Linear Discriminant Functions

- General form:

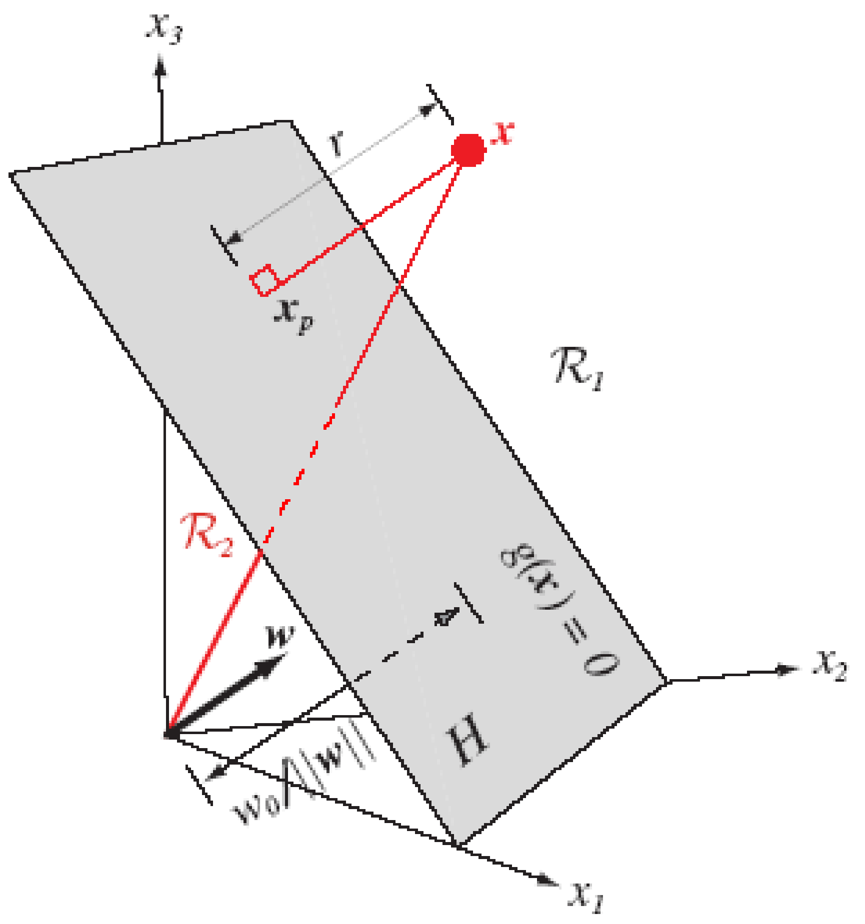
$$g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0$$

w is the *weight vector*, and

w_0 is the *bias* or *threshold weight*

- 2 classes:
  - One function, g(**x**), and then:
  - decide ω_1 if $g(\mathbf{x}) > 0$, and
    ω_2 otherwise
  - if $g(\mathbf{x}) = 0$, decide arbitrarily

w gives the "orientation" of *H*, and
w_0 gives the "distance" from the origin to *H*



Fisher's Classifier

- Given a dataset with labeled samples:

$$D = \{\mathbf{x}_{11}, \mathbf{x}_{12}, \ldots, \mathbf{x}_{1n_1}, \mathbf{x}_{21}, \mathbf{x}_{22}, \ldots, \mathbf{x}_{2n_2}\}$$

- Two data subsets (or datasets)

$$D_1 = \{\mathbf{x}_{11}, \mathbf{x}_{12}, \ldots, \mathbf{x}_{1n_1}\}$$

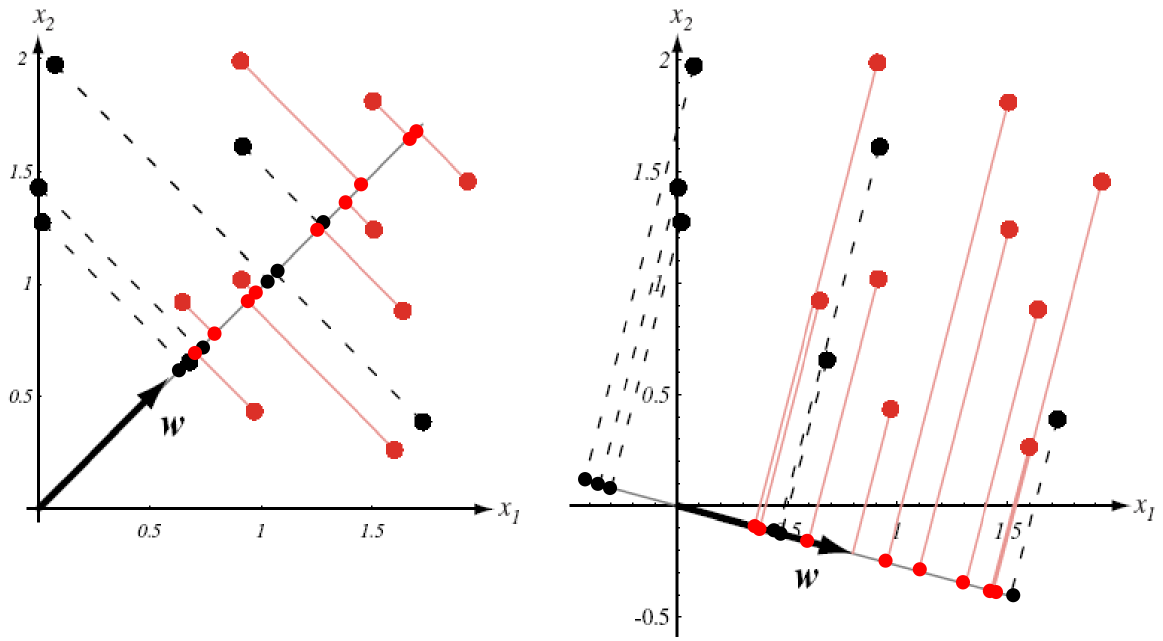
$$D_2 = \{\mathbf{x}_{21}, \mathbf{x}_{22}, \ldots, \mathbf{x}_{2n_2}\}$$

  samples $\in$ to ω_1 and ω_2 respectively, where $n = n_1 + n_2$
- Perform a linear transformation of each **x**: $y_{ij} = \mathbf{w}^t \mathbf{x}_{ij}$
- obtaining two new datasets

$$Y_1 = \{y_{11}, y_{12}, \ldots, y_{1n_1}\}$$ and

$$Y_2 = \{y_{21}, y_{22}, \ldots, y_{2n_2}\}$$

- ||**w**|| = 1 means that each y_{ij} is the projection of $\mathbf{x}_{ij}$ onto a line in the direction of **w**
- For now, don't care about the *magnitude* of **w**



Naïve approach

- What is the best direction of **w**?
- **Define:** *sample mean*, $\mathbf{m}_i$, as:

$$\mathbf{m}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in D_i} \mathbf{x}$$

- Then, sample mean in the *projected line* is:

$$\tilde{m}_i = \frac{1}{n_i} \sum_{y \in Y_i} y$$

$$= \frac{1}{n_i} \sum_{\mathbf{x} \in D_i} \mathbf{w}^t \mathbf{x} = \mathbf{w}^t \mathbf{m}_i$$

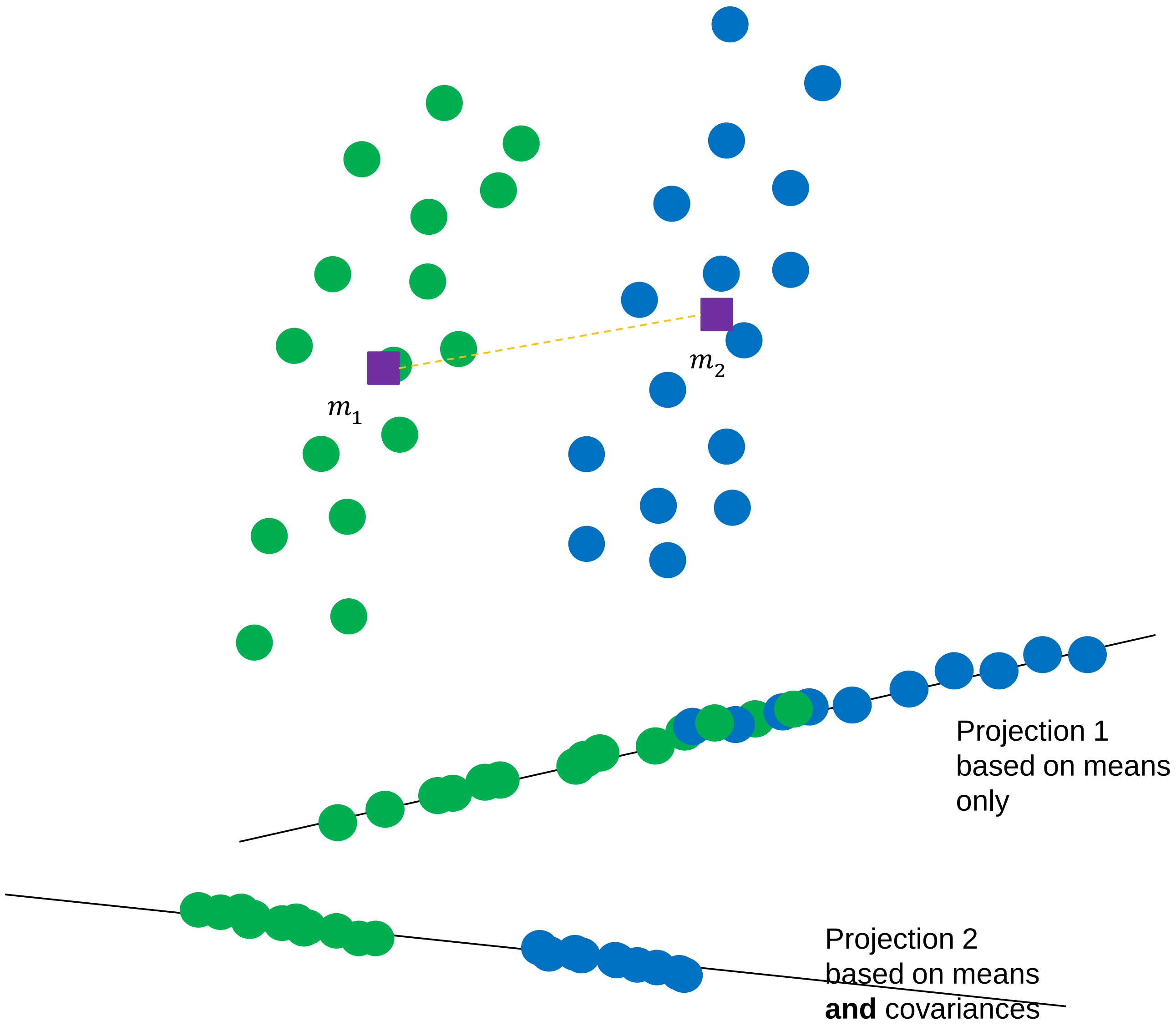
- Thus, $\tilde{m}_i$ is the projection of $\mathbf{m}_i$

- The distance between the projected means is given by:

$$\left| \tilde{m}_1 - \tilde{m}_2 \right| = \left| \mathbf{w}^t (\mathbf{m}_1 - \mathbf{m}_2) \right| \qquad (1)$$

- Then, different **w**'s will give us different "between-mean" values, and
- we want to maximize the class "separability"
- Find a vector **w** that maximizes (1)

Is this Naïve approach good enough?



- Use the variances $\tilde{s}_i^2 = \frac{1}{n_i} \sum_{y \in Y_i} (y - \tilde{m}_i)^2$
- *within-class variance*: $\tilde{s}_1^2 + \tilde{s}_2^2$
- Find a vector **w** that maximizes:

$$J(\mathbf{w}) = \frac{|\tilde{m}_1 - \tilde{m}_2|^2}{\tilde{s}_1^2 + \tilde{s}_2^2} \qquad (2)$$

- $J(.)$ has to be expressed in terms of **w**
- Sample *covariance matrix*:

$$\mathbf{S}_i = \frac{1}{n_i} \sum_{\mathbf{x} \in D_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^t$$

and the *within-class covariance matrix*:

$$\mathbf{S}_W = \frac{1}{n}\left(n_1 \mathbf{S}_1 + n_2 \mathbf{S}_2\right) = p_1 \mathbf{S}_1 + p_2 \mathbf{S}_2$$

where $p_i = \frac{n_i}{n}$

- Express the sum of the covariances as:

$$\tilde{s}_1^2 + \tilde{s}_2^2 = \mathbf{w}^t \mathbf{S}_W \mathbf{w}$$

- Separation of projected means as:

$$\left(\tilde{m}_1 - \tilde{m}_2\right)^2 = \mathbf{w}^t \mathbf{S}_B \mathbf{w}$$

where

$$\mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^t$$

is the *between-class scatter matrix*.

- Thus, we can write $J(.)$ in terms of $\mathbf{S}_B$ and $\mathbf{S}_W$ as:

$$J(\mathbf{w}) = \frac{\mathbf{w}^t \mathbf{S}_B \mathbf{w}}{\mathbf{w}^t \mathbf{S}_W \mathbf{w}} \qquad (3)$$

- The vector **w** that maximizes *J*(.) must satisfy: $\mathbf{S}_B\mathbf{w} = \lambda\mathbf{S}_W\mathbf{w}$
- If $\mathbf{S}_W$ is *not singular*:

$$\mathbf{S}_W^{-1}\mathbf{S}_B\mathbf{w} = \lambda\mathbf{w}$$

- The solution **w** is an eigenvector of $\mathbf{S}_W^{-1}\mathbf{S}_B$
- Since $\mathbf{S}_B\mathbf{w}$ is in the direction of $\mathbf{m}_1 - \mathbf{m}_2$, and

  λ is a "scaling factor" of **w**,

  the solution is given by

$$\mathbf{w} = \mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

- Note: there is only one non-zero eigenvalue of $\mathbf{S}_W^{-1}\mathbf{S}_B$

- Once obtained the direction of **w**,
- Complete linear classifier:

$$g(\mathbf{x}) = \mathbf{w}^t\mathbf{x} + w_0$$

  i.e., find w_0
- A naïve approach is to assume that the *class conditional* probabilities in the projected line are *identical*, and thus:

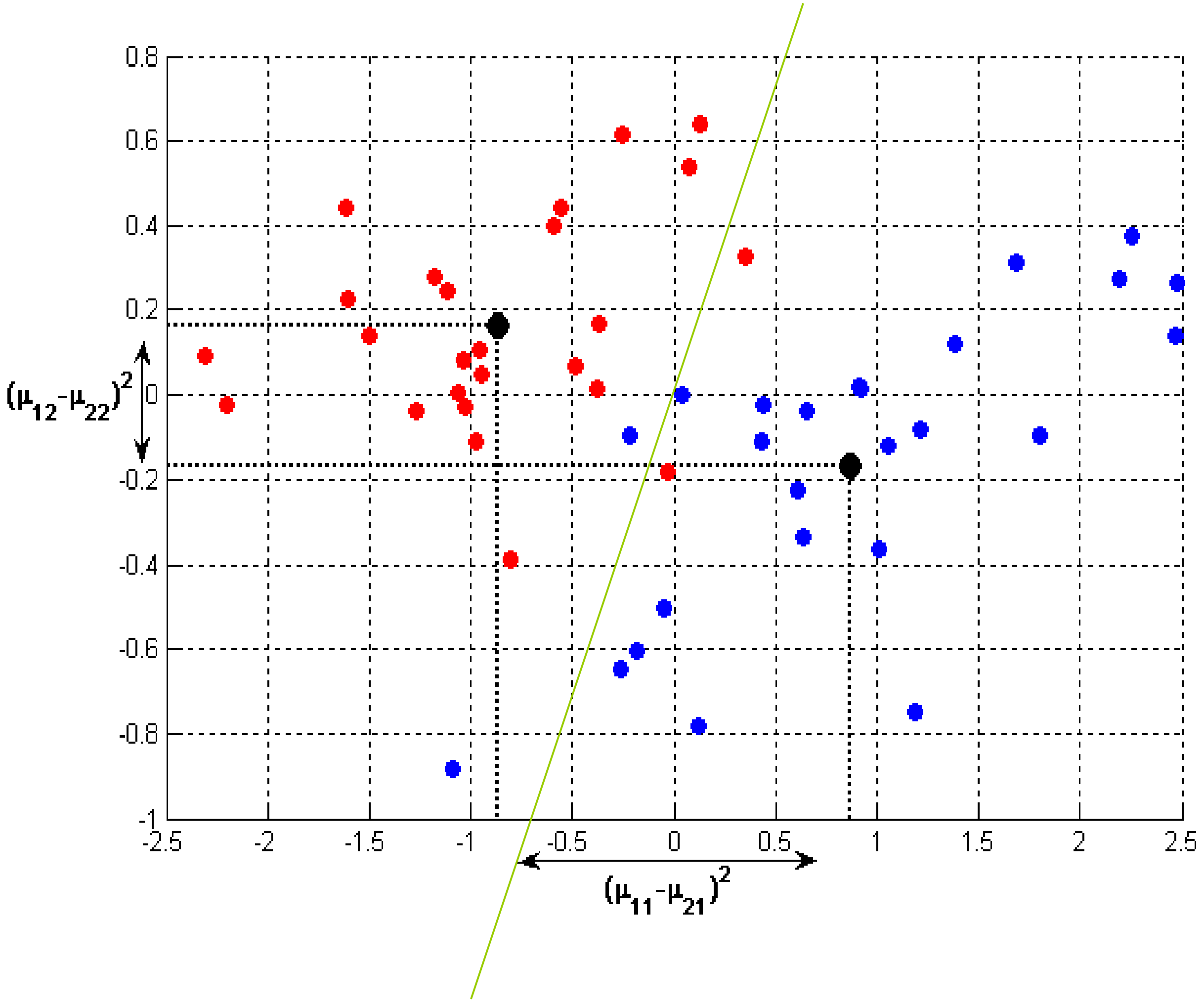
$$w_0 = -\frac{1}{2}(\tilde{m}_1 + \tilde{m}_2) - \ln\frac{P(\omega_1)}{P(\omega_2)}$$

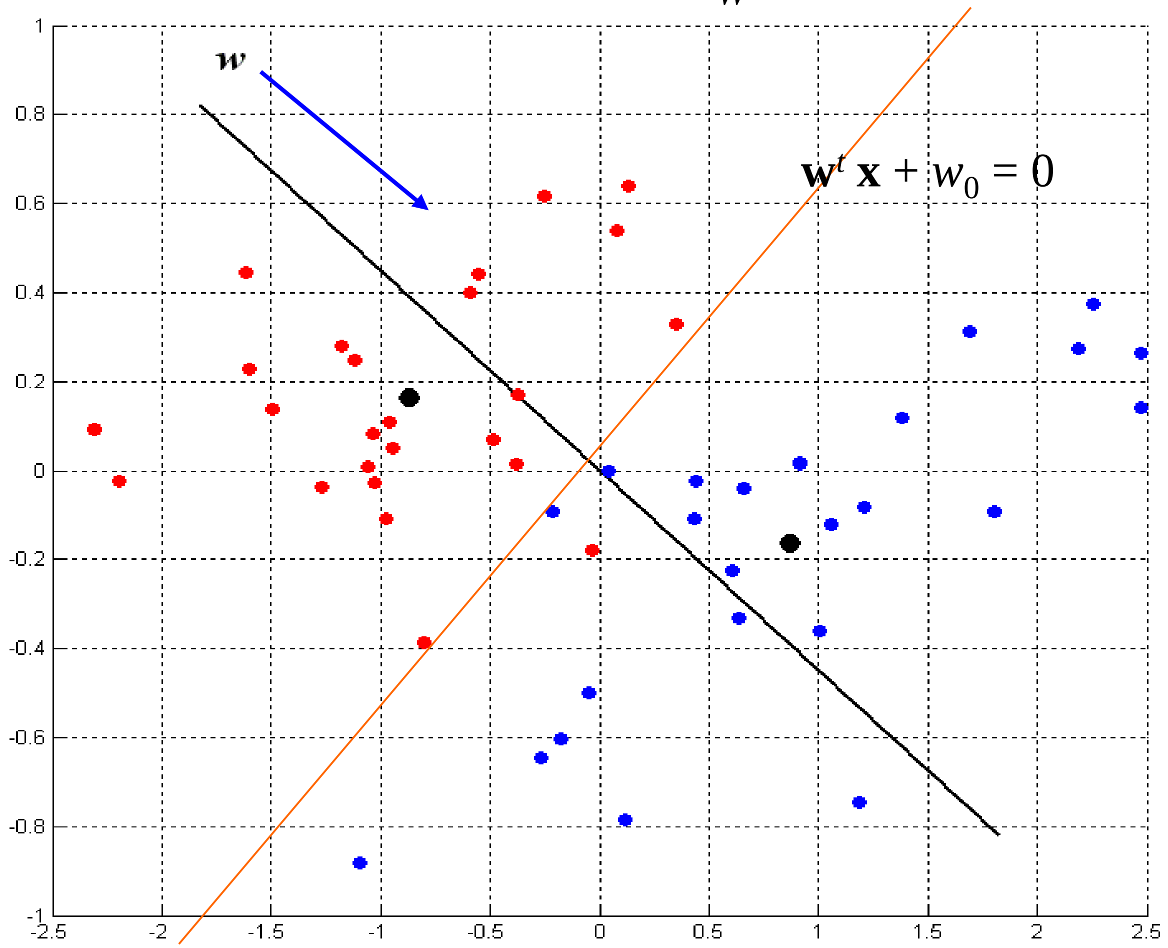
- w_0 is the middle point between the two sample means in the *projected* data

Example: means vs variances

$$J(\mathbf{w}) = |\tilde{m}_1 - \tilde{m}_2| = |\mathbf{w}^t(\mathbf{m}_1 - \mathbf{m}_2)|$$

$$J(\mathbf{w}) = \frac{\mathbf{w}^t \mathbf{S}_B \mathbf{w}}{\mathbf{w}^t \mathbf{S}_W \mathbf{w}}$$





Example 2

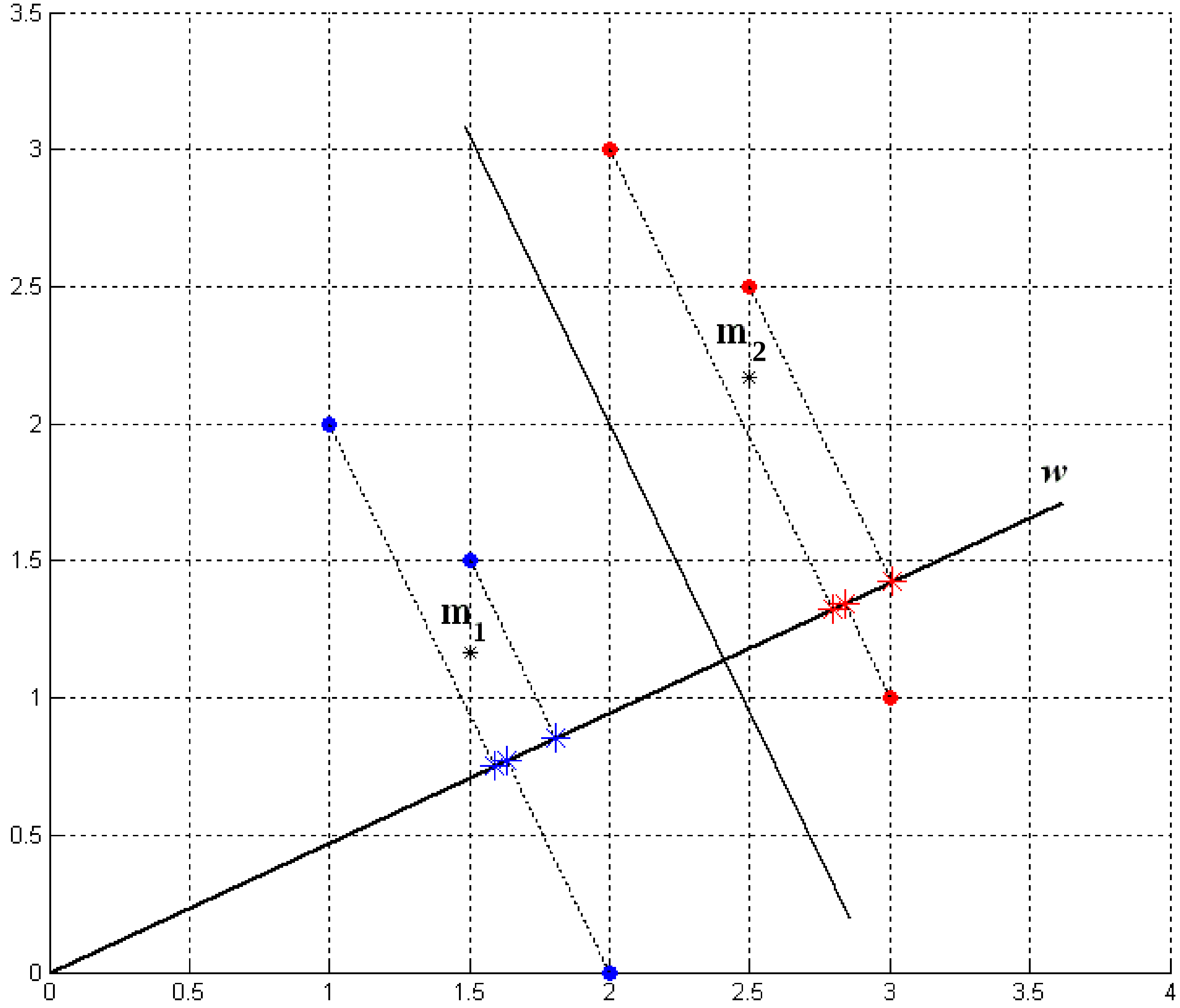
$$D_1 = \begin{bmatrix} 1.5 & 1.5 \\ 1 & 2 \\ 2 & 0 \end{bmatrix} \quad D_2 = \begin{bmatrix} 3 & 1 \\ 2 & 3 \\ 2.5 & 2.5 \end{bmatrix} \quad p_1 = p_2 = 0.5$$

$$\mathbf{m}_1 = \begin{bmatrix} 1.5 \\ 1.1667 \end{bmatrix} \mathbf{m}_2 = \begin{bmatrix} 2.5 \\ 2.1667 \end{bmatrix} \mathbf{S}_1 = \begin{bmatrix} 0.25 & -0.5 \\ -0.5 & 1.0833 \end{bmatrix} \mathbf{S}_2 = \begin{bmatrix} 0.25 & -0.5 \\ -0.5 & 1.0833 \end{bmatrix}$$

$$\mathbf{S}_W = p_1\mathbf{S}_1 + p_2\mathbf{S}_2 = \begin{bmatrix} 0.25 & -0.5 \\ -0.5 & 1.0833 \end{bmatrix} \qquad S_w^{-1} = \begin{bmatrix} 52 & 24 \\ 24 & 12 \end{bmatrix}$$

$$\mathbf{w} = \mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2) = \begin{bmatrix} -76 \\ -36 \end{bmatrix}$$

Example 2 Graphically



Generalized Linear Classifiers

Augmented Feature Vector

- We've seen that the form of a linear classifier is:

$$g(\mathbf{x}) = \mathbf{w}^t \mathbf{x} + w_0$$

- we can write this function as:

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i = \sum_{i=0}^{d} w_i x_i$$

where $x_0 = 1$

- In NN, w_0 is called "bias"

- The *augmented feature vector*, **y**, is:

$$\mathbf{y} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix} = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}$$

- Similarly, the *augmented weight vector*:

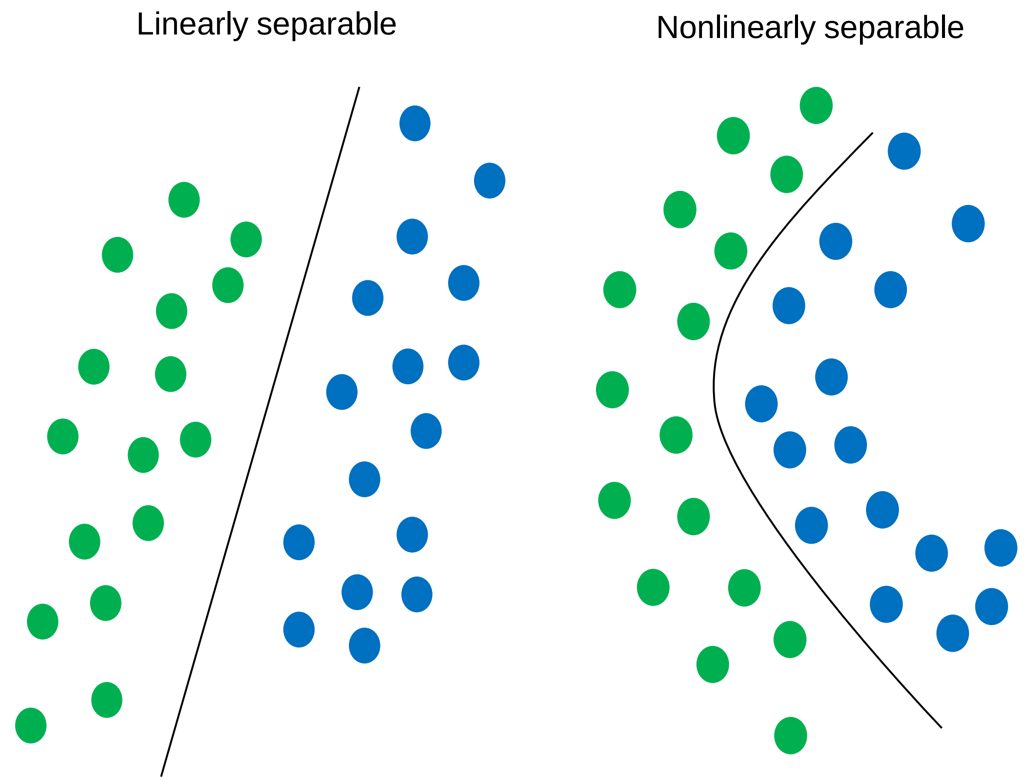
$$\mathbf{a} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix} = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix}$$

- This implies a mapping from the *d*-dim. space onto the (*d*+1)-dim. space
- Classifier: $\mathbf{a}^t \mathbf{y} = 0$

Linearly Separable Classes

- A set of n samples $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n$, labeled either ω_1 or ω_2
- Aim: find the weights of $\mathbf{a}$, used in the linear classifier $g(\mathbf{x}) = \mathbf{a}^t\,\mathbf{y}$
- A solution $\mathbf{a}$ that correctly classifies *all* the training samples, implies

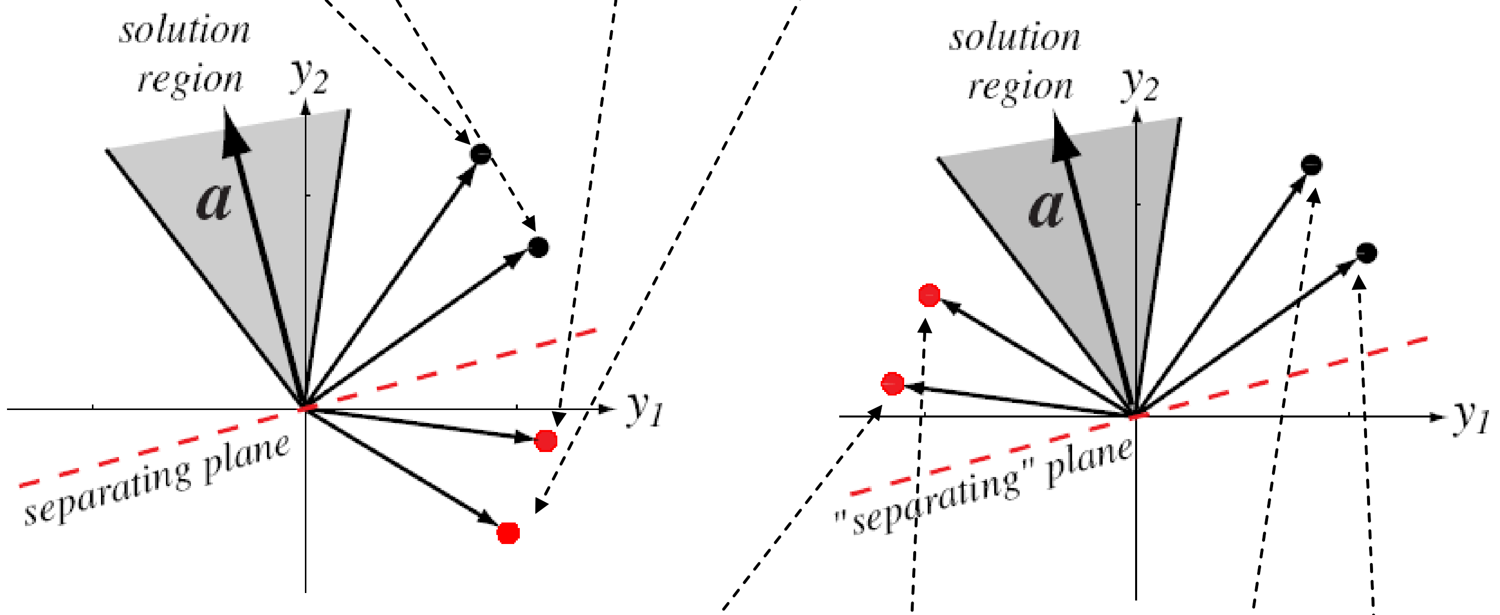
  $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n$ are *linearly separable*
  - $\mathbf{y}_i \in \omega_1$ **correctly** classified if $\mathbf{a}^t\,\mathbf{y}_i > 0$,
  - $\mathbf{y}_i \in \omega_2$ … …. if $\mathbf{a}^t\,\mathbf{y}_i < 0$



Normalization

- Replace all samples of ω_2 by their *negatives*

ω_1: $\{[2,3]^t,[3,2]^t\}$; ω_2: $\{[3,-0.5]^t,[2,-1.5]^t\}$



Normalized samples:

ω_2: $\{[-3, 0.5]^t,[-2,1.5]^t\}$; ω_1: $\{[2,3]^t,[3,2]^t\}$

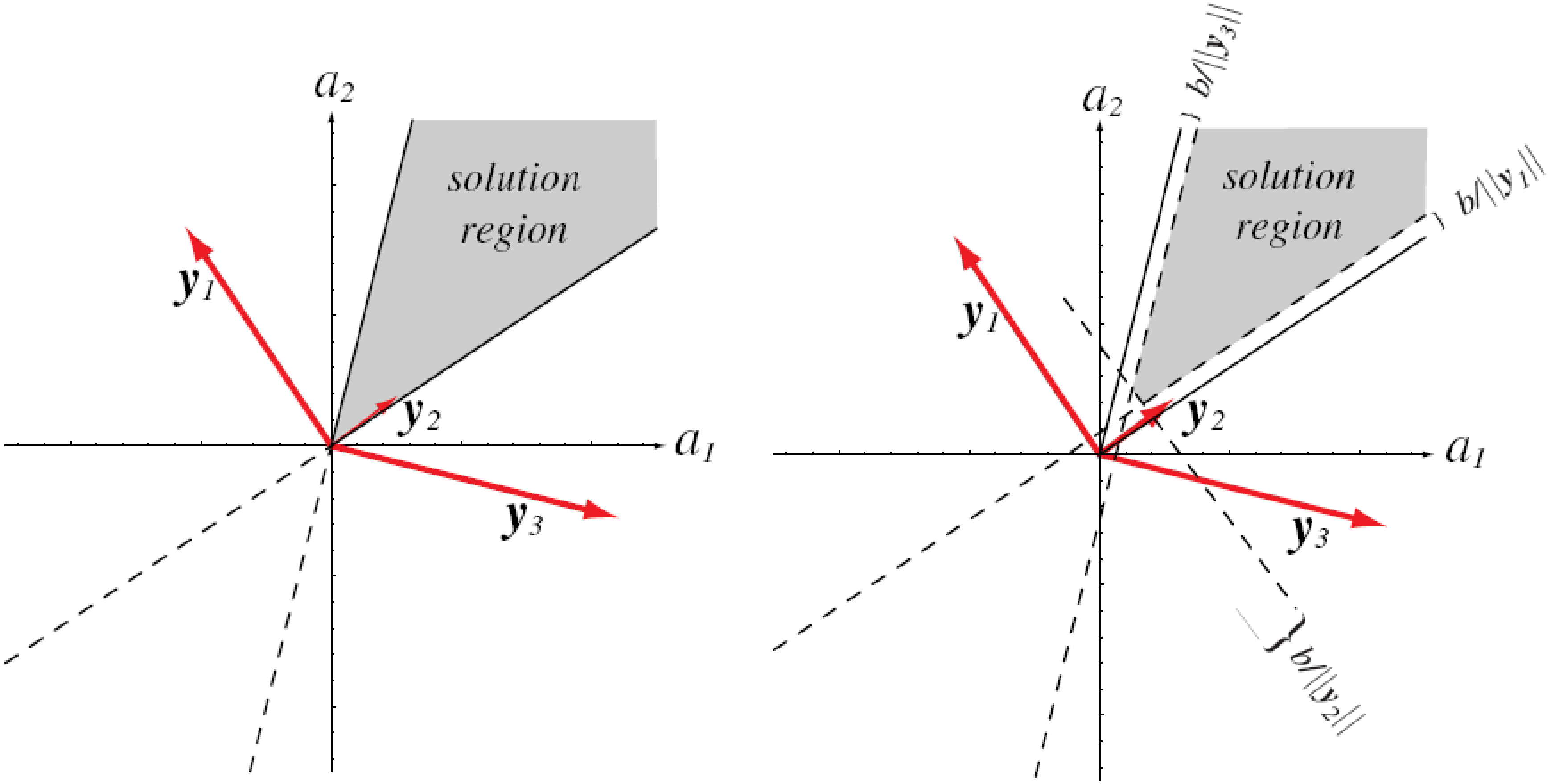
- It is then clear that if a solution vector **a** exists

  it may not be **unique**
- Thus, many approaches can be proposed
- **One way** is to look at a unit-length vector **a**

  that *maximizes* the *minimum* distance from the

  hyperplane to the samples
- **Another way:** Seek for the minimum-length vector **a** that satisfies $\mathbf{a}^t \mathbf{y}_i > b$
  - for all $\mathbf{y}_i$ and
  - for some positive value b.

- Say, we have $D = \{\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3\}$, samples in 2D space
- … three samples… already normalized…



Approaches for Linearly Separable Case

- Gradient descent procedures
- Newton's algorithm
- The perceptron criterion function/algorithm
- Relaxation procedures
  - Batch relaxation
  - Single-sample relaxation
- Minimum squared-error procedures
- Widrow-Hoff or LMS procedure
- Ho-Kashyap procedure
- Support vector machine (SVM)
- … many others

The Perceptron Criterion

- Find a criterion function to solve the set of inequalities $\mathbf{a}^t\ \mathbf{y}_i > 0$
- Solution: $J(.)$ is the number of samples "misclassified" by **a**.
- It gives a "piecewise" criterion function, for which the gradient descent algorithm can be used
- The *perceptron criterion function*:

$$J_p(\mathbf{a}) = \sum_{\mathbf{y}\in Y(\mathbf{a})} (-\mathbf{a}^t\mathbf{y})$$

where $Y(\mathbf{a})$ is the set of samples *misclassified* by **a**.

- Normalizing all samples
- A sample **y** is misclassified if $\mathbf{a}^t\ \mathbf{y} \leq 0$
- implies that for all $\mathbf{y} \in Y(\mathbf{a})$,

$$\mathbf{a}^t\ \mathbf{y} \leq 0 \ \Rightarrow\ -\mathbf{a}^t\ \mathbf{y} > 0$$

- $J_p(\mathbf{a})$ is **either** positive or zero, but **never** negative
- $J_p(\mathbf{a})$ is zero only when $Y(\mathbf{a})$ is *empty*
- Geometric interpretation of $J_p(\mathbf{a})$:
  - It is $\propto$ to the *sum* of distances from the *misclassified* samples to the discriminant function given by **a**

- Use $J_p(\mathbf{a})$ in the Gradient Descent algorithm
- *Gradient operator* ∇:

$$\nabla J_p(\mathbf{a}) = \sum_{\mathbf{y} \in Y(\mathbf{a})} (-\mathbf{y})$$

  - because the gradient operator of J_p is $\partial J_p / \partial a_j$

$$\frac{\partial}{\partial \mathbf{x}} \mathbf{y}^t \mathbf{x} = \mathbf{y}$$

- Update rule:

$$\mathbf{a}(k+1) \leftarrow \mathbf{a}(k) + \eta(k) \sum_{\mathbf{y} \in Y(k)} \mathbf{y}$$

where $Y(k)$ is the set of samples misclassified by $\mathbf{a}(k)$

Algorithm **Batch Perceptron**

Input: A threshold θ

begin Initialize **a**, $\eta(1)$, $k \leftarrow 0$

    repeat

        $k \leftarrow k + 1$

        $\mathbf{a} \leftarrow \mathbf{a} + \eta(k) \sum_{\mathbf{y} \in Y(k)} \mathbf{y}$

    until $\left| \eta(k) \sum_{\mathbf{y} \in Y(k)} \mathbf{y} \right| < \theta$

end

Variants

- Algorithm called “batch perceptron”
  - use all samples in $J(.)$
- “single-sample” perceptron:

  if $\mathbf{y}^k$ is misclassified by $\mathbf{a}$

  $$\mathbf{a} \leftarrow \mathbf{a} + \mathbf{y}^k \qquad (4)$$
- Repeated until no $\mathbf{y}^k$ is misclassified
- Proved to converge if the samples are

  “linearly separable”
- Can still be used in nonlinearly separable
- (4) is also called “fixed-increment” rule,
- since $\eta(.)$ is constant for all iterations

Relaxation procedures

- Descent criterion:

$$J_q(\mathbf{a}) = \sum_{\mathbf{y} \in Y} \left(\mathbf{a}^t \mathbf{y}\right)^2$$

- Regularization/normalization:

$$J_r(\mathbf{a}) = \frac{1}{2} \sum_{\mathbf{y} \in Y} \frac{\left(\mathbf{a}^t \mathbf{y} - b\right)^2}{||\mathbf{y}||^2}$$

- aka “minimum square error”
- Lead to a “smoother” surface of the optimization problem

Nonlinearly Separable Case

- Perceptron and relaxation are usually called

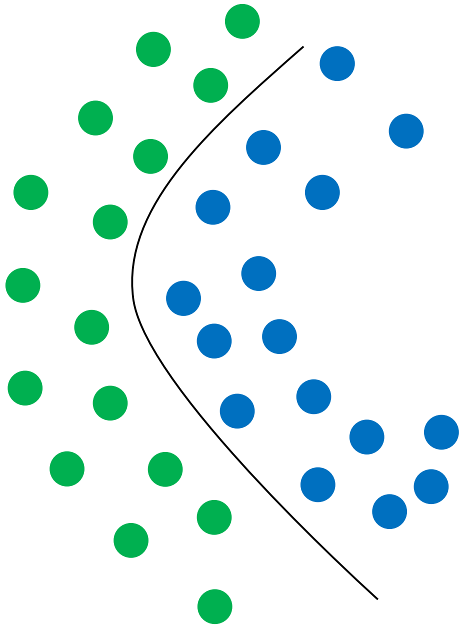
  error-correcting procedures
- It does work on nonlinearly separable
- In the nonlinearly separable case,

  relaxation procedures work better

$$J_r(\mathbf{a}) = \frac{1}{2} \sum_{\mathbf{y} \in Y} \frac{\left(\mathbf{a}^t \mathbf{y} - b\right)^2}{||\mathbf{y}||^2}$$

Solution using the

minimum squared-error procedure



Minimum Squared-error (MSE)

- *Normalizing* all samples:

  $\mathbf{a}^t\,\mathbf{y} > 0$ for all $\mathbf{y}$
- Consider $\mathbf{a}^t\,\mathbf{y}_i = b_i$

  where b_i is an *arbitrarily specified positive constant*
- Aim: find solution to

  $\mathbf{a}^t\,\mathbf{y}_i = b_i$

- Problem in matrix-like form: **Ya** = **b**

$$\begin{bmatrix} y_{10} & y_{11} & \cdots & y_{1d} \\ y_{20} & y_{21} & \cdots & y_{2d} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ y_{n0} & y_{n1} & \cdots & y_{nd} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_d \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ \vdots \\ \vdots \\ b_n \end{bmatrix}$$

- **Y** is an $n \times (d+1)$ matrix
- The i^{th} row is vector $\mathbf{y}_i$ (normalized)
- **b** is a vector (of arbitrary constants)
- **a** is the weight vector

Aim: Find a solution vector **a** to **Ya** = **b**

- If **Y** is square, no problem…

  find **a** = $\mathbf{Y}^{-1}$ **b**, and we are done
- But in general, **Y** is *rectangular*
- Instead: minimize the error between **Ya** and **b**, as:

$$\mathbf{e} = \mathbf{Ya} - \mathbf{b}$$

or:
$$J_s(\mathbf{a}) = \|\mathbf{Ya} - \mathbf{b}\|^2 = \sum_{i=1}^{n} (\mathbf{a}^t \mathbf{y}_i - b_i)^2$$

Gradient:
$$\nabla J_s = \sum_{i=1}^{n} 2(\mathbf{a}^t \mathbf{y}_i - b_i)\mathbf{y}_i = 2\mathbf{Y}^t(\mathbf{Ya} - \mathbf{b})$$

- **Solution:** $\mathbf{Y}^t$ **Y** is a square matrix, hopefully, nonsingular, we have:

$$\mathbf{a} = (\mathbf{Y}^t \mathbf{Y})^{-1} \mathbf{Y}^t \mathbf{b} = \mathbf{Y}^\dagger \mathbf{b}$$

- We know what $\mathbf{Y}^\dagger$ is:
- the *pseudoinverse*
- The pseudoinverse, in general exists, but
- if it doesn't, we can find it as:

$$\mathbf{Y}^\dagger \equiv \lim_{\varepsilon \to 0} \left(\mathbf{Y}^t \mathbf{Y} + \varepsilon \mathbf{I} \right)^{-1} \mathbf{Y}^t$$

- It can be shown that the limit always exists, and **a** = $\mathbf{Y}^\dagger$ **b** is a solution to **Ya** = **b**
- Reasonable choice: **b** = $\mathbf{1}_n$

  a solution exists in most of the cases

Example

- Class 1: $[1,2]^t$ and $[2,0]^t$
- Class 2: $[3,1]^t$ and $[2,3]^t$
- Decision boundary:

$$\mathbf{a}^t \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} = 0$$

- Lets find **a**
- Create

$$\mathbf{Y} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 0 \\ -1 & -3 & -1 \\ -1 & -2 & -3 \end{bmatrix}$$

- and find

$$\mathbf{Y}^+ = (\mathbf{Y}^t\mathbf{Y})^{-1}\mathbf{Y}^t = \begin{bmatrix} 5/4 & 13/12 & 3/4 & 7/12 \\ -1/2 & -1/6 & -1/2 & -1/6 \\ 0 & -1/3 & 0 & -1/3 \end{bmatrix}$$

- Set the margins $\mathbf{b} = [1,1,1,1]^t$
- Solution $\mathbf{a} = \mathbf{Y}^\dagger \mathbf{b} = [11/3,-4/3,-2/3]^t$

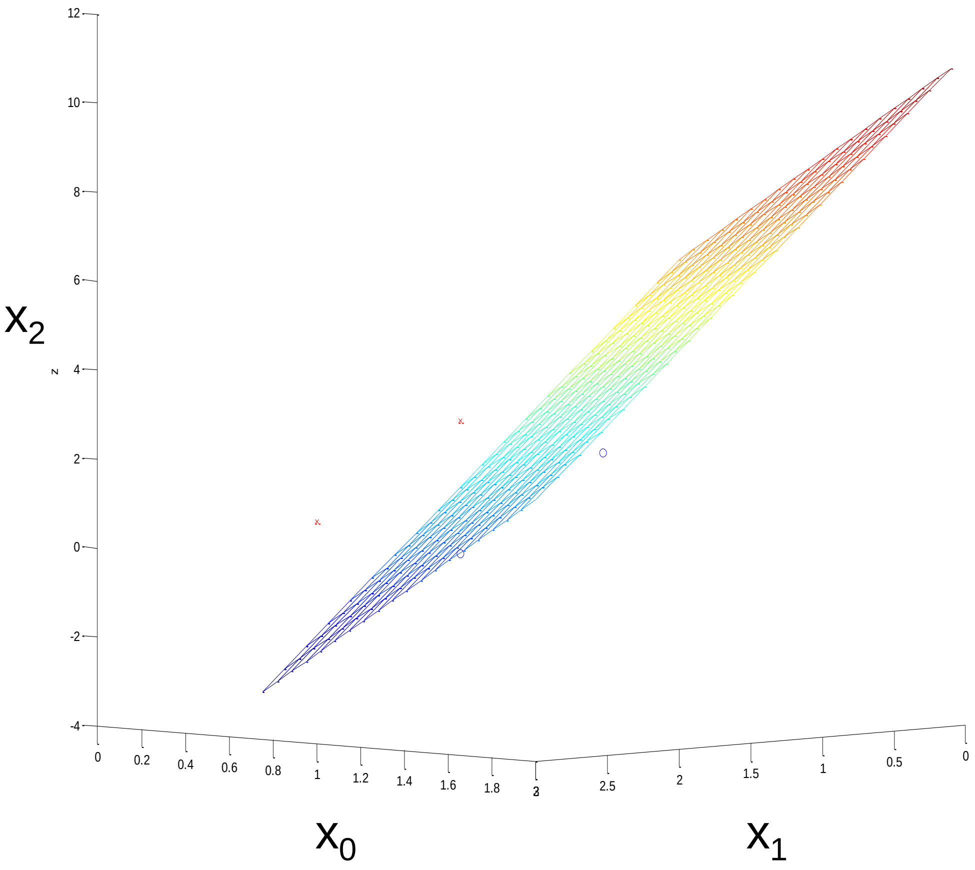
$$g(\mathbf{y}) = \frac{11}{3}x_0 - \frac{4}{3}x_1 - \frac{2}{3}x_2 = 0$$

Decide ω_1 if $g(\mathbf{y}) > 0$,

otherwise decide ω_2 when $g(\mathbf{y}) \le 0$

- Classify: $\mathbf{x} = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$

- Augmented vector: $\mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}$

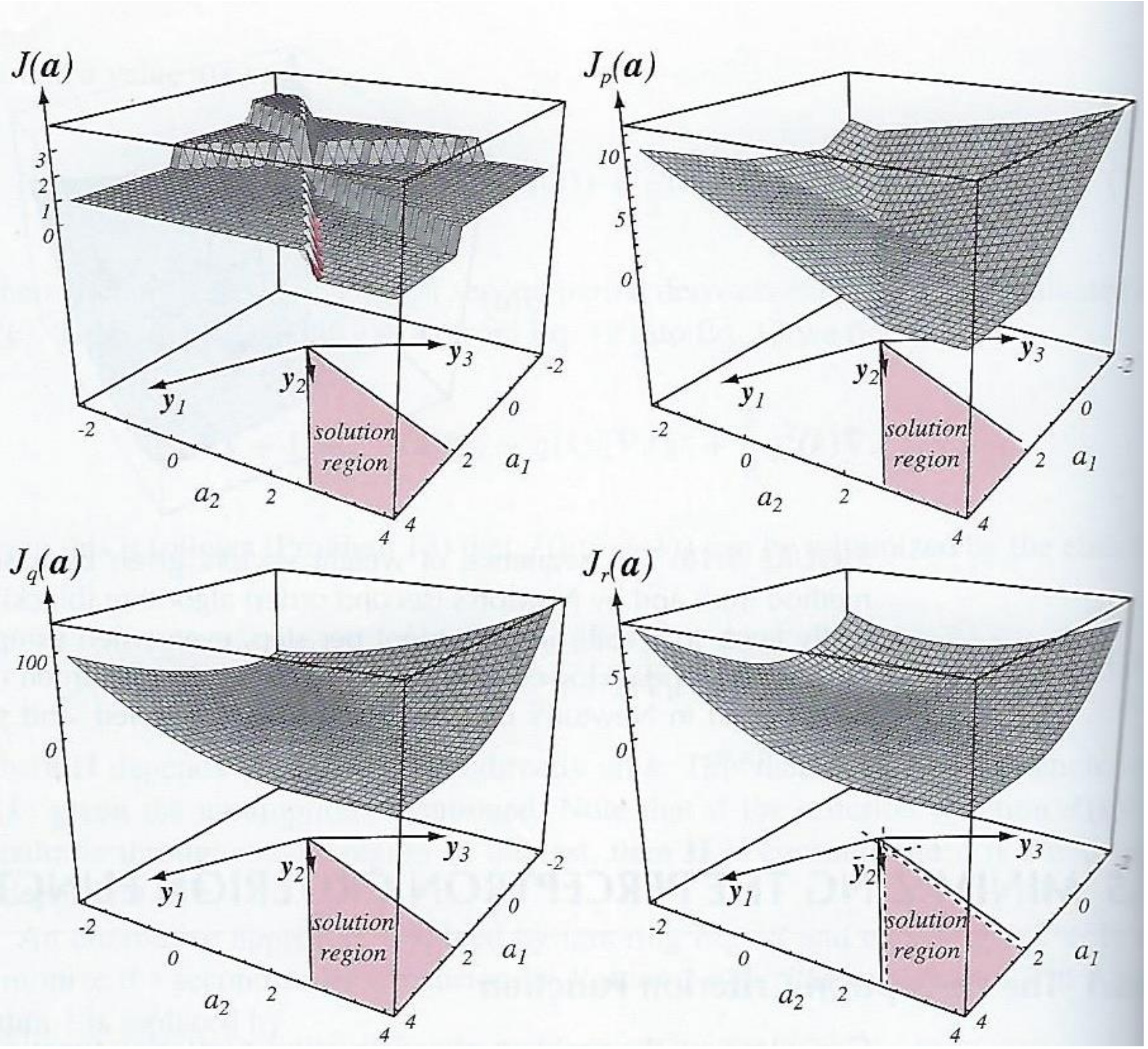


$$g(\mathbf{y}) = \frac{11}{3} - \frac{4}{3}2 - \frac{2}{3}2 = \frac{11}{3} - \frac{8}{3} - \frac{4}{3} = -\frac{1}{3} < 0$$

$$\Rightarrow \text{ decide } \mathbf{x} \in \omega_2$$

Optimization Landscape - Relaxation

Number of misclassified samples



$$J_p(\mathbf{a}) = \sum_{\mathbf{y}\in Y(\mathbf{a})} (-\mathbf{a}^t\mathbf{y})$$

$$J_q(\mathbf{a}) = \sum_{\mathbf{y}\in Y} \left(\mathbf{a}^t\mathbf{y}\right)^2$$

$$J_r(\mathbf{a}) = \frac{1}{2}\sum_{\mathbf{y}\in Y} \frac{\left(\mathbf{a}^t\mathbf{y} - b\right)^2}{\|\mathbf{y}\|^2}$$

Support Vector Machines (SVM)

- Most widely-used technique for classification
- Suitable for small training datasets
- Works well with a large number of features
- Excellent generalization power

Main idea:

- Derive a *linear* (could be nonlinear) classifier on the basis of a convex optimization problem
- Make use of "support vectors" to derive the classifier

- Consider a dataset that contains *labeled* samples

  drawn from two classes, ω_1 and ω_2 :

$$D = \{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n\}$$

- Let z_k be the "identifier" for the class,
- where for each $\mathbf{y}_i$:

$$z_k = \begin{cases} +1 & \text{if } \mathbf{y}_i \in \omega_1 \\ -1 & \text{if } \mathbf{y}_i \in \omega_2 \end{cases}$$

Augmented space

- As before, the linear classifier in the *augmented* space is:

$$g(\mathbf{y}) = \mathbf{a}^t \mathbf{y}$$

- Recall:
  - $a_0 = w_0$ (the threshold or bias)
  - $y_0 = 1$ (the threshold is not changed)
- **Two cases:**
  - Linearly separable classes
  - Nonlinearly separable classes

Linearly separable case:

- A *separating* hyperplane satisfies:

for $k = 1, \ldots, n$

- Though the margin is *any* positive distance from the hyperplane to the samples

Aim of the SVM:

- Find the separating hyperplane with the *largest margin*
- But using only the *support vectors*
- The *larger* the margin, the better the classifier

Linearly separable case:

- A *separating* hyperplane satisfies:

$$z_k g(\mathbf{y}_k) \geq 1$$

for k = 1, …, n

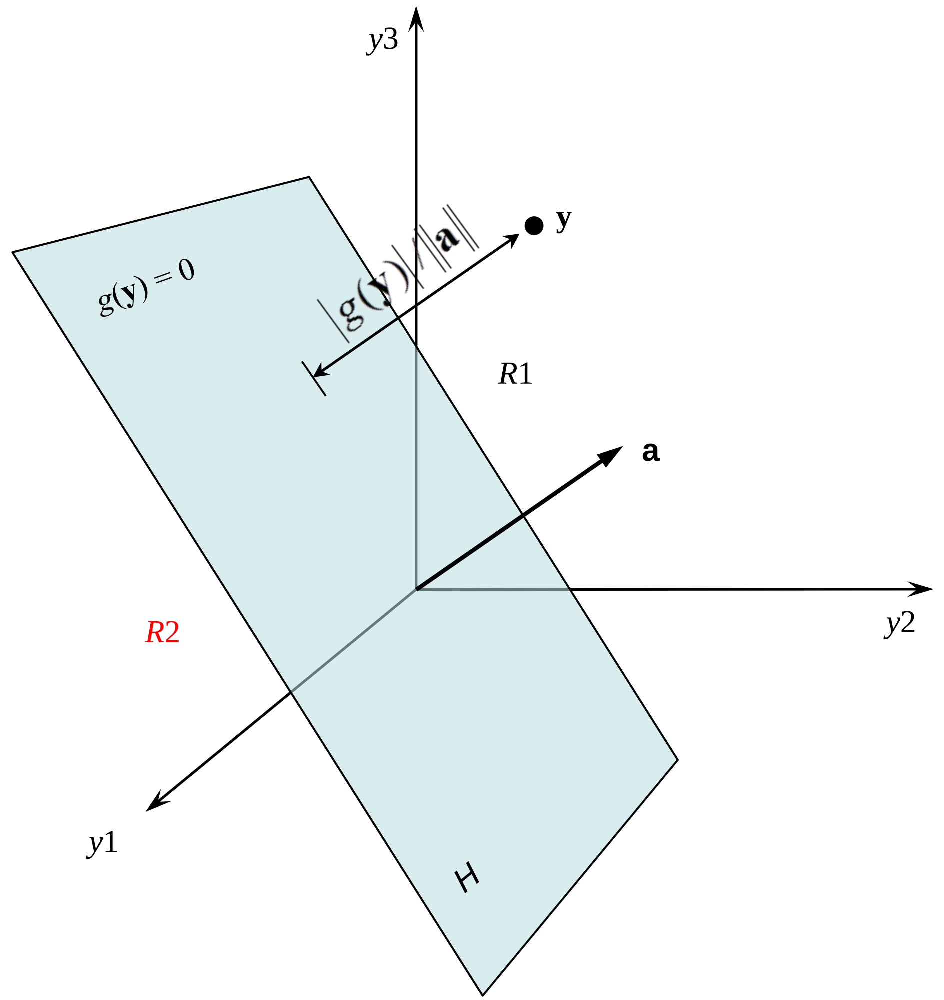
- Though the margin is *any* positive distance from the hyperplane to the samples

Aim of the SVM:

- Find the separating hyperplane with the *largest margin*
- But using only the *support vectors*
- The *larger* the margin, the better the classifier

Recall:

- The distance from any sample $\mathbf{y}$ to H: $|g(\mathbf{y})| / \|\mathbf{a}\|$
- Or equivalently $\frac{z_k g(\mathbf{y})}{\|\mathbf{a}\|}$



Support Vectors

Linearly separable case:

- A positive margin *b* exists,
- then…

Rewrite the problem:

- Find the vector(s) **a** that maximize(s) *b*, where:

$$\frac{z_k g(\mathbf{y}_k)}{\|\mathbf{a}\|} \geq b \qquad (2)$$

Note:

- The solution vector can be "scaled" and still preserve the *direction* of the hyperplane
- To *force* uniqueness of the solution, impose the constraint $b\,||\mathbf{a}|| = 1$
- In other words…

- Want to minimize $||\mathbf{a}||^2$
  while keeping the margin fixed.
- Why are they called *support vector machines*?
- They rely on the "support vectors" to derive the classifier.
- Which are the support vectors?
  … the ones whose margin is *minimal*

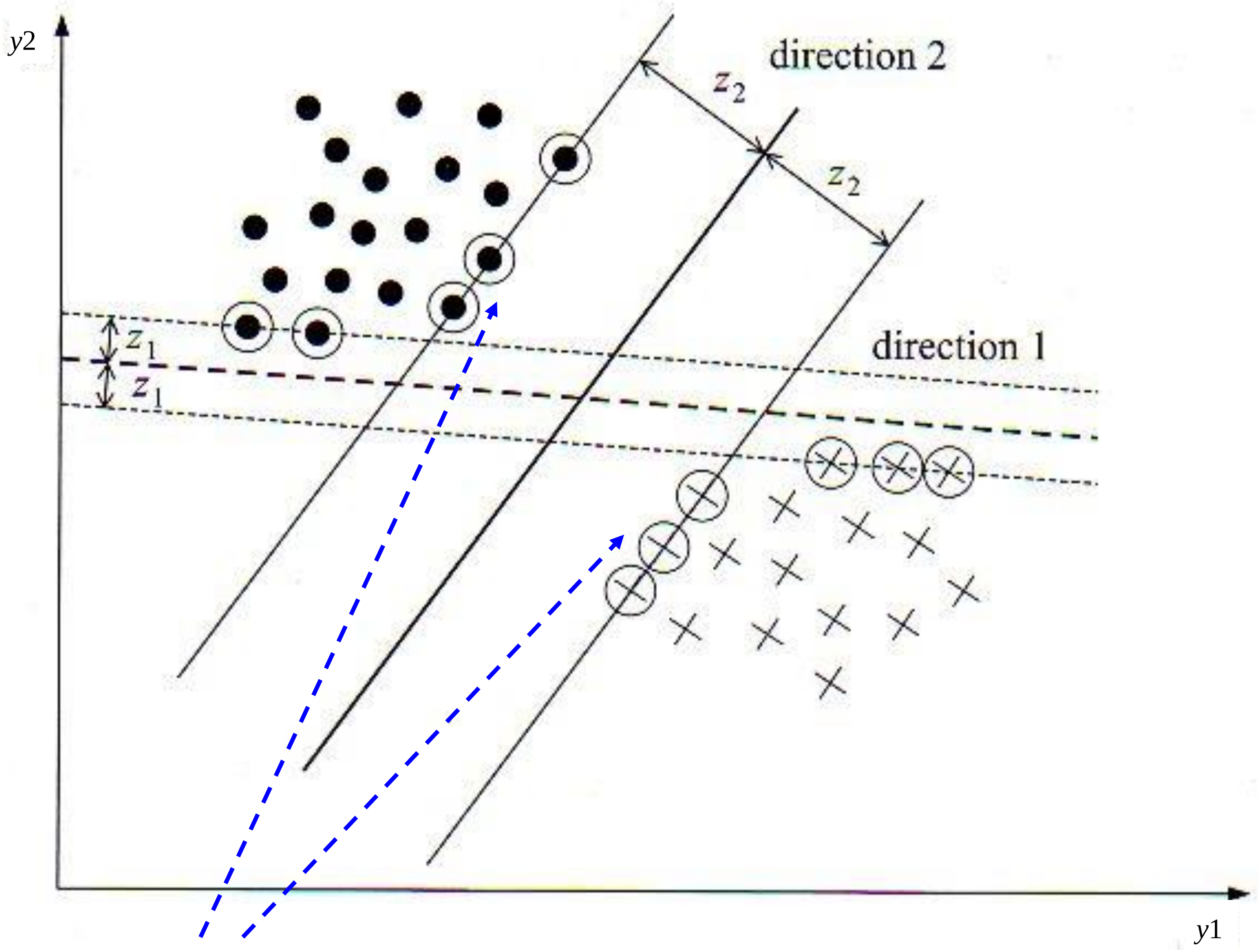
Or, put in other words:

- We intend to find samples that are the "hardest" to classify

Recall:

- We want to find the hyperplane that maximizes the margin

Graphically



support vectors

Reformulate the problem

- Lets keep the margin fixed, *say* b = 1

  and minimize $||\mathbf{a}||^2$
- Rewriting (2), yields a

  constrained optimization problem…
- Minimize:

$$\frac{1}{2}\|\mathbf{a}\|^2$$

- Subject to:

$$z_k \mathbf{a}^t \mathbf{y}_k = 1 \quad \text{or} \quad z_k \mathbf{a}^t \mathbf{y}_k - 1 = 0$$

  for all k = 1, .., n

Lagrange Multipliers

- Using *Lagrange undetermined multipliers*, transformed into an *unconstrained* optimization problem:
- Objective function:

$$L(\mathbf{a},\boldsymbol{\alpha}) = \underbrace{\frac{1}{2}\|\mathbf{a}\|^2}_{\text{Objective function}} - \sum_{k=1}^{n} \underbrace{\alpha_k}_{\text{Multipliers}} \underbrace{\left(z_k \mathbf{a}^t \mathbf{y}_k - 1\right)}_{\text{Constraints}} \qquad (3)$$

where $\alpha_k \geq 0$ are the undetermined multipliers

- Aim:
  - Minimize L with respect to **a**, and
  - Maximize it wrt to $\alpha_k \geq 0$

Dual Problem

Duality:

- Lagrangian treatment of optimization problems leads to an interesting dual representation, usually easier to solve than the “primal” problem

Besides:

- In the SVM, the so-called Karush-Kuhn-Tucker conditions allow us to use
  another representation of this problem,
  easier to solve, and
  involving fewer variables than the
  whole training set.

- Thus, (3) is now expressed in terms of α, as maximizing:

$$L(\boldsymbol{\alpha}) = \sum_{k=1}^{n} \alpha_k - \frac{1}{2} \sum_{k,j=1}^{n} \alpha_k \alpha_j z_k z_j \mathbf{y}_j^t \mathbf{y}_k \tag{4}$$

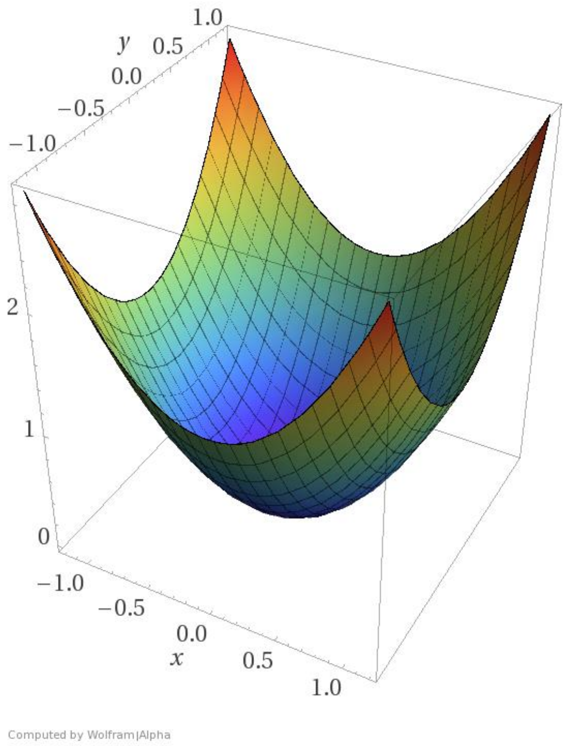
subject to the following constraints:

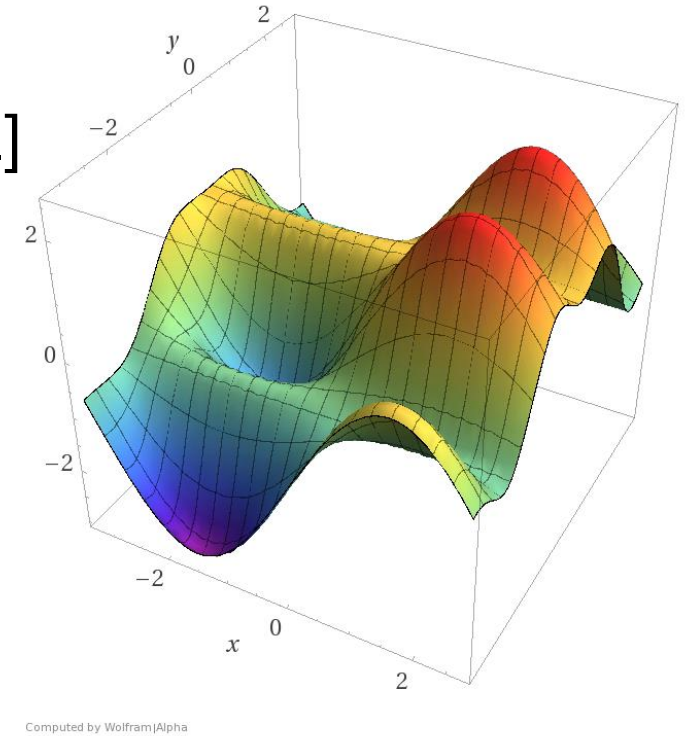
$$\sum_{k=1}^{n} z_k \alpha_k = 0, \quad \text{and } \alpha_k \geq 0$$

- Need to obtain values of α_k
- n_s (support) vectors are those for which $\alpha_k \neq 0$
- Soln. vector **a** given by: $\mathbf{a} = \sum_{k=1}^{n_s} \alpha_k z_k \mathbf{y}_k$
- Classification: $\mathbf{a}^t \mathbf{y} > 0$ decide $\mathbf{y} \in \omega_1$
  otherwise decide $\mathbf{y} \in \omega_2$

Convex Optimization

- Yields a *quadratic* constrained optimization problem.
- It is convex and the constraints are linear
  - form a convex set of feasible solutions
  - Has a unique global optima
- For more details see Ch. 21 of [1]

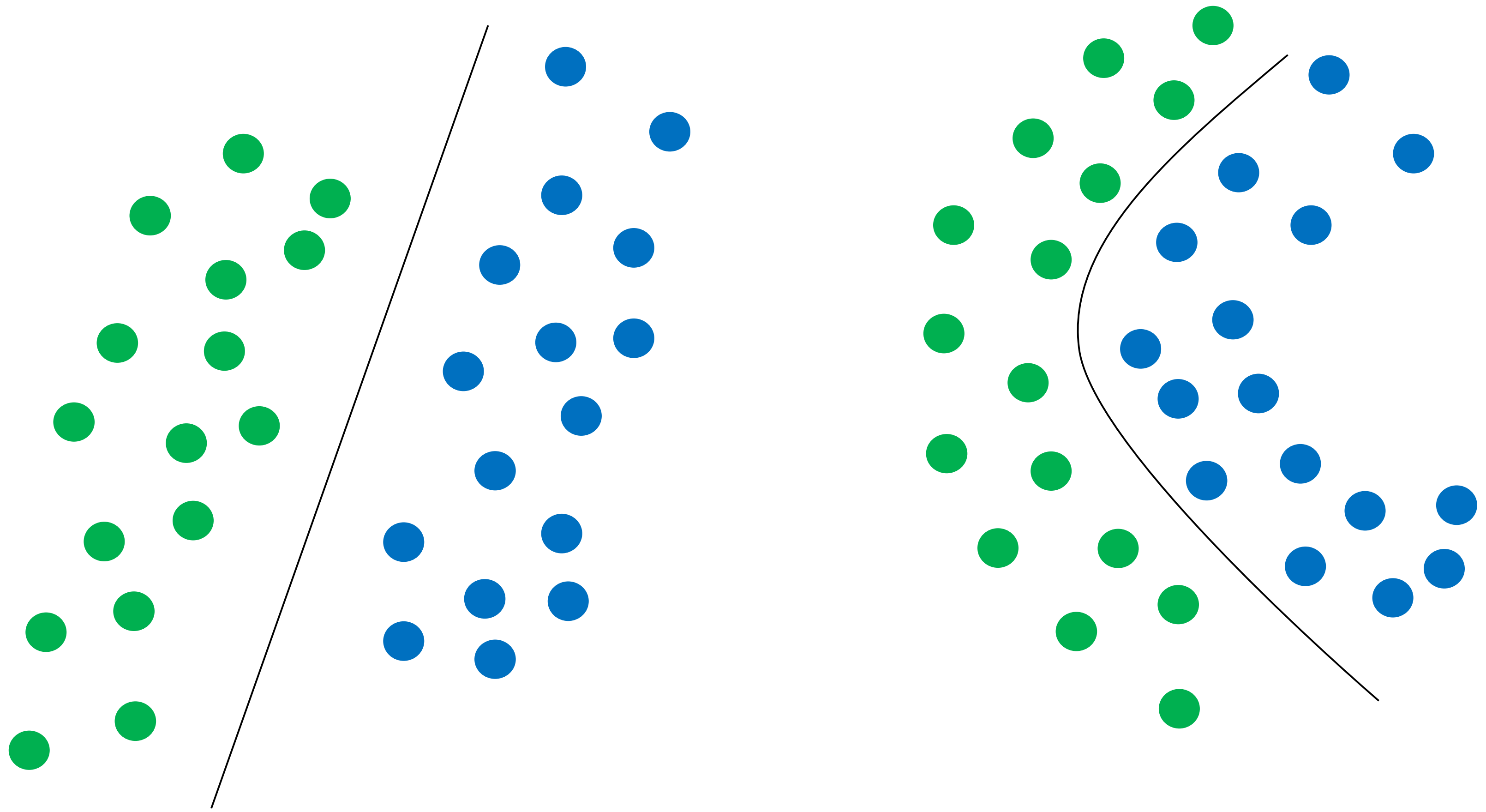




Linear vs Nonlinearly Separable

Linearly separable

Nonlinearly separable



Mapping Functions

Generalized Discriminant Functions

- **Quadratic Discriminant:**

$$g(\mathbf{x}) = \mathbf{x}^t \mathbf{W} \mathbf{x} + \mathbf{w}^t \mathbf{x} + w_0$$

- where
  - **W** is a matrix,
  - **w** is a vector, and
  - w_0 is a threshold weight
- This is the general form of the Bayesian classifier with normal distributions (Ch. 2)
- It can also be generalized to …

  a *polynomial* discriminant function
- Note: for now, we will classify a vector **x** instead of **y**

Polynomial Discriminant Functions

- A *linear* discriminant function

$$g(\mathbf{x}) = \mathbf{w}^t \mathbf{x} + w_0$$

- can be written as:

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i$$

- A *quadratic* discriminant function

$$g(\mathbf{x}) = \mathbf{x}^t \mathbf{W} \mathbf{x} + \mathbf{w}^t \mathbf{x} + w_0$$

- can be written as:

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i + \sum_{i=1}^{d} \sum_{j=1}^{d} w_{ij} x_i x_j$$

Polynomial Discriminant Functions

- We can continue adding more terms like this:

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} w_i x_i + \sum_{i=1}^{d}\sum_{j=1}^{d} w_{ij} x_i x_j + \sum_{i=1}^{d}\sum_{j=1}^{d}\sum_{k=1}^{d} w_{ijk} x_i x_j x_k$$

- and so on…

  yielding *polynomial discriminant functions*.

- Clearly, a k^{th} order polynomial requires $O(d^k)$ terms !!
- But…
  - do we need all these terms?
  - Probably not…

Phi Functions

- Indeed, we can use "truncated" series expansions of some arbitrary function $g(\mathbf{x})$…

  to get the *generalized linear discriminant function*:

$$g(\mathbf{x}) = \sum_{i=1}^{\hat{d}} a_i \phi_i(\mathbf{x})$$

  or written in another way:

$$g(\mathbf{x}) = \mathbf{a}^t \mathbf{y}$$

- The *weight vector* $\mathbf{a}$ is a $\hat{d}$-dimensional vector, and

  the idea is that $\hat{d} >>> d$
- We have now $\hat{d}$ functions called the "phi functions" $\boldsymbol{\phi}$(.)

  and are *arbitrary* functions of $\mathbf{x}$

Mapping + SVM

- Such functions are *not linear* on **x**,

  but are *linear* on **y**.
- So, then the idea of finding a linear function in a "higher-dimensional" space, say the **y**-space (feature space).
- The linear function defines a hyperplane in the **y**-space,
  - which passes through the origin of the system
- Also called *homogeneous* linear discriminant function
- Thus, two problems:
  - Find a mapping from **x** to **y**
  - Find a good linear discriminant function in the **y**-space

    (we already know how to get this one, but will see another way)
  - Now, once we map to the new space, we classify **y**

Example 1

- Consider this quadratic discriminant function on *x*

$$g(x) = a_0 + a_1 x + a_2 x^2$$

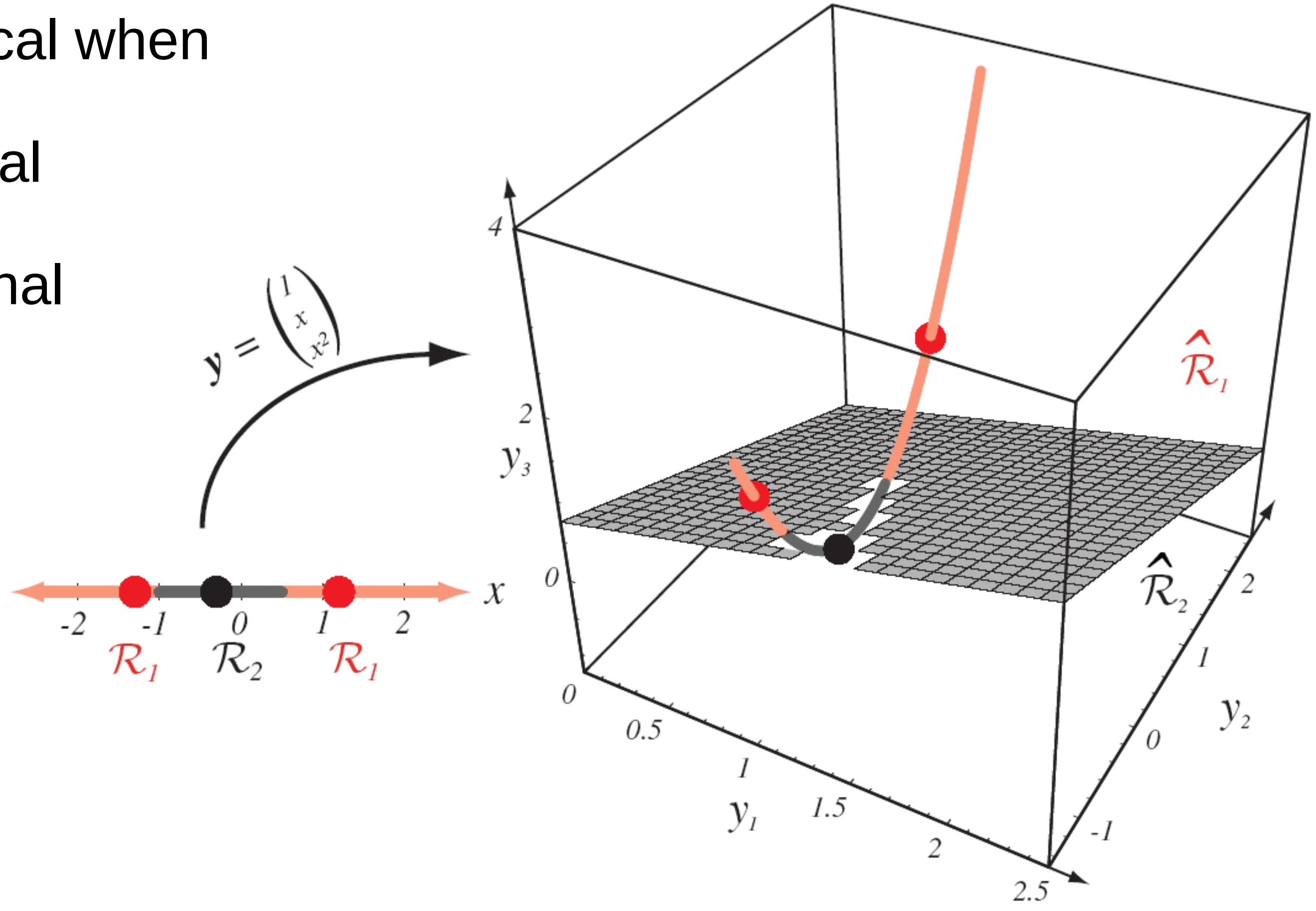
… it is a *one-variable* function (domain is in 1D space)

- Now, lets apply a mapping from *x* to **y** from the 1D space to the 3D space
- Resulting in a vector **y** as follows (example):

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}$$

Graphically

- The data in the 3D space remains 1D, and lie in a *parabola*
- if x follows a distn $px(x)$, assume defined in $(-\infty,\infty)$,
- Then $\mathbf{y}$ follows another distn. $p\mathbf{y}(\mathbf{y})$,
  - being 0 in every $\mathbf{y} \notin$ the parabola
- This case is typical when mapping from a *lower*-dimensional space to a *higher*-dimensional space.



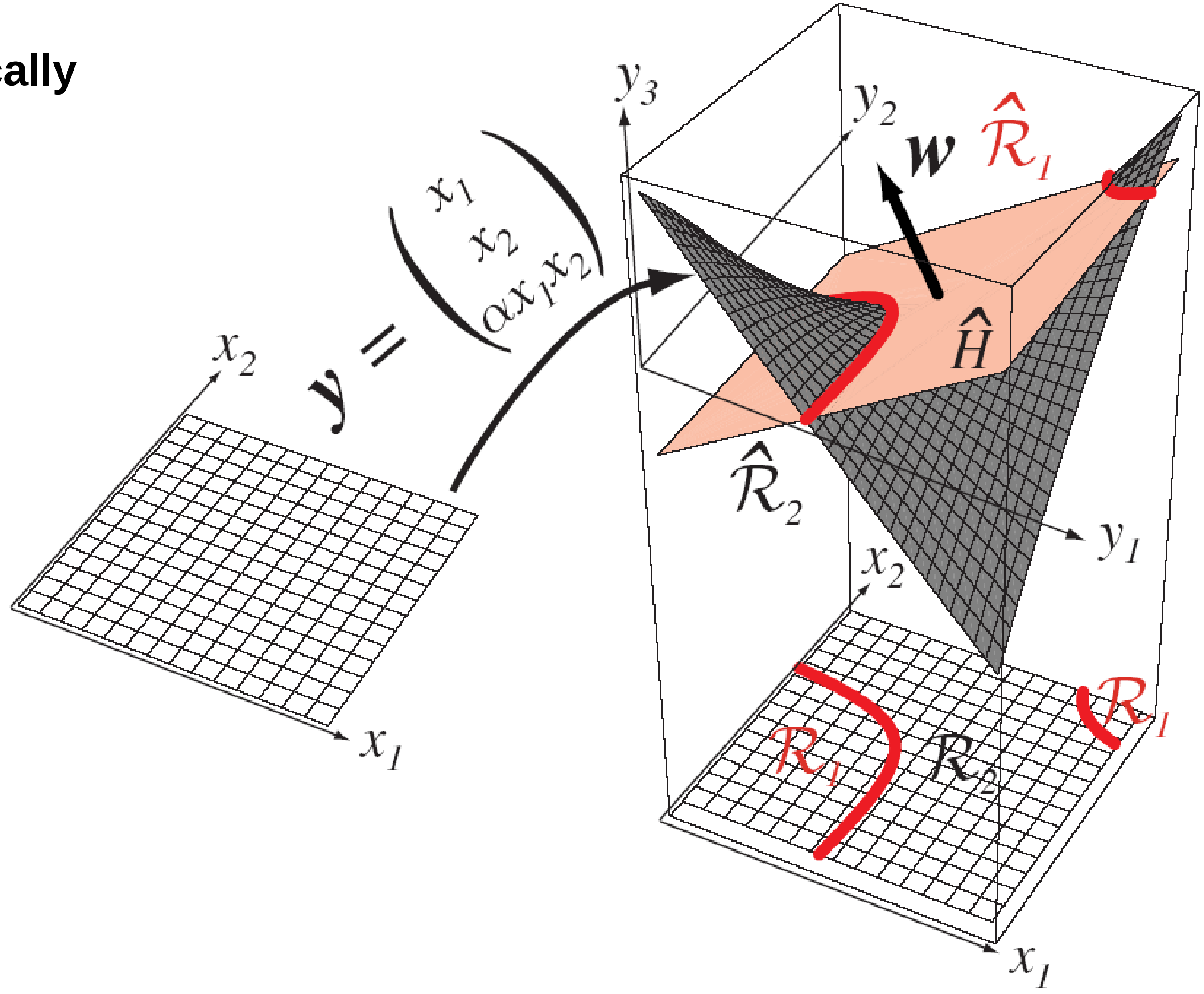
Example 2

- Let **x** = [x_1, x_2]^t in 2D space mapped to **y** in the 3D space:

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \\ \alpha x_1 x_2 \end{bmatrix}$$

- This transformation places all data in an *arbitrary surface* in 3D (see next page)
- The classifier in 2D space is a hyperbola that divides the space into two regions.
- It is equivalent to a plane in the 3D space!

Graphically



Moral: Data **nonlinearly** separable in *some* space
may become **linearly** separable in *another* space!

Example 3

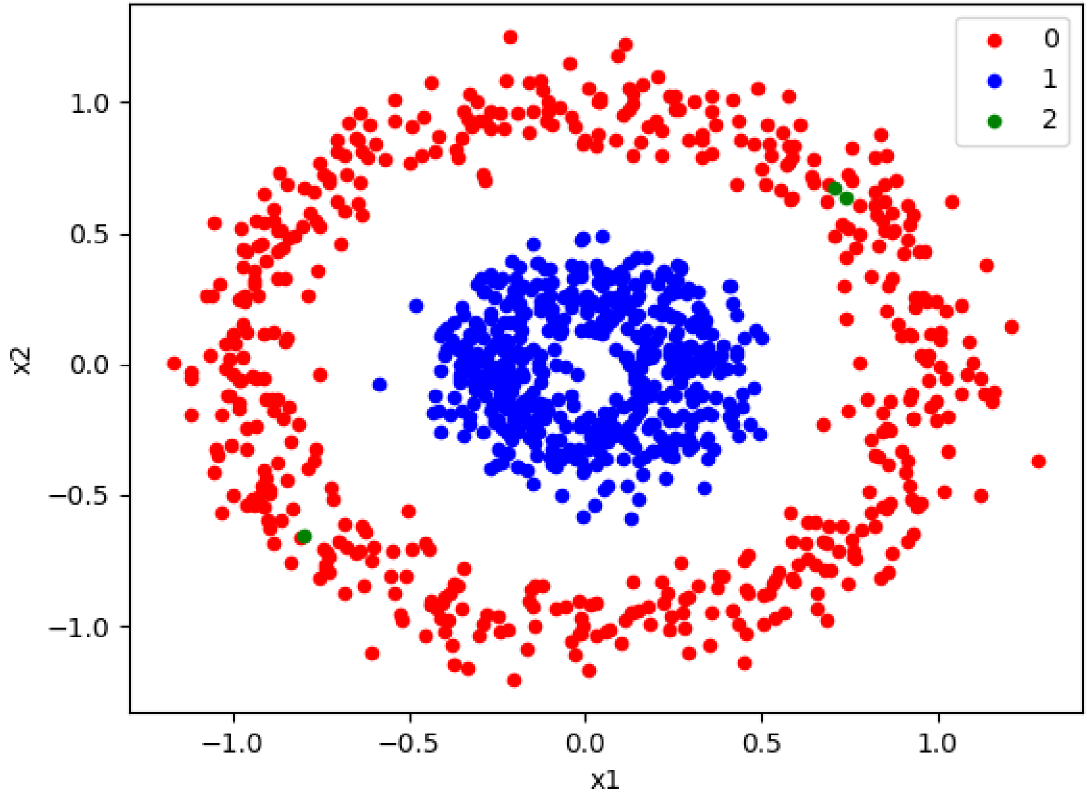
- Let **x** = $[x_1, x_2]^t$ in 2D space mapped to **y** in the 2D space:

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_1^2 + x_2^2 \end{bmatrix}$$

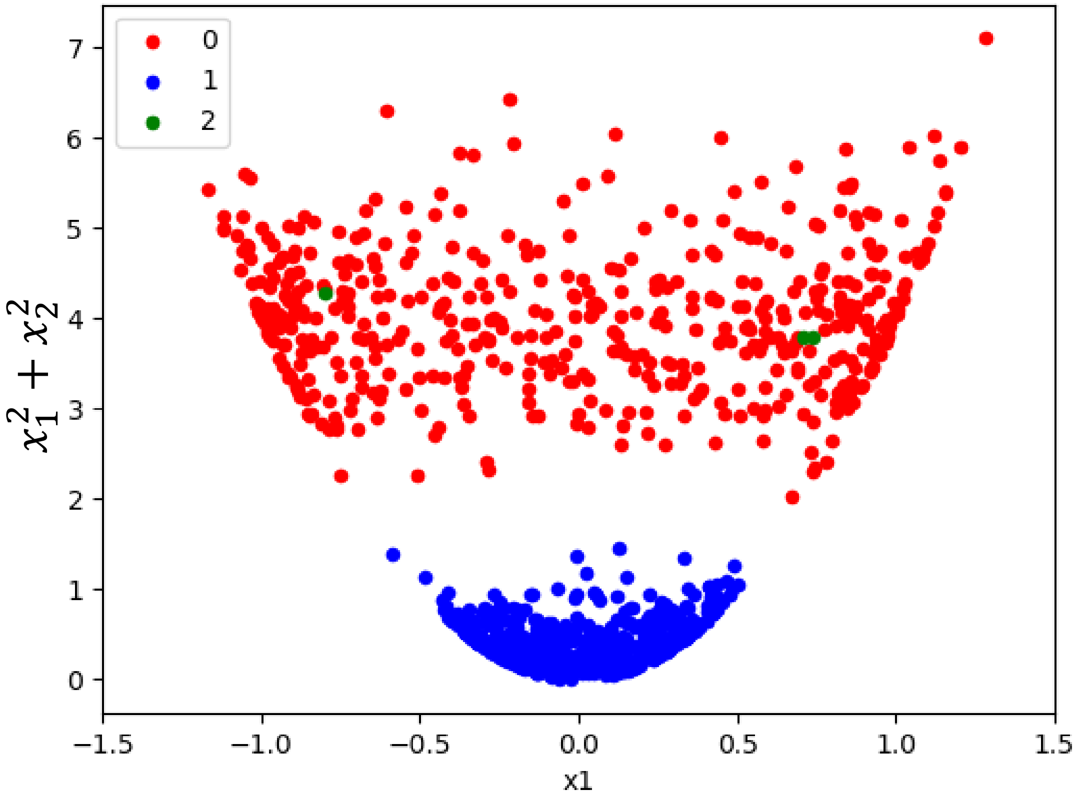
- This transformation places all data in an *arbitrary parabolic* form in 2D (see next page)
- The classifier in the original 2D space has a circular form (circle) to divide the space into two regions.
- It is equivalent to a line in the new 2D space!

Graphically

Original 2D space:

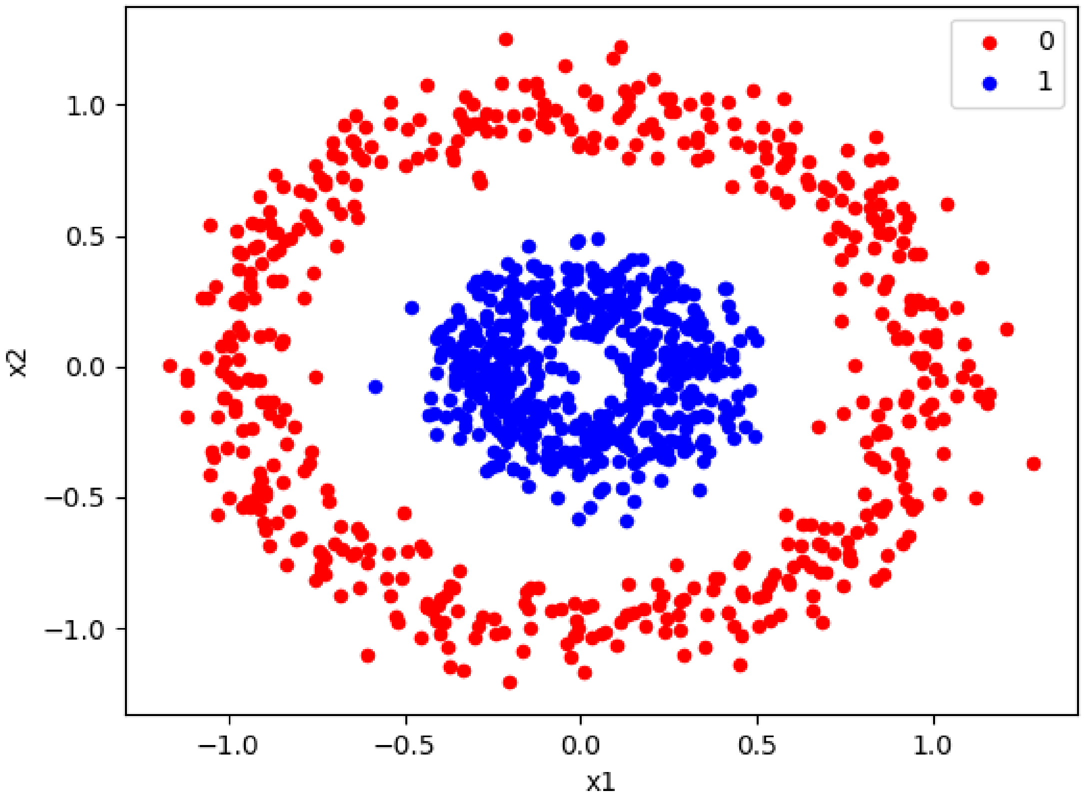


New 2D space:

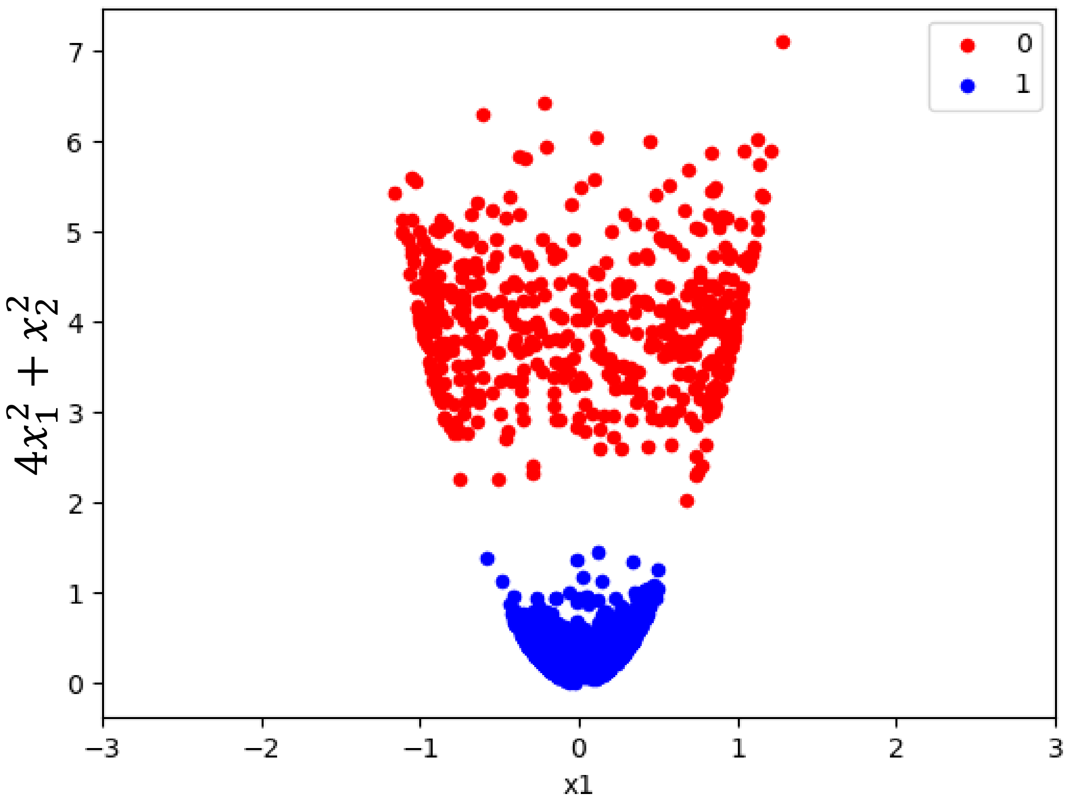


Graphically – cont'd

Original 2D space:



New 2D space:



Explicit Mapping

- Lets transform each vector $\mathbf{x}_k$ (a d-dim. vector)

  into a new one $\mathbf{y}_k$ in the $\hat{d}$-dim. space as:

  $$\mathbf{y}_k = \phi(\mathbf{x}_k)$$

  where, ideally, $\hat{d} \gg d$ and

  $\phi(\cdot)$ is an *arbitrary*, (typically) *nonlinear* function of $\mathbf{x}$

  called "phi function"

Note: It could be the case that ϕ is a linear function

- Then, derive the SVM classifier in the $\hat{d}$-dimensional space, and we are done
- However:
  - $\hat{d}$ is typically very large or it could be infinite!

Kernels

For the phi function:

y = $\boldsymbol{\phi}$(**x**), where $\boldsymbol{\phi}: \Re^d \rightarrow \Re^{\hat{d}}$

or $\mathbf{x} = [x_1, x_2, \ldots, x_d]^t \rightarrow \mathbf{y} = \boldsymbol{\phi}(\mathbf{x}) = [\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots, \phi_{\hat{d}}(\mathbf{x})]^t$

$\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots, \phi_{\hat{d}}(\mathbf{x})$ are *arbitrary functions* of **x**

… and the corresponding kernel is:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \boldsymbol{\phi}^t(\mathbf{x}_i)\, \boldsymbol{\phi}(\mathbf{x}_j) = \mathbf{y}_i^t\, \mathbf{y}_j$$

The kernel is a function of two vectors, and is defined as the inner product of these vectors

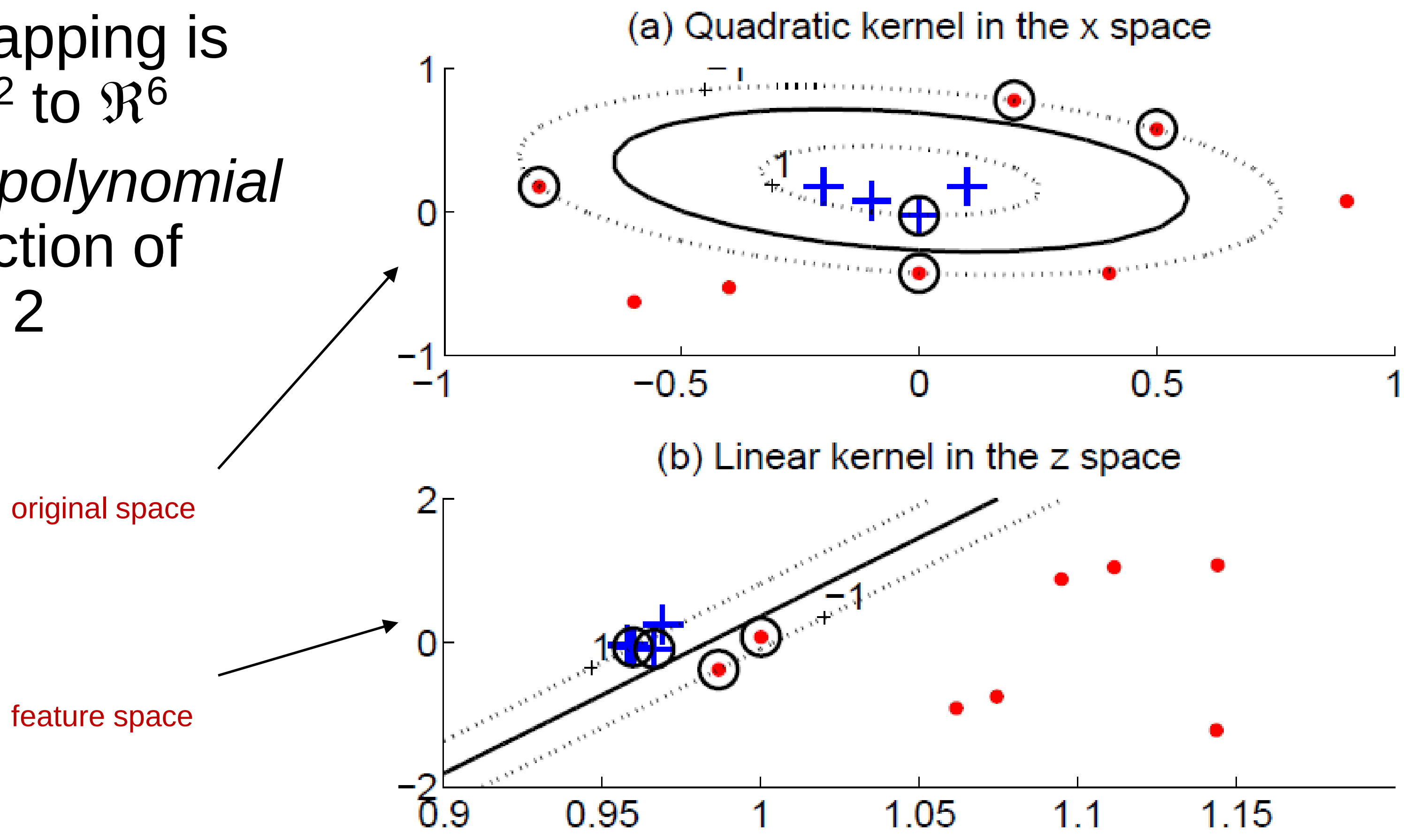
Notes:

- $\hat{d}$ can be even ∞
- Classification is nonlinear on $\Re^d$ but can linear on $\Re^{\hat{d}}$

Example 1

Polynomial phi function:

- Let $\mathbf{x}=[x_1,x_2]^t \rightarrow \mathbf{y}=\phi(\mathbf{x})=[x_1^2,x_2^2,\sqrt{2}x_1x_2,\sqrt{2}x_1,\sqrt{2}x_2,1]^t$ be a mapping
- This mapping is from $\Re^2$ to $\Re^6$
- Called *polynomial* phi function of degree 2



Kernels - examples

- <u>Linear (dot):</u>
  $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^t \mathbf{x}_j$
  (linear phi function)

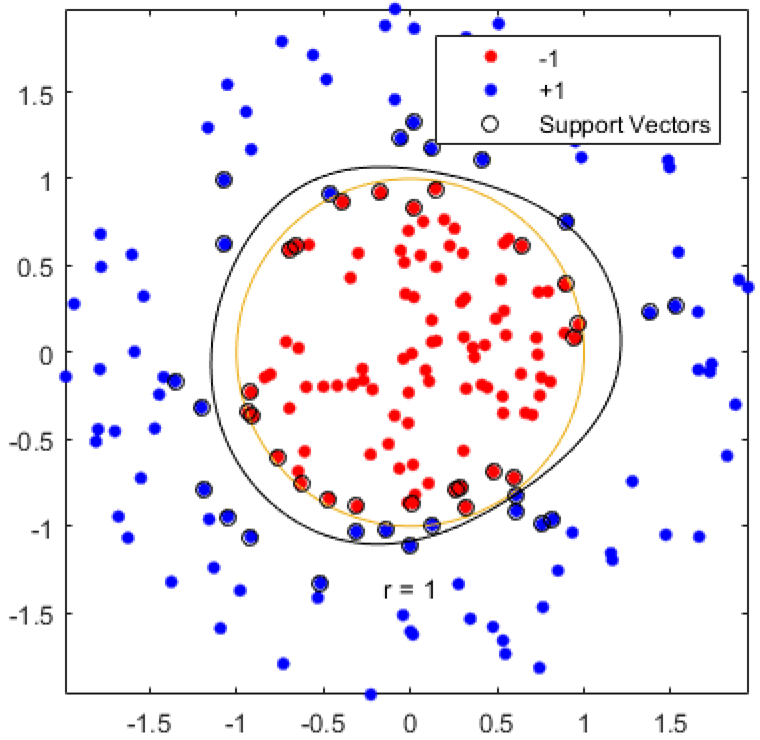
- <u>Polynomial:</u>
  $K(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i^t \mathbf{x}_j + 1)^q$, $q > 0$

  If $q = 2$: $(\mathbf{x}_i^t \mathbf{x}_j + 1)^2 = \mathbf{y}_i^t \mathbf{y}_j$
  where, for $d=2$: $\mathbf{y} = \boldsymbol{\phi}(\mathbf{x}) = [x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1]^t$

  (polynomial phi function)

Radial basis function (RBF):

$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\left\| \mathbf{x}_i - \mathbf{x}_j \right\|^2}{2\sigma^2} \right)$$



- Also known as *Gaussian* kernel
- σ controls the shape of the separating function
- σ is also known as “gamma” or γ

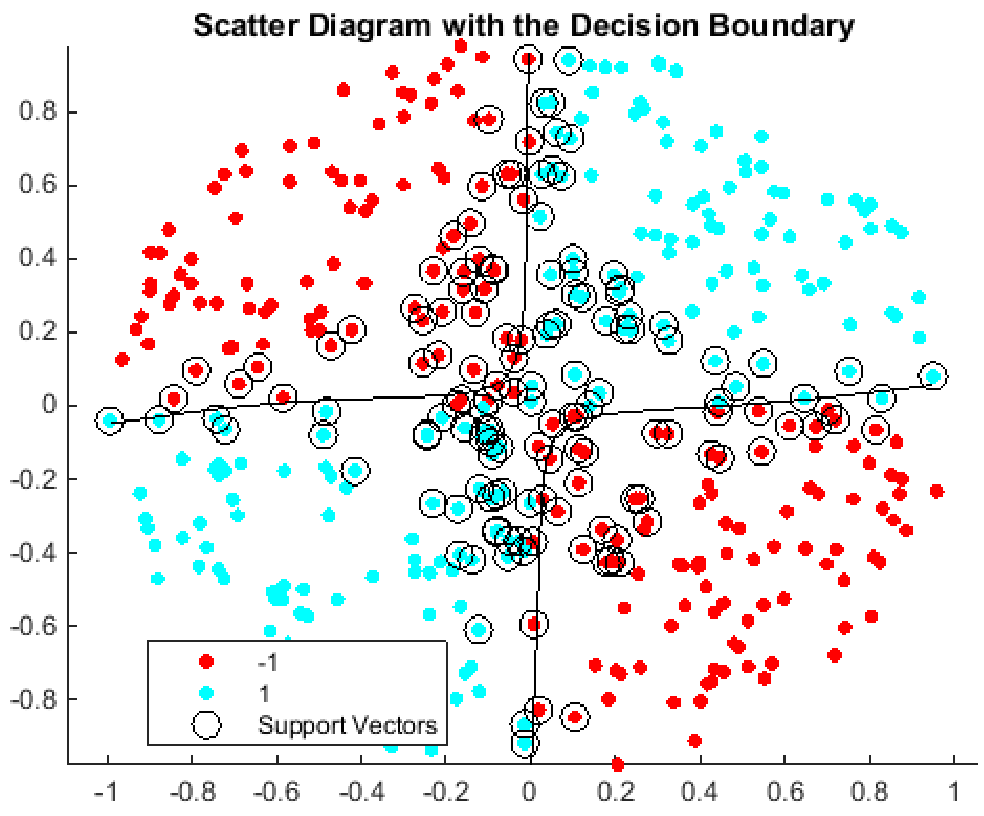
Hyperbolic tangent:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \tanh\left(\beta\, \mathbf{x}_i^t \mathbf{x}_j + \gamma\right)$$

for values of β and γ that satisfy Mercer´s conditions

(e.g. $\beta = 2$ and $\gamma = 1$)

Aka *sigmoid* kernel or *multilayer perceptron* (neural network)



Other kernels:

- Anova
- Fourier series
- Three-layer (or multi-layer) neural network
- Spline
- B-spline
- Additive
- Tensor product
- Graph kernels
- and more …

Mercer's Conditions

- Let $\mathbf{x} \in \Re^d$ and $\boldsymbol{\phi} : \Re^d \to \mathcal{H}$
  $\boldsymbol{\phi}$ has $\hat{d}$ components, $\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots, \phi_{\hat{d}}(\mathbf{x})$
  where *H* is a Hilbert space
  (a complete linear space + inner product)
- $K(\mathbf{x}, \mathbf{z}) = \boldsymbol{\phi}^t(\mathbf{x})\, \boldsymbol{\phi}(\mathbf{z})$ is a symmetric function
  that satisfies:
  $$\int K(\mathbf{x},\mathbf{z}) g(\mathbf{x}) g(\mathbf{z}) d\mathbf{x} d\mathbf{z} \geq \mathbf{0}$$
  for any $g(\mathbf{x})$, $\mathbf{x} \in \Re^d$ such that
  $$\int g^2(\mathbf{x}) d\mathbf{x} < \infty$$
- $K(.,.)$ is a positive semidefinite kernel
- For a finite set of vectors $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$,
  K is a positive semidefinite matrix

The Kernel Trick in SVM

- An advantage of using kernels:
  - The solution can be found without an explicit mapping to the higher dimensional space
- Recall: $$L(\boldsymbol{\alpha}) = \sum_{k=1}^{n} \alpha_k - \frac{1}{2} \sum_{k,j=1}^{n} \alpha_k \alpha_j z_k z_j \mathbf{y}_j^t \mathbf{y}_k \qquad (4)$$
- L function in terms of kernels:
$$L(\boldsymbol{\alpha}) = \sum_{k=1}^{n} \alpha_k - \frac{1}{2} \sum_{k,j=1}^{n} \alpha_k \alpha_j z_k z_j K(\mathbf{x}_j, \mathbf{x}_k) \qquad (5)$$
- subject to the following constraints:
$$\sum_{k=1}^{n} z_k \alpha_k = 0, \quad \text{and } \alpha_k \geq 0$$
- Obtain values of α_k
- n_s (support) vectors are those for which $\alpha_k \neq 0$

Classification

- With kernel:

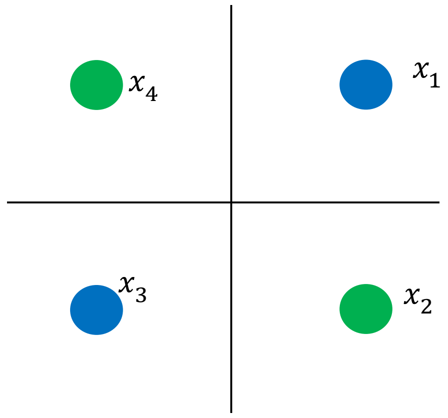
$g(\mathbf{x}) = \sum_{i=1}^{n_s} \alpha_i z_i K(\mathbf{x}_i, \mathbf{x})$ projects $\mathbf{x}$ onto the 1D space

$$\begin{aligned} g(\mathbf{x}) > 0 \quad &\text{decide} \quad \mathbf{x} \in \omega_1 \\ \text{otherwise } &\text{decide} \quad \mathbf{x} \in \omega_2 \end{aligned}$$

- With explicit mapping:

$$\begin{aligned} \mathbf{a}^t \mathbf{y} = \mathbf{a}^t \boldsymbol{\phi}(\mathbf{x}) > 0 \ &\text{decide} \quad \mathbf{x} \in \omega_1 \\ \text{otherwise } &\text{decide} \quad \mathbf{x} \in \omega_2 \end{aligned}$$

Example



- The XOR classification problem
- 4 samples:

  $\mathbf{x}_1 = [1,1]^t$ and $\mathbf{x}_3 = [-1,-1]^t \in \omega_1$

  $\mathbf{x}_2 = [1,-1]^t$ and $\mathbf{x}_4 = [-1,1]^t \in \omega_2$

- Lets use a *degree*-2 polynomial phi-function and explicit mapping
- So, mapping from 2D to 6D:

$$\mathbf{y} = \boldsymbol{\phi}(\mathbf{x}) = \left[1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2\right]^t$$

- Eq. (4) results in:

$$L(\boldsymbol{\alpha}) = \sum_{k=1}^{4} \alpha_k - \frac{1}{2} \sum_{k,j=1}^{4} \alpha_k \alpha_j z_k z_j \mathbf{y}_j^t \mathbf{y}_k \qquad (6)$$

subject to:

$$\sum_{k=1}^{4} \alpha_k z_k = 0, \quad \text{and } \alpha_k \geq 0$$

Expanding:

$$L(\boldsymbol{\alpha}) = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 - \frac{1}{2}(9\alpha_1^2 - 2\alpha_1\alpha_2 - 2\alpha_1\alpha_3 + 2\alpha_1\alpha_4$$

$$+ 9\alpha_2^2 + 2\alpha_2\alpha_3 - 2\alpha_1\alpha_3 + 2\alpha_2\alpha_4 + 9\alpha_3^2 - 2\alpha_3\alpha_4 + 9\alpha_4^2)$$

subject to:

$$\alpha_1 - \alpha_2 + \alpha_3 - \alpha_4 = 0, \ \alpha_k \geq 0, \ k = 1,2,3,4$$

Solution:

- Optimal values for the undetermined multipliers:

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \frac{1}{8} \neq 0$$

- Optimal vector **a** given by:

$$\mathbf{a} = \sum_{k=1}^{4} \alpha_k z_k \boldsymbol{\phi}(\mathbf{x}_k) = [0,0,0,\frac{1}{\sqrt{2}},0,0]$$

- In this example, *all* 4 training samples are support vectors

- So, the *optimal* hyperplane is given by:

$$\mathbf{a}^t \boldsymbol{\phi}(\mathbf{x}) = 0, \quad \text{or}$$

$$[0,0,0,\frac{1}{\sqrt{2}},0,0]\left[1,\sqrt{2}x_1,\sqrt{2}x_2,\sqrt{2}x_1x_2,x_1^2,x_2^2\right]^t = 0$$

- Solving for **y**, we have:

$$x_1 x_2 = 0$$

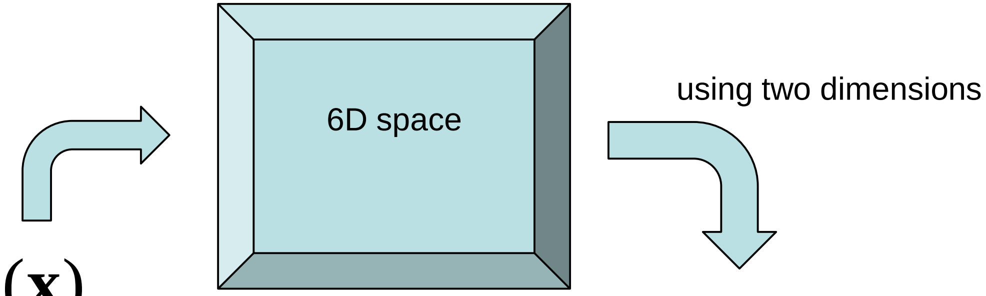
- The margin *b* is given by:

$$b = 1/\|\mathbf{a}\| = \sqrt{2}$$

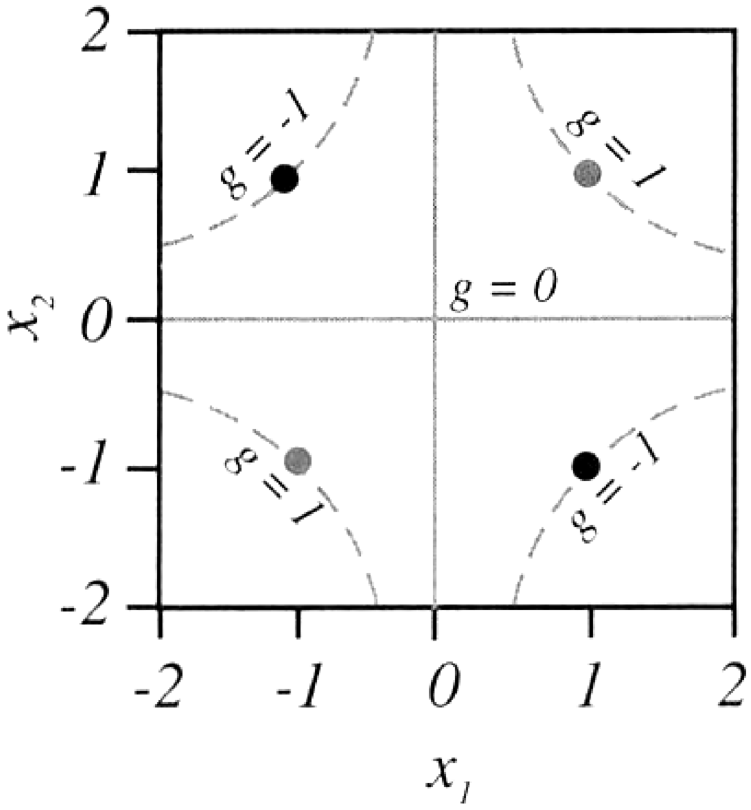
Notes:

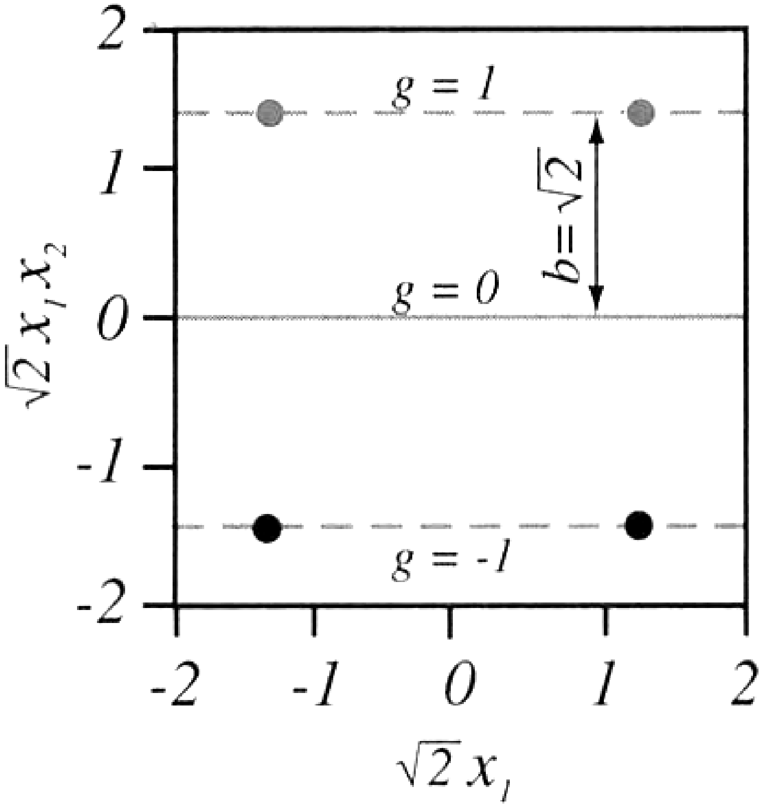
- A 2D representation/classifier is good enough
- Mapping to 6D not required at classification time
- Even a 1D classifier is enough!

The XOR problem graphically



$$\mathbf{y} = \phi(\mathbf{x})$$





Lets classify:

$$\mathbf{x} = \begin{bmatrix} 0.5 & 0.5 \end{bmatrix}$$

$$\boldsymbol{\phi}(\mathbf{x}) = \mathbf{y} = [1, \sqrt{2}(0.5), \sqrt{2}(0.5), \sqrt{2}(0.5)(0.5), 0.25, 0.25]^t$$

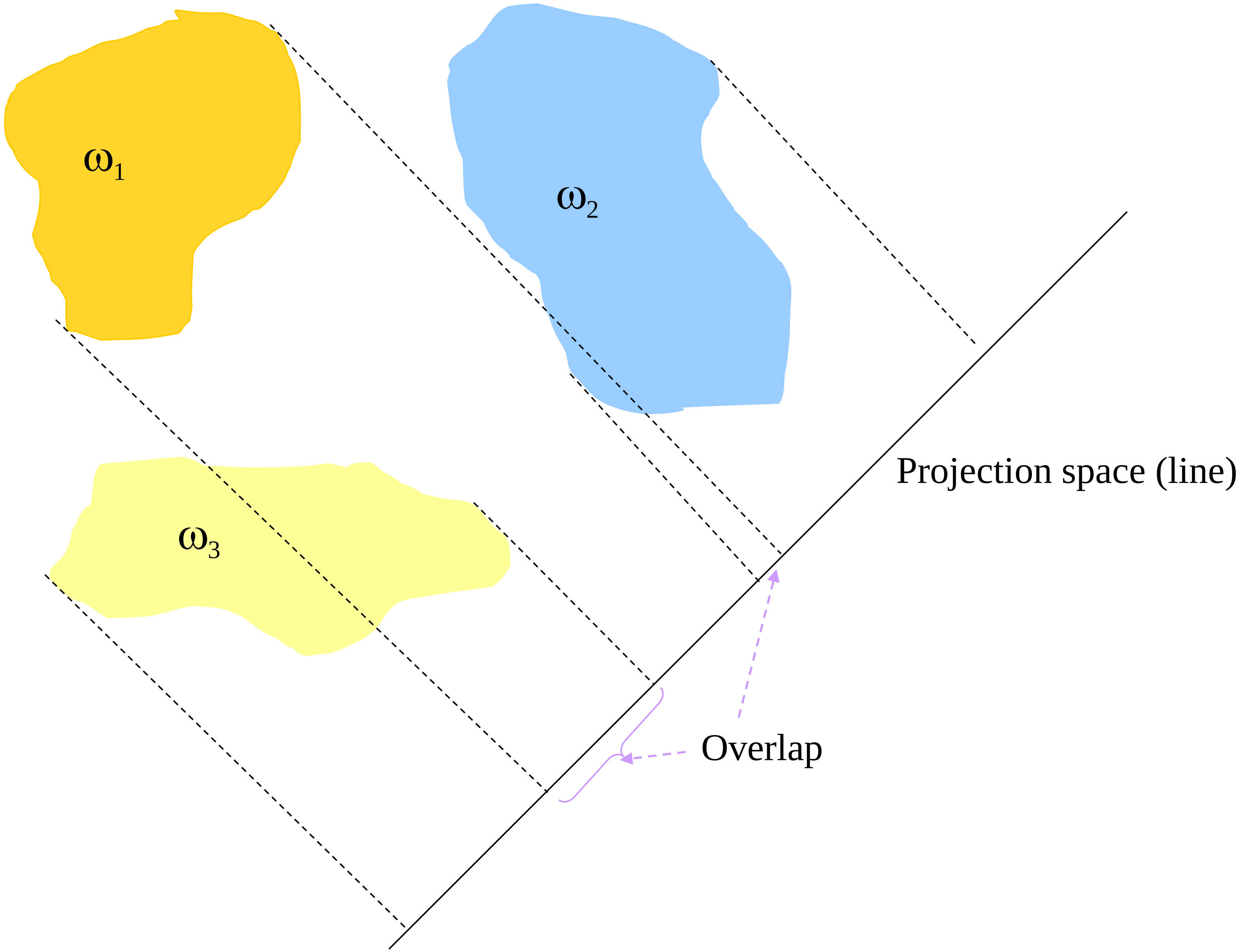
$$\mathbf{a}^t\mathbf{y} = [0,0,0,\frac{1}{\sqrt{2}},0,0]\begin{bmatrix} 1 \\ \sqrt{2}(0.5) \\ \sqrt{2}(0.5) \\ \sqrt{2}(0.5)(0.5) \\ 0.25 \\ 0.25 \end{bmatrix} = \frac{1}{\sqrt{2}}\sqrt{2}(0.5)(0.5)$$

$$\Rightarrow \mathbf{a}^t\mathbf{y} = 0.25 > 0 \Rightarrow \text{ decide } \mathbf{x} \in \omega_1$$

The Multi-Class Case

- Assume we have *c* classes: $\omega_1, \omega_2, \ldots, \omega_c$
- Various approaches:
  - All at once
  - One against all
  - One against one
  - Linear machine: Divide the space into *c* regions

All at once



One against all

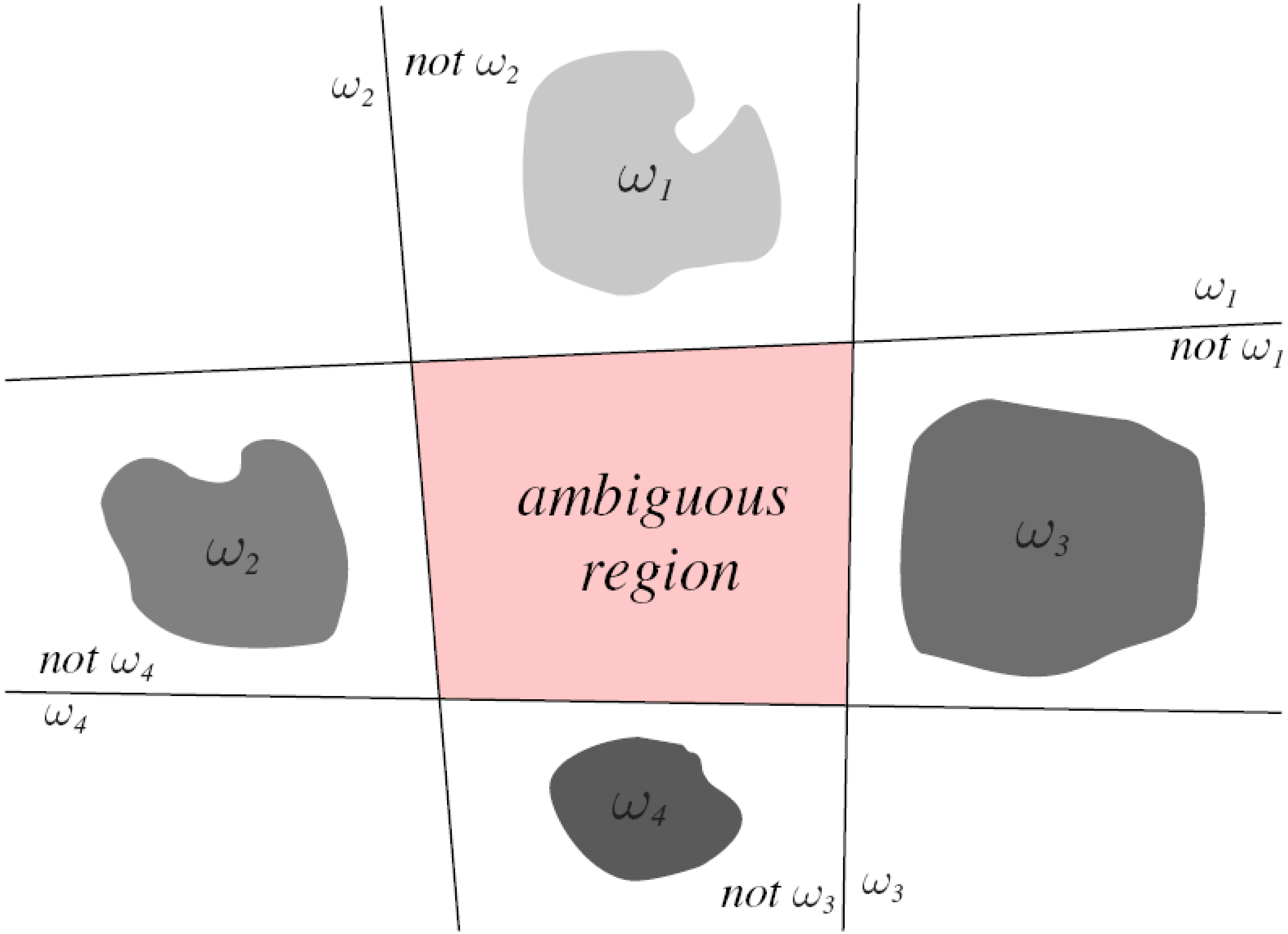
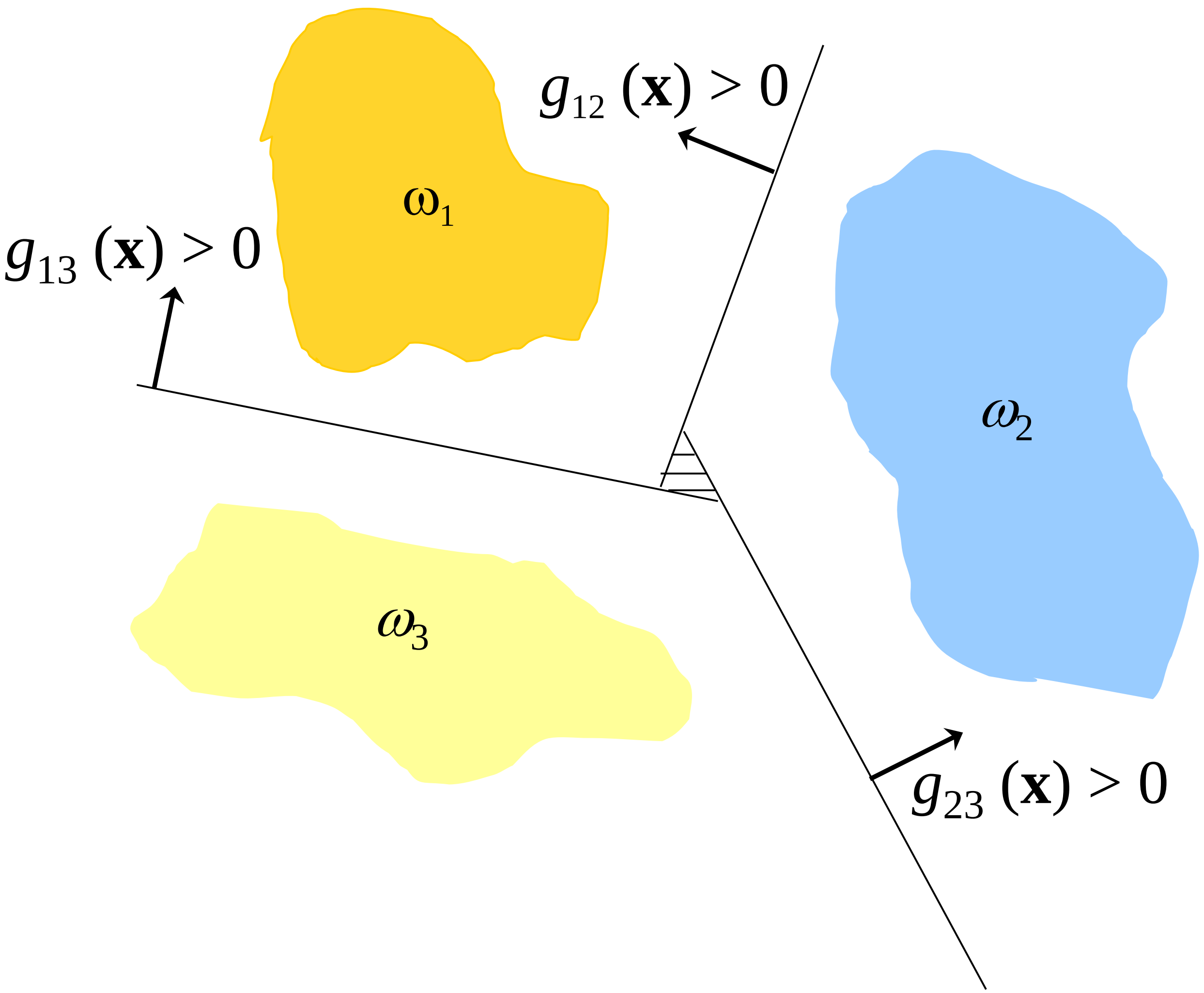


Image from Duda et al.

One against one



Tools for SVM

- **Resources:**
  - Kernel machines: http://www.kernel-machines.org/
  - SVMs: www.support-vector-machines.org
- **Tools:**
  - LibSVM: Interface with various languages including Matlab/Octave (http://www.csie.ntu.edu.tw/~cjlin/libsvm/)
  - WEKA (by installing LibSVM or others)
  - Scikit: SVM/SVC (http://scikit-learn.org/stable/modules/svm.html)
  - SVM Light: http://svmlight.joachims.org/
  - OSU SVM: http://sourceforge.net/projects/svm/)
- **In Matlab:**
  - Bioinformatics toolbox http://www.mathworks.com/help/toolbox/bioinfo/ref/svmtrain.html
  - Syntax:
    - SVMStruct = svmtrain(Training,Group)
    - SVMStruct = svmtrain(Training,Group,Name,Value)

SVM in Scikit

- Available as part of the standard APIs
- Support two-class, multi-class and one-class classification
- Allows for different kernels: linear, polynomial, RBF, sigmoid, and custom kernels
- Multi-class implements the one-against-one approach
- Can deal with unbalanced classification problems via weight parameters
- Supports regression and density estimation
- Documentation:
  - http://scikit-learn.org/stable/modules/svm.html

Linear Classifiers in Scikit

- Linear Discriminant Analysis (LDA)
  - https://scikit-learn.org/0.16/modules/generated/sklearn.lda.LDA.html
- Linear and Quadratic classifiers in Scikit:
  - https://scikit-learn.org/stable/modules/lda_qda.html
- Mean square error (MSE) for regression
  - https://scikit-learn.org/stable/modules/generated/sklearn.metrics.mean_squared_error.html
- Perceptron
  - https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.Perceptron.html
- Multi-layer Perceptron (no GPU support)
  - https://scikit-learn.org/stable/modules/neural_networks_supervised.html

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