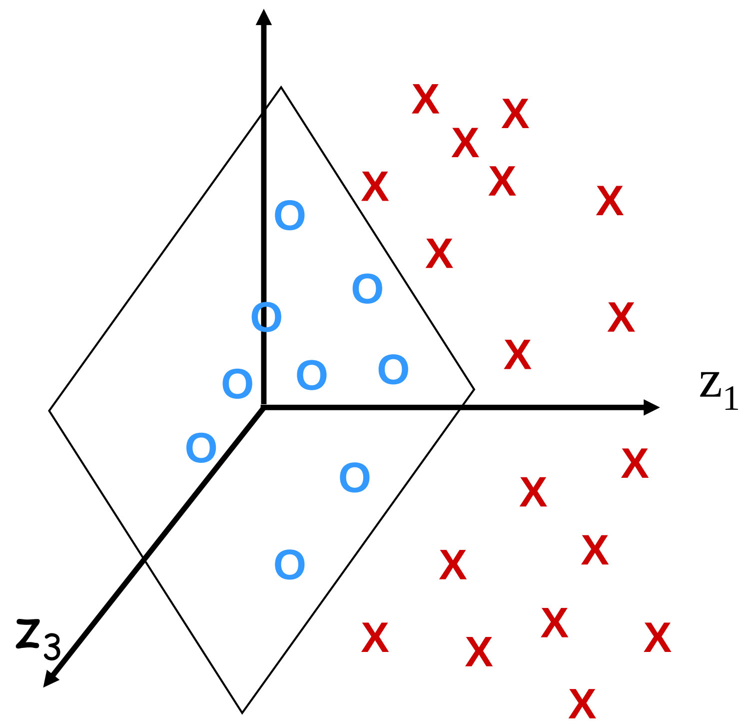
For n=2, d=2, the kernel $K(x, z) = (x \cdot z)^d$ corresponds to

$$(x_1, x_2) \rightarrow \Phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1 x_2)$$

Original space



Φ-space

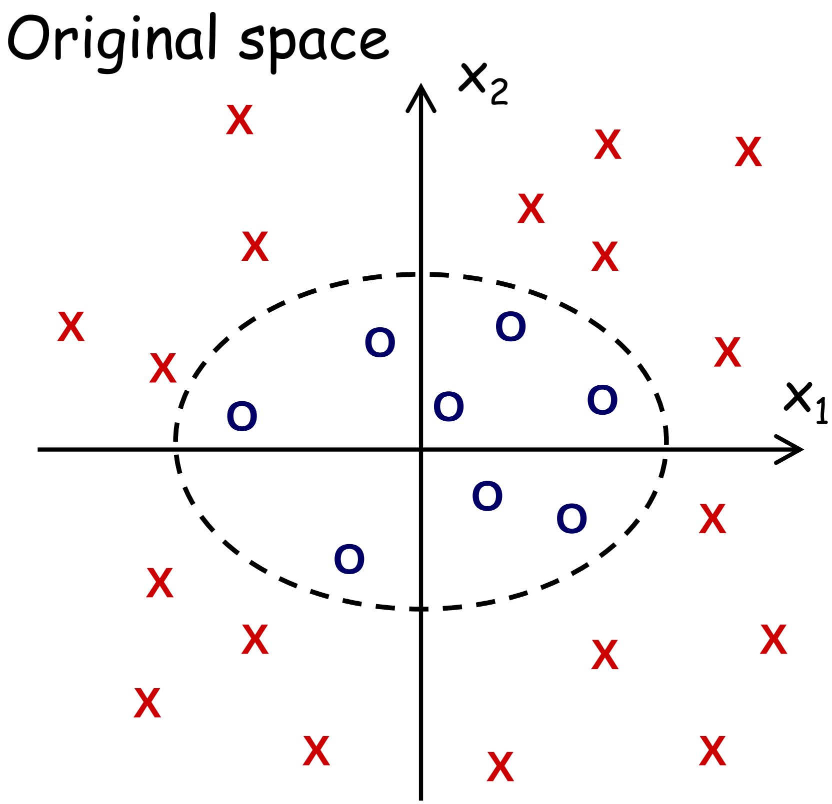


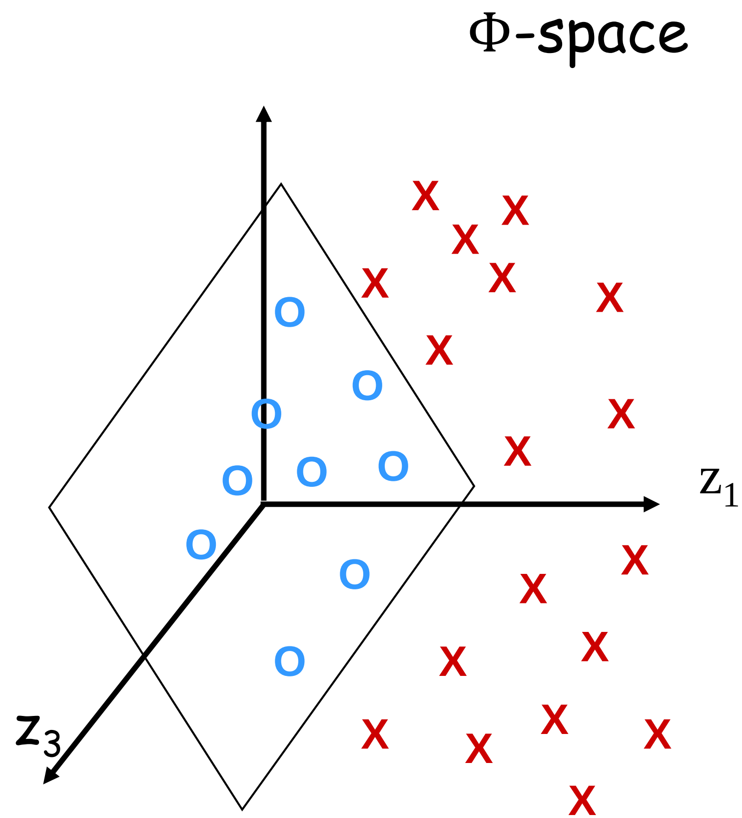
Example

$\phi: R^2 \rightarrow R^3$, $(x_1, x_2) \rightarrow \Phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$

$$\phi(x) \cdot \phi(z) = \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right) \cdot (z_1^2, z_2^2, \sqrt{2}z_1z_2)$$

$$= (x_1z_1 + x_2z_2)^2 = (x \cdot z)^2 = K(x, z)$$





Kernels

Definition

$K(\cdot,\cdot)$ is a kernel if it can be viewed as a legal definition of inner product:

- $\exists\ \phi: X \to R^N$ s.t. $K(x,z) = \phi(x) \cdot \phi(z)$
  - Range of ϕ is called the Φ-space.
  - N can be very large.

- But think of ϕ as implicit, not explicit!!!!

Example

Note: feature space might not be unique.

$\phi: R^2 \rightarrow R^3, (x_1, x_2) \rightarrow \Phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$

$\phi(x) \cdot \phi(z) = \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right) \cdot (z_1^2, z_2^2, \sqrt{2}z_1z_2)$

$= (x_1z_1 + x_2z_2)^2 = (x \cdot z)^2 = K(x, z)$

$\phi: R^2 \rightarrow R^4, (x_1, x_2) \rightarrow \Phi(x) = (x_1^2, x_2^2, x_1x_2, x_2x_1)$

$\phi(x) \cdot \phi(z) = (x_1^2, x_2^2, x_1x_2, x_2x_1) \cdot (z_1^2, z_2^2, z_1z_2, z_2z_1)$

$= (x \cdot z)^2 = K(x, z)$

Avoid explicitly expanding the features

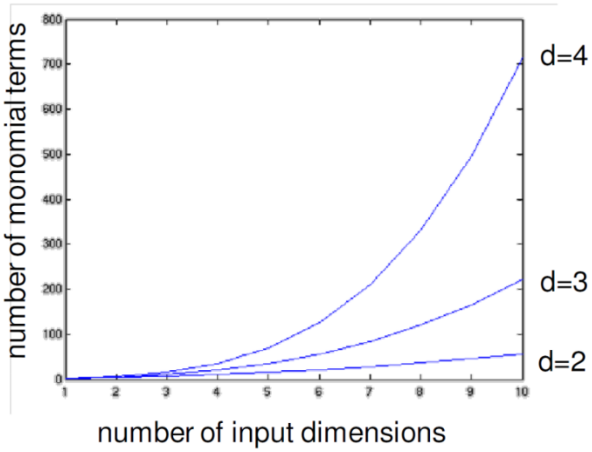
Feature space can grow really large and really quickly….

Crucial to think of ϕ as implicit, not explicit!!!!

- Polynomial kernel degreee d, $k(x,z) = (x^\top z)^d = \phi(x) \cdot \phi(z)$
  - $x_1^d, x_1 x_2 \dots x_d, x_1^2 x_2 \dots x_{d-1}$
  - Total number of such feature is

$$\binom{d+n-1}{d} = \frac{(d+n-1)!}{d!\,(n-1)!}$$

  - $d = 6, n = 100$, there are 1.6 billion terms



$O(n)$ $computation!$

$$k(x,z) = (x^\top z)^d = \phi(x) \cdot \phi(z)$$

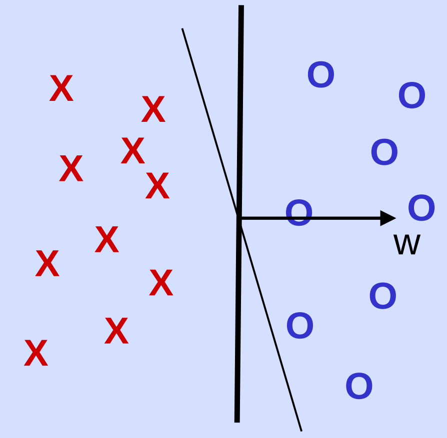
Kernelizing a learning algorithm

- **If all computations involving instances are in terms of inner products then**:
  - Conceptually, work in a very high diml space and the alg's performance depends only on linear separability in that extended space.
  - Computationally, only need to modify the algo by replacing each $x \cdot z$ with a $K(x, z)$.

- **Examples of kernalizable algos:**
  - classification: Perceptron, SVM.
  - regression: linear, ridge regression.
  - clustering: k-means.

Kernelizing the Perceptron Algorithm

- Set t=1, start with the all zero vector w_1.
- Given example x, predict + iff $w_t \cdot x \geq 0$
- On a mistake, update as follows:
  - Mistake on positive, $w_{t+1} \leftarrow w_t + x$
  - Mistake on negative, $w_{t+1} \leftarrow w_t - x$



Easy to kernelize since w_t is weighted sum of incorrectly classified examples $w_t = a_{i_1} x_{i_1} + \cdots + a_{i_k} x_{i_k}$

Replace $w_t \cdot x = a_{i_1} x_{i_1} \cdot x + \cdots + a_{i_k} x_{i_k} \cdot x$ with

$a_{i_1} K(x_{i_1}, x) + \cdots + a_{i_k} K(x_{i_k}, x)$

Note: need to store all the mistakes so far.

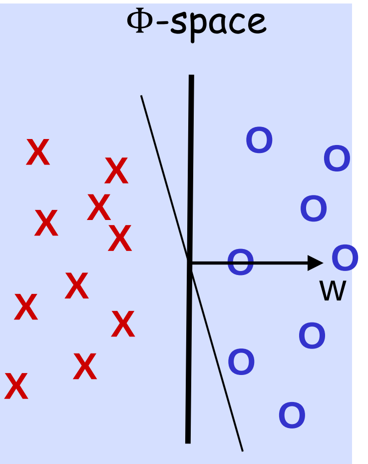
Kernelizing the Perceptron Algorithm

- Given x, predict + iff

$$\phi(x_{i_{t-1}}) \cdot \phi(x)$$

$$a_{i_1} K(x_{i_1}, x) + \cdots + a_{i_{t-1}} K(x_{i_{t-1}}, x) \geq 0$$

- On the t th mistake, update as follows:
  - Mistake on positive, set $a_{i_t} \leftarrow 1$; store x_{i_t}
  - Mistake on negative, $a_{i_t} \leftarrow -1$; store x_{i_t}



Perceptron $w_t = a_{i_1} x_{i_1} + \cdots + a_{i_k} x_{i_k}$

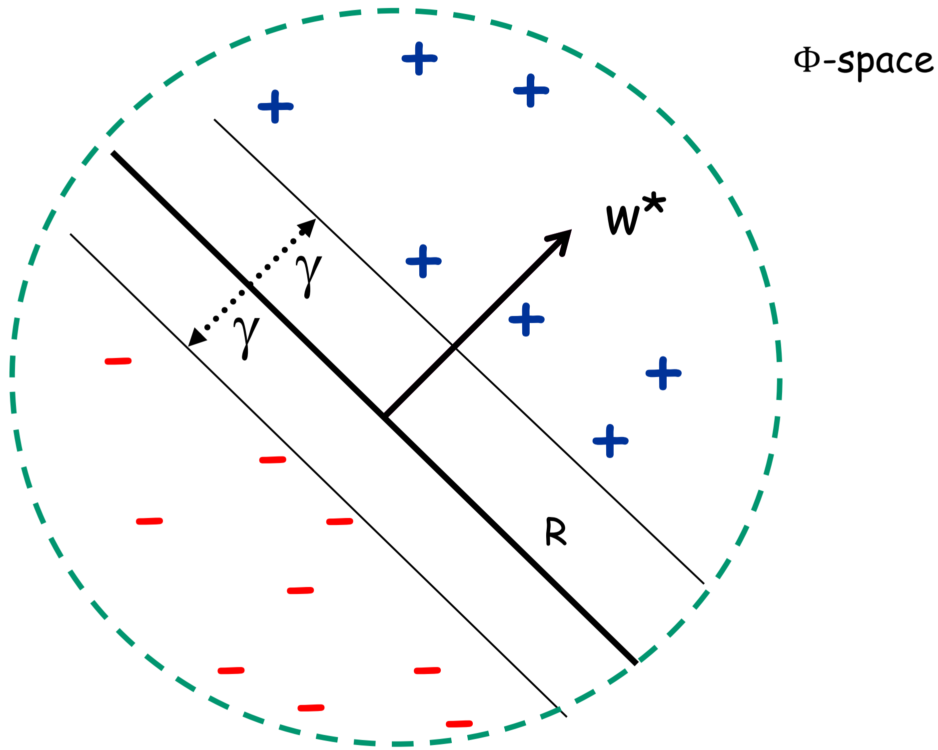
$$w_t \cdot x = a_{i_1} x_{i_1} \cdot x + \cdots + a_{i_k} x_{i_k} \cdot x \quad \rightarrow \quad a_{i_1} K(x_{i_1}, x) + \cdots + a_{i_k} K(x_{i_k}, x)$$

Exact same behavior/prediction rule as if mapped data in the ϕ-space and ran Perceptron there!

Do this implicitly, so computational savings!!!!!

Generalize Well if Good Margin

- If data is linearly separable by margin in the ϕ-space, then small mistake bound.
- If margin γ in ϕ-space, then Perceptron makes $\left(\frac{R}{\gamma}\right)^2$ mistakes.



Kernels: More Examples

- Linear: $\mathrm{K}(\mathrm{x}, \mathrm{z}) = \mathrm{x} \cdot z$

- Polynomial: $\mathrm{K}(\mathrm{x}, z) = (\mathrm{x} \cdot z)^{\mathrm{d}}$ or $\mathrm{K}(\mathrm{x}, z) = (1 + \mathrm{x} \cdot z)^{\mathrm{d}}$

- Gaussian: $\mathrm{K}(\mathrm{x}, z) = \exp\left[-\frac{||x-z||^2}{2\,\sigma^2}\right]$

- Laplace Kernel: $\mathrm{K}(\mathrm{x}, z) = \exp\left[-\frac{||x-z||}{2\,\sigma^2}\right]$

- Kernel for non-vectorial data, e.g., measuring similarity between sequences.

Properties of Kernels

Theorem (Mercer)

K is a kernel if and only if:

- K is symmetric
- For any set of training points $x_1, x_2, \ldots, x_m$ and for any $a_1, a_2, \ldots, a_m \in R$, we have:

$$\sum_{i,j} a_i a_j K(x_i, x_j) \geq 0$$

$$a^T K a \geq 0$$

I.e., $K = (K(x_i, x_j))_{i,j=1,\ldots,n}$ is positive semi-definite.

Kernel Methods

- Offer great modularity.

- No need to change the underlying learning algorithm to accommodate a particular choice of kernel function.
- Also, we can substitute a different algorithm while maintaining the same kernel.

Kernel, Closure Properties

Easily create new kernels using basic ones!

Fact: If $K_1(\cdot,\cdot)$ and $K_2(\cdot,\cdot)$ are kernels $c_1 \geq 0, c_2 \geq 0$,

then $K(x, z) = c_1 K_1(x, z) + c_2 K_2(x, z)$ is a kernel.

Key idea: concatenate the ϕ spaces.

$$\phi(x) = (\sqrt{c_1}\, \phi_1(x), \sqrt{c_2}\, \phi_2(x))$$

$$\phi(x) \cdot \phi(z) = c_1\, \underbrace{\phi_1(x) \cdot \phi_1(z)}_{K_1(x,z)} + c_2\, \underbrace{\phi_2(x) \cdot \phi_2(z)}_{K_2(x,z)}$$

Kernel, Closure Properties

Easily create new kernels using basic ones!

Fact: If $K_1(\cdot,\cdot)$ and $K_2(\cdot,\cdot)$ are kernels,

then $K(x,z) = K_1(x,z)K_2(x,z)$ is a kernel.

Key idea: $\phi(x) = \left(\phi_{1,i}(x)\ \phi_{2,j}(x)\right)_{i\in\{1,\dots,n\},\, j\in\{1,\dots,m\}}$

$$\phi(x)\cdot\phi(z) = \sum_{i,j} \phi_{1,i}(x)\ \phi_{2,j}(x)\phi_{1,i}(z)\ \phi_{2,j}(z)$$

$$= \sum_{i} \phi_{1,i}(x)\ \phi_{1,i}(z)\left(\sum_{j} \phi_{2,j}(x)\ \phi_{2,j}(z)\right)$$

$$= \sum_i \phi_{1,i}(x)\ \phi_{1,i}(z)K_2(x,z) = K_1(x,z)\ K_2(x,z)$$

Kernels, Discussion

- If all computations involving instances are in terms of inner products then:
  - Conceptually, work in a very high diml space and the alg's performance depends only on linear separability in that extended space.
  - Computationally, only need to modify the algo by replacing each $x \cdot z$ with a $K(x, z)$.

- Lots of Machine Learning algorithms are kernalizable:
  - classification: Perceptron, SVM.
  - regression: linear regression.
  - clustering: k-means.

Kernels, Discussion

- If all computations involving instances are in terms of inner products then:
  - Conceptually, work in a very high diml space and the alg's performance depends only on linear separability in that extended space.
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How to choose a kernel:

- Kernels often encode domain knowledge (e.g., string kernels)
- Use Cross-Validation to choose the parameters, e.g., σ for Gaussian Kernel $K(x, z) = \exp\left[-\frac{||x-z||^2}{2\,\sigma^2}\right]$
- Learn a good kernel; e.g., [Lanckriet-Cristianini-Bartlett-El Ghaoui-Jordan'04]