COMS 4771
Perceptron and Kernelization

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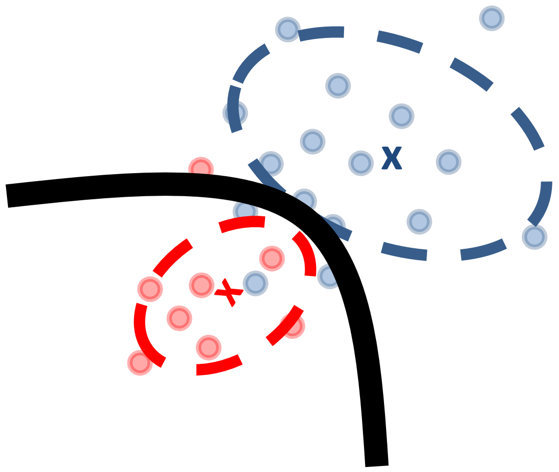
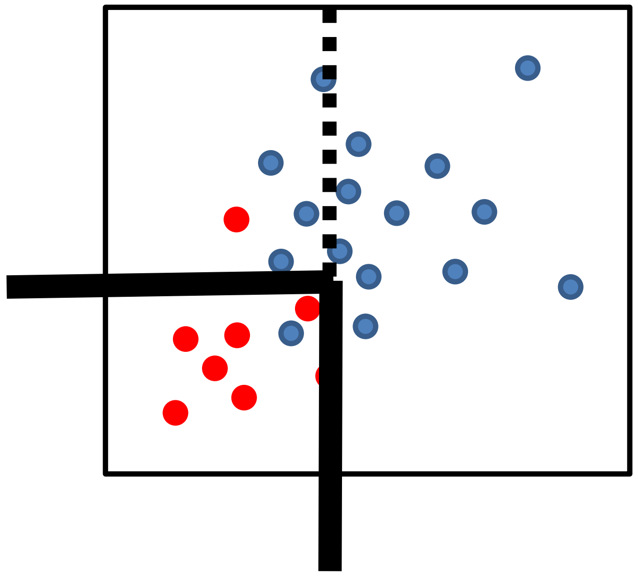
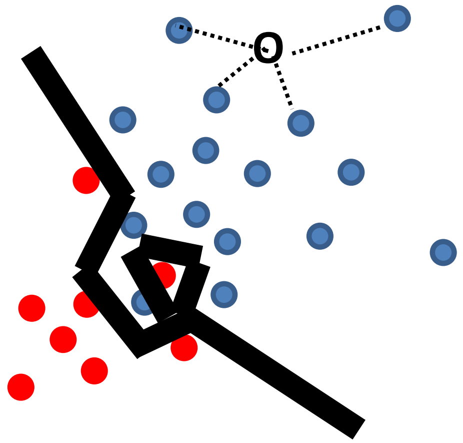
Last time...

- Generative vs. Discriminative Classifiers
- Nearest Neighbor (NN) classification
- Optimality of *k*-NN
- Coping with drawbacks of *k*-NN
- Decision Trees
- The notion of overfitting in machine learning

A Closer Look Classification

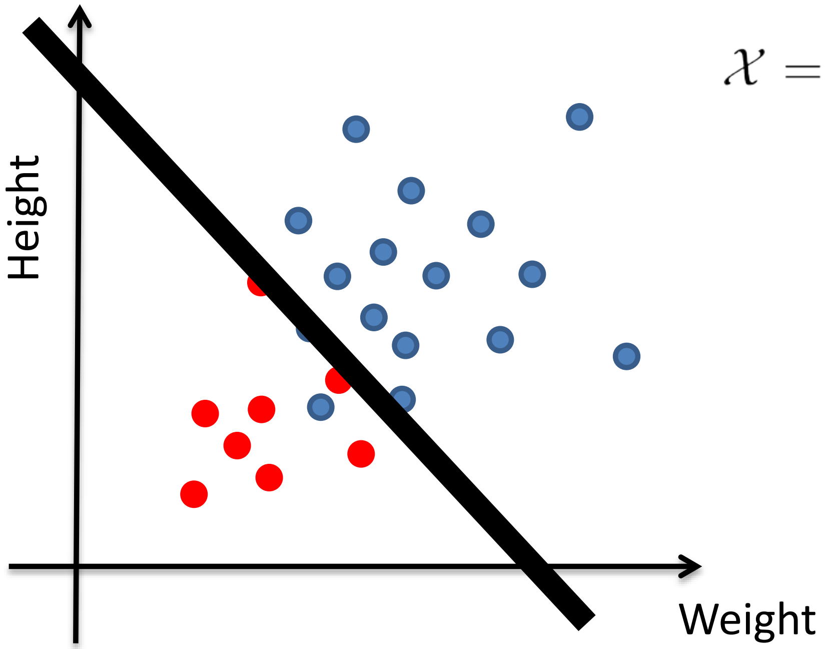






Knowing the boundary is enough for classification

Linear Decision Boundary



$$\mathcal{X} = \mathbf{R}^2 = \text{Weight} \times \text{Height}$$

🟦	male data
🟥	female data

Assume binary classification y= {-1,+1}

(What happens in multi-class case?)

Learning Linear Decision Boundaries

g = decision boundary

d=1 case: $g(x) = w_1 x + w_0$

general: $g(\vec{x}) = \vec{w} \cdot \vec{x} + w_0$

f = linear classifier

$$f(\vec{x}) := \begin{cases} +1 & \text{if } g(\vec{x}) \geq 0 \\ -1 & \text{if } g(\vec{x}) < 0 \end{cases}$$

$$= \text{sign}(\vec{w} \cdot \vec{x} + w_0)$$

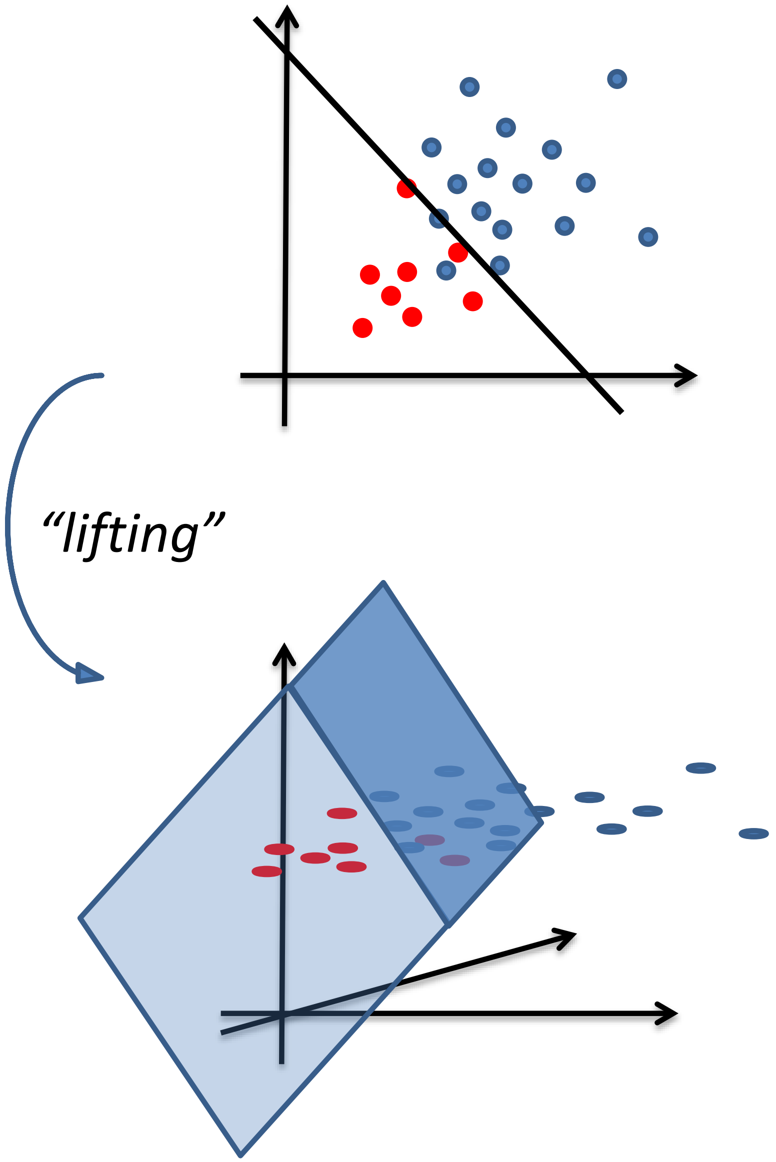
# of parameters to learn in $\mathbf{R}^d$*?*

Dealing with w_0

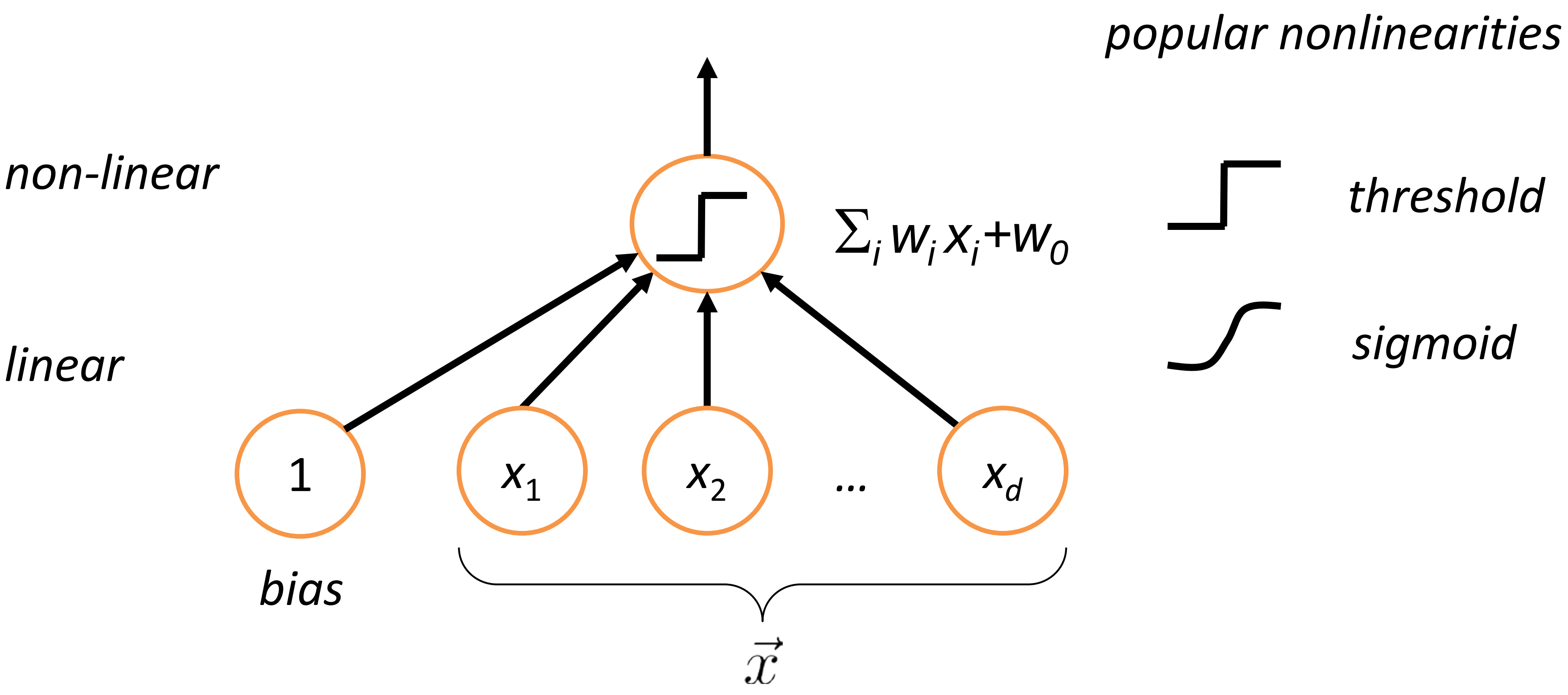
$$g(\vec{x}) = \vec{w} \cdot \vec{x} + w_0$$

$$= \underbrace{\begin{bmatrix} \vec{w} \\ w_0 \end{bmatrix}}_{\vec{w}'} \cdot \underbrace{\begin{bmatrix} \vec{x} \\ 1 \end{bmatrix}}_{\vec{x}'}$$ *bias*

$$g(\vec{x}') = \vec{w}' \cdot \vec{x}'$$ *homogeneous*

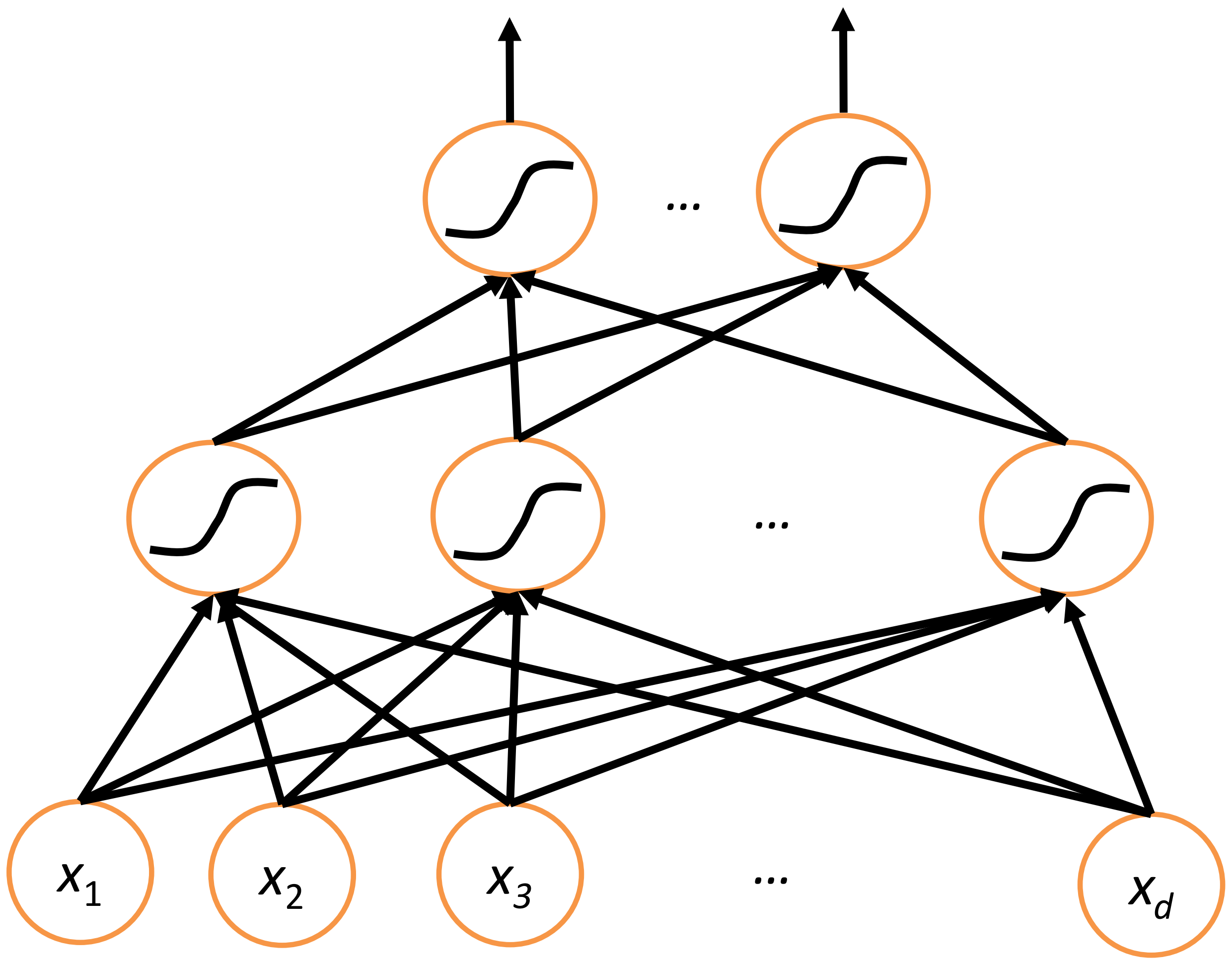


The Linear Classifier



A basic computational unit in a neuron

Can Be Combined to Make a Network



Amazing fact:

Can approximate any smooth function!

An artificial neural network

How to Learn the Weights?

Given labeled training data (bias included): $(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots (\vec{x}_n, y_n)$

Want: $\vec{w}$, which **minimizes** the training error, i.e.

$$\arg\min_{\vec{w}} \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\left[\operatorname{sign}(\vec{w} \cdot \vec{x}_i) \neq y_i\right]$$

$$= \arg\min_{\vec{w}} \sum_{\substack{x_i \\ \text{s.t.} y_i = +1}} \mathbf{1}[\vec{x}_i \cdot \vec{w} < 0] + \sum_{\substack{x_i \\ \text{s.t.} y_i = -1}} \mathbf{1}[\vec{x}_i \cdot \vec{w} \geq 0]$$

*How do we **minimize**?*

- Cannot use the standard technique (take derivate and examine the stationary points). Why?

Unfortunately: *NP-hard to solve or even approximate!*

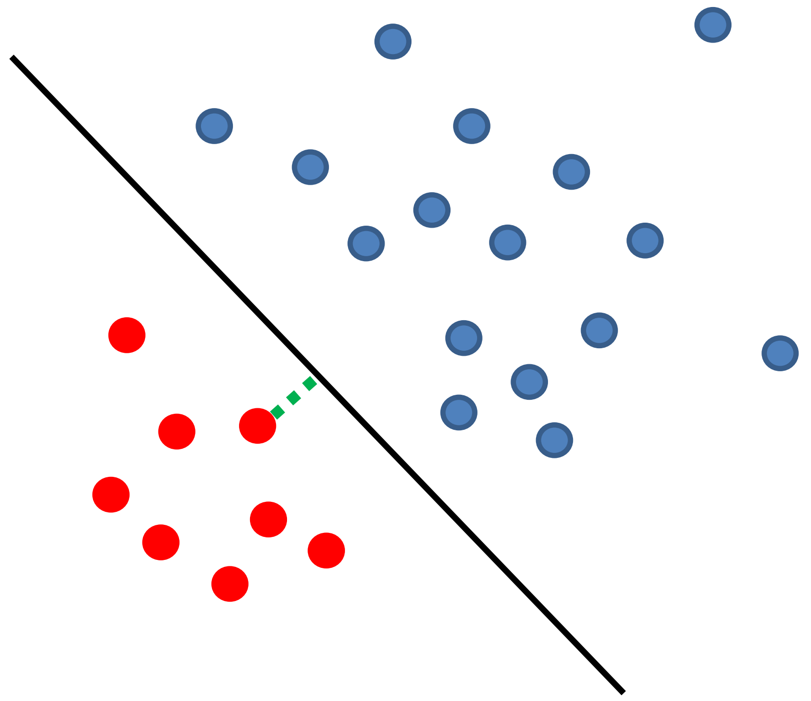
Finding Weights (Relaxed Assumptions)

Can we approximate the weights if we make reasonable assumptions?

What if the training data is linearly separable?

Linear Separability

Say there is a **linear** decision boundary which can **perfectly separate** the training data



distance of the closest point to the boundary (margin γ)

Finding Weights

Given: labeled training data S = $(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots (\vec{x}_n, y_n)$

Want to determine: is there a $\vec{w}$ which satisfies $y_i(\vec{w} \cdot \vec{x}_i) \geq 0$ (for all *i*)

i.e., is the training data linearly separable?

Since there are d+1 variables and |S| constraints, it is possible to solve efficiently it via a (constraint) optimization program. (How?)

*Can find it in a much **simpler** way!*

The Perceptron Algorithm

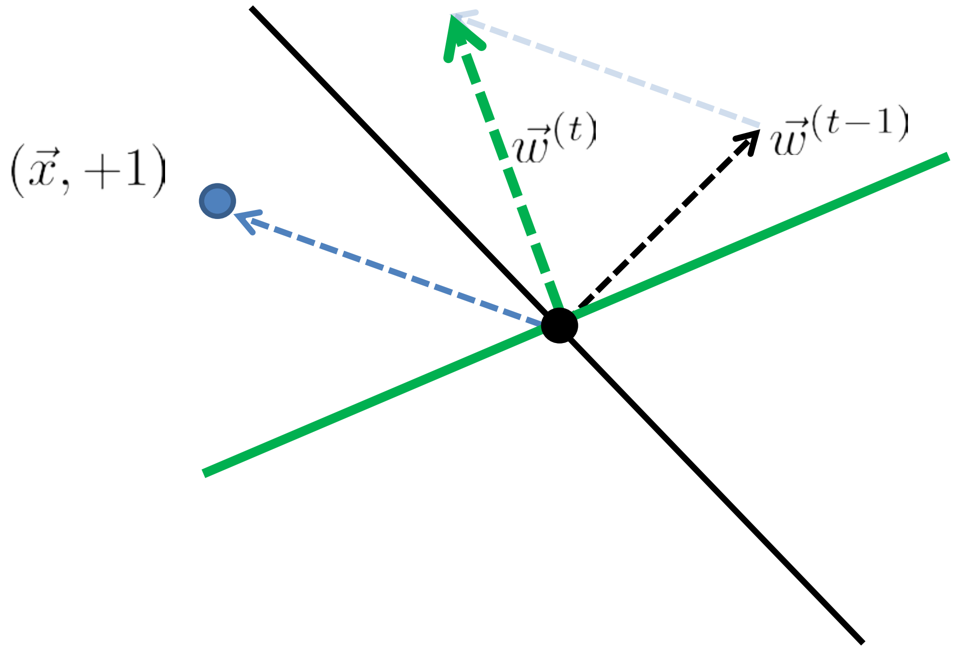
Given: labelled training data S = $(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots (\vec{x}_n, y_n)$

```
Initialize $\vec{w}^{(0)}$ = 0
For t = 1,2,3,…
    If exists $(\vec{x}, y) \in S$ s.t. $\text{sign}(\vec{w}^{(t-1)} \cdot \vec{x}) \neq y$
```

$$\vec{w}^{(t)} \leftarrow \begin{cases} \vec{w}^{(t-1)} + \vec{x} & \text{if } y = +1 \\ \vec{w}^{(t-1)} - \vec{x} & \text{if } y = -1 \end{cases} \qquad = \vec{w}^{(t-1)} + y\vec{x}$$

(terminate when no such training sample exists)

Perceptron Algorithm: Geometry

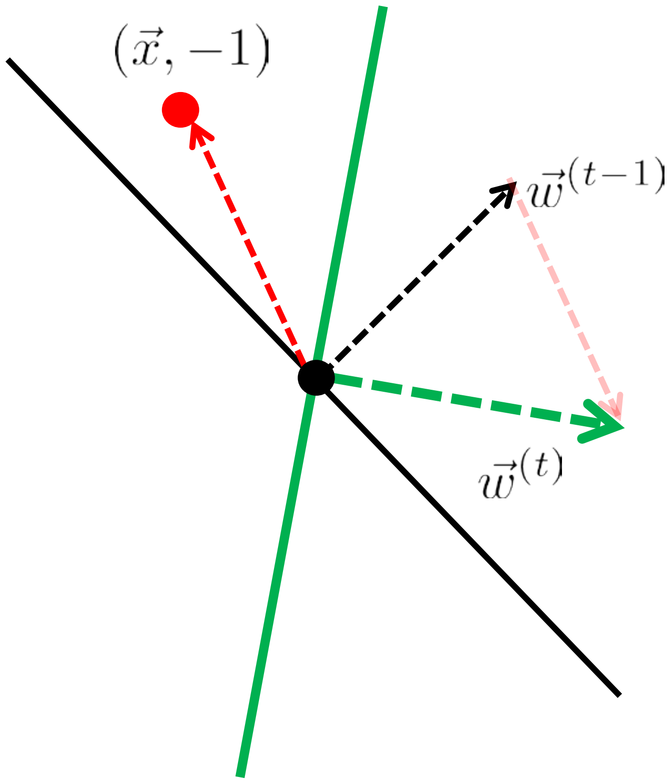


$$\text{sign}(\vec{w}^{(t-1)} \cdot \vec{x}) \neq +1$$

$$\vec{w}^{(t)} \leftarrow \vec{w}^{(t-1)} + \vec{x}$$

$$\text{sign}(\vec{w}^{t} \cdot \vec{x}) = +1$$

Perceptron Algorithm: Geometry



$$\text{sign}(\vec{w}^{(t-1)} \cdot \vec{x}) \neq -1$$

$$\vec{w}^{(t)} \leftarrow \vec{w}^{(t-1)} - \vec{x}$$

$$\text{sign}(\vec{w}^{t} \cdot \vec{x}) = -1$$

The Perceptron Algorithm

Input: labelled training data S = $(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots (\vec{x}_n, y_n)$

```
Initialize $\vec{w}^{(0)}$ = 0
For t = 1,2,3,…
    If exists $(\vec{x}, y) \in S$ s.t. $\mathrm{sign}(\vec{w}^{(t-1)} \cdot \vec{x}) \neq y$
```

$$\vec{w}^{(t)} \leftarrow \begin{cases} \vec{w}^{(t-1)} + \vec{x} & \text{if } y = +1 \\ \vec{w}^{(t-1)} - \vec{x} & \text{if } y = -1 \end{cases} \qquad = \vec{w}^{(t-1)} + y\vec{x}$$

(terminate when no such training sample exists)

Question: *Does the perceptron algorithm terminates? If so, when?*

Perceptron Algorithm: Guarantee

Theorem (Perceptron mistake bound):

Assume there is a (unit length) $\vec{w}^*$ that can separate the training sample S with margin γ

Let R = $\max_{\vec{x} \in S} ||\vec{x}||$

Then, the perceptron algorithm will make at most $T := \left(\frac{R}{\gamma}\right)^2$ mistakes.

Thus, the algorithm will terminate in T rounds!

umm… but what about the generalization or the test error?

Proof

Key quantity to analyze:

How far is $\vec{w}^{(t)}$ from $\vec{w}^*$?

Suppose the perceptron algorithm makes a mistake in iteration *t*, then

$$\begin{aligned} \vec{w}^{(t)} \cdot \vec{w}^* &= (\vec{w}^{(t-1)} + y\vec{x}) \cdot \vec{w}^* \\ &\geq \vec{w}^{(t-1)} \cdot \vec{w}^* + \gamma \end{aligned}$$

$$\begin{aligned} \|\vec{w}^{(t)}\|^2 &= \|\vec{w}^{(t-1)} + y\vec{x}\|^2 \\ &= \|\vec{w}^{(t-1)}\|^2 + 2y(\vec{w}^{(t-1)} \cdot \vec{x}) + \|y\vec{x}\|^2 \\ &\leq \|\vec{w}^{(t-1)}\|^2 + R^2 \end{aligned}$$

Proof (contd.)

for all iterations *t*

$$\begin{aligned} \vec{w}^{(t)} \cdot \vec{w}^* &\geq \vec{w}^{(t-1)} \cdot \vec{w}^* + \gamma \\ \|\vec{w}^{(t)}\|^2 &\leq \|\vec{w}^{(t-1)}\|^2 + R^2 \end{aligned}$$

So, after T rounds

$$T\gamma \leq \vec{w}^{(T)} \cdot \vec{w}^* \leq \|\vec{w}^{(T)}\|\|\vec{w}^*\| \leq R\sqrt{T}$$

Therefore: $T \leq \left(\frac{R}{\gamma}\right)^2$

■

What Good is a Mistake Bound?

- It’s an upper bound on the number of mistakes made by an ***online algorithm*** on an **arbitrary sequence** of examples

  i.e. no i.i.d. assumption and not loading all the data at once!

- Online algorithms with small mistake bounds can be used to develop classifiers with **good generalization error**!

Other Simple Variants on the Perceptron

Voted perceptron

Average perceptron

Winnow

…

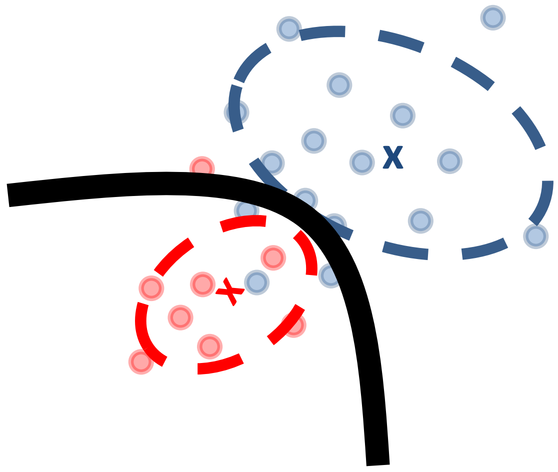
Linear Classification

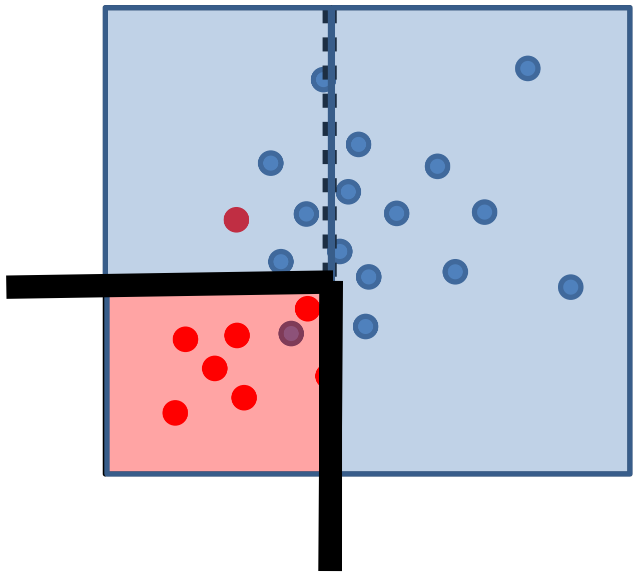
Linear classification simple,

but… *when is real-data (even approximately) linearly separable?*

What about non-linear decision boundaries?

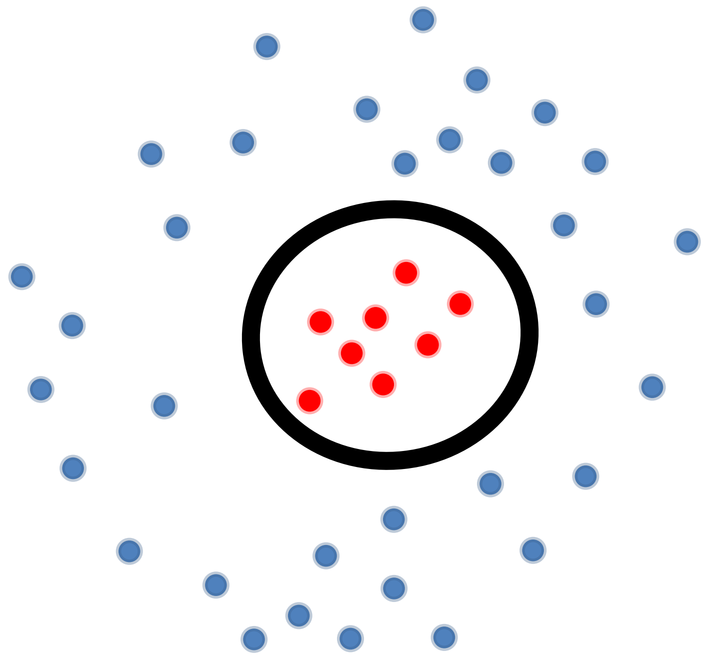
Non linear decision boundaries are common:





Generalizing Linear Classification

Suppose we have the following training data:



d=2 case:

$$g(\vec{x}) = w_1 x_1^2 + w_2 x_2^2 + w_0$$

say, the decision boundary is some sort of ellipse

e.g. circle of radius r:

$$w_1 = 1$$
$$w_2 = 1$$
$$w_0 = -r^2$$

separable via a circular decision boundary

$\boxed{\textit{not linear in } \vec{x} \textit{ !}}$

But g *is* Linear in *some* Space!

$$g(\vec{x}) = w_1 \boxed{x_1^2} + w_2 \boxed{x_2^2} + w_0$$

non linear in x_1 & x_2

$$= w_1 \boxed{\chi_1} + w_2 \boxed{\chi_2} + w_0$$

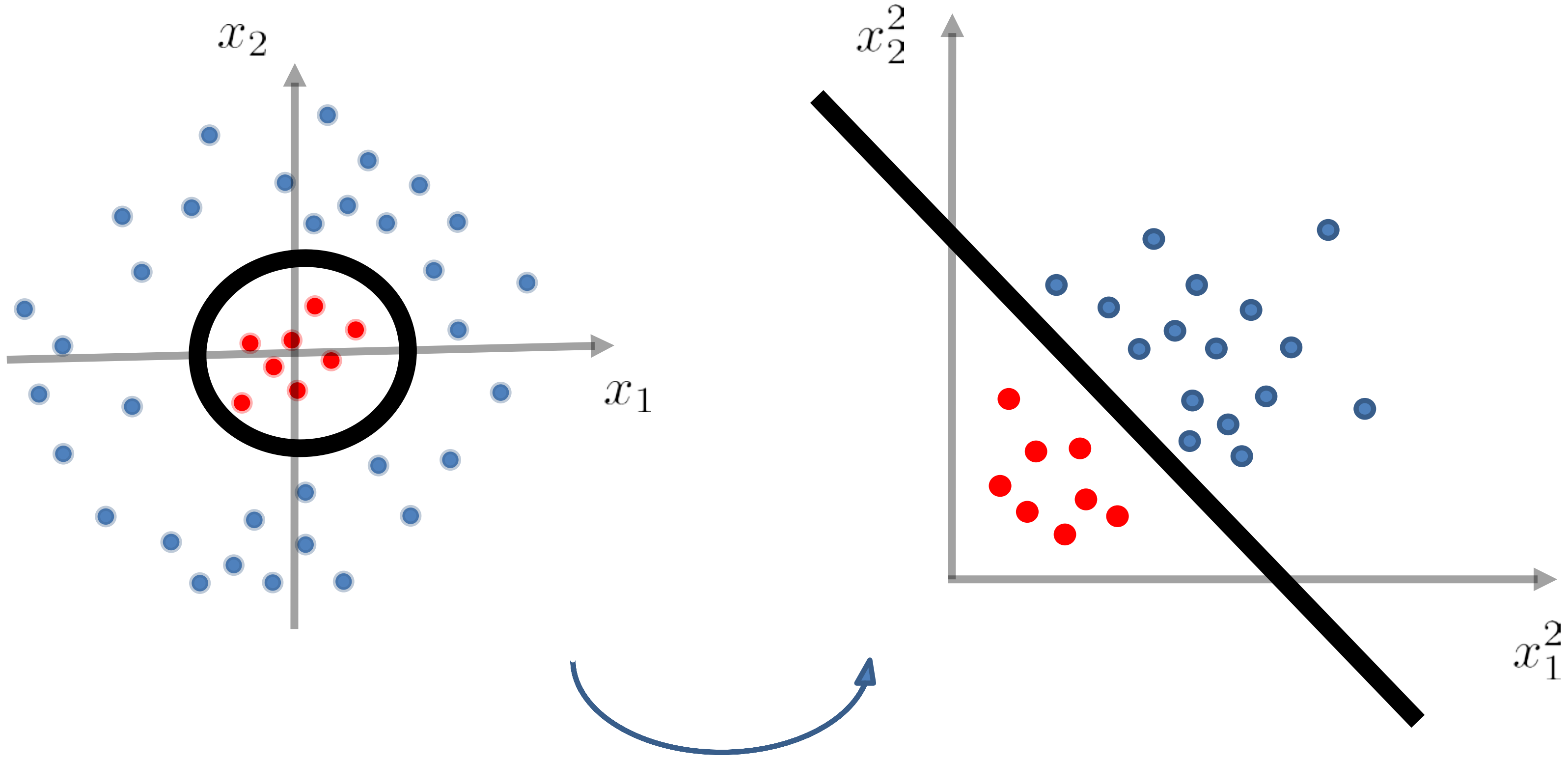
linear in χ_1 & χ_2 !

So if we apply a feature transformation on our data:

$$\phi(x_1, x_2) \mapsto (x_1^2, x_2^2)$$

Then *g* becomes linear in ϕ - transformed feature space!

Feature Transformation Geometrically



$$\phi(x_1, x_2) \mapsto (x_1^2, x_2^2)$$

Feature Transform for Quadratic Boundaries

R^2 *case: (generic quadratic boundary)*

$$g(\vec{x}) = w_1 x_1^2 + w_2 x_2^2 + w_3 x_1 x_2 + w_4 x_1 + w_5 x_2 + w_0$$
$$= \sum_{p+q\leq 2} w_{p,q}\; x_1^p x_2^q$$

feature transformation:

$$\phi(x_1, x_2) \mapsto (x_1^2, x_2^2, x_1x_2, x_1, x_2, 1)$$

R^d *case: (generic quadratic boundary)*

This captures all pairwise interactions between variables

$$g(\vec{x}) = \sum_{i,j=1}^{d} \sum_{p+q\leq 2} w_{i,j}^{p,q}\; x_i^p x_j^q$$

feature transformation:

$$\phi(x_1, x_2) \mapsto (x_1^2, x_2^2, \ldots, x_d^2, x_1x_2, \ldots, x_{d-1}x_d, x_1, x_2, 1)$$

Data is Linearly Separable in some Space!

Theorem:

Given n labeled points $(\vec{x}_1, y_1), (\vec{x}_2, y_2), \ldots (\vec{x}_n, y_n)$ $y_i = \{-1,+1\}$,

there exists a feature transform where the data points are linearly separable.

(this feature transform is sometimes called the Kernel transform)

the proof is almost trivial!

Proof

Given *n* points, consider the mapping into $\mathbf{R}^n$:

$$\phi(\vec{x}_i) \mapsto \begin{pmatrix} 0 \\ \vdots \\ 0 \\ y_i \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

(zero in all coordinates except in coordinate i)

Then, the decision boundary induced by linear weighting $\vec{w}^* = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$ perfectly separates the input data!

■

Transforming the Data into Kernel Space

Pros:

Any problem becomes **linearly separable**!

Cons:

What about computation? Generic kernel transform is typically $\Omega(n)$

*Some useful kernel transforms map the input space into **infinite dimensional space**!*

What about model complexity?

Generalization performance typically degrades with model complexity

The Kernel Trick (to Deal with Computation)

Explicitly working in generic Kernel space $\phi(\vec{x}_i)$ takes time Ω(n)

But the dot product between two data points in kernel space can be computed relatively quickly

$\phi(\vec{x}_i) \cdot \phi(\vec{x}_j)$ *can compute fast*

Example: quadratic kernel transform for data in **R**^{d}

explicit transform	*O*(d^2)	$(x_1^2, \ldots, x_d^2, x_1 x_2, \ldots, x_{d-1} x_d, x_1, x_2, 1)$
dot products	*O(d)*	$(1 + \vec{x}_i \cdot \vec{x}_j)^2$

RBF (radial basis function) kernel transform for data in **R**^{d}

explicit transform	infinite dimension!
dot products	*O(d)*

The Kernel Trick

The trick is to perform classification in such a way that it **only accesses the data** in terms of dot products (so it can be done quicker)

Example: the `kernel Perceptron’

Recall: $\vec{w}^{(t)} \leftarrow \vec{w}^{(t-1)} + y\vec{x}$

Equivalently $\vec{w} = \sum_{k=1}^{n} \alpha_k y_k \vec{x}_k$ *α_k = # of time mistake was made on x_k*

Thus, classification becomes

$$f(\vec{x}) := \text{sign}(\vec{w} \cdot \vec{x}) \quad = \text{sign}\big(\vec{x} \cdot \sum_{k=1}^{n} \alpha_k y_k \vec{x}_k\big) \quad = \text{sign}\big(\sum_{k=1}^{n} \alpha_k y_k (\vec{x}_k \cdot \vec{x})\big)$$

Only accessing data in terms of dot products!

The Kernel Trick: for Perceptron

classification in original space:

$$f(\vec{x}) = \text{sign}\Big(\sum_{k=1}^{n} \alpha_k y_k (\vec{x}_k \cdot \vec{x})\Big)$$

If we were working in the transformed Kernel space, it would have been

$$f(\phi(\vec{x})) = \text{sign}\Big(\sum_{k=1}^{n} \alpha_k y_k \big(\phi(\vec{x}_k) \cdot \phi(\vec{x})\big)\Big)$$

Algorithm:

```
Initialize $\vec{\alpha}$ = 0
For t = 1,2,3,…, T
    If exists $(\vec{x}_i, y_i) \in S$ s.t. $\text{sign}\Big(\sum_{k=1}^{n} \alpha_k y_k \big(\phi(\vec{x}_k) \cdot \phi(\vec{x}_i)\big)\Big) \neq y_i$
    $\alpha_i \leftarrow \alpha_i + 1$
```

implicitly working in non-linear kernel space!

The Kernel Trick: Significance

$$\sum_{k=1}^{n} \alpha_k y_k \left(\phi(\vec{x}_k) \cdot \phi(\vec{x})\right)$$

dot products are a measure of similarity

Can be replaced by any user-defined measure of similarity!

*So, we can work in any user-defined non-linear space **implicitly** **without** the potentially heavy computational cost*

What We Learned…

- Decision boundaries for classification
- Linear decision boundary (linear classification)
- The Perceptron algorithm
- Mistake bound for the perceptron
- Generalizing to non-linear boundaries (via Kernel space)
- Problems become linear in Kernel space
- The Kernel trick to speed up computation

Questions?

Next time…

Support Vector Machines (SVMs)!