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Machine Learning

Chapter 5

Linear Discriminant Functions

Contents

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Decision-Making Approaches

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- Probabilistic Approaches
  - Based on the underlying *probability densities* of training sets.
  - For example, *Bayesian decision rule* assumes that the underlying probability densities were available.
- Discriminating Approaches
  - Assume we know the proper *forms for the discriminant functions*.
  - Use the samples to estimate the values of *parameters of the classifier*.

Discriminant Function

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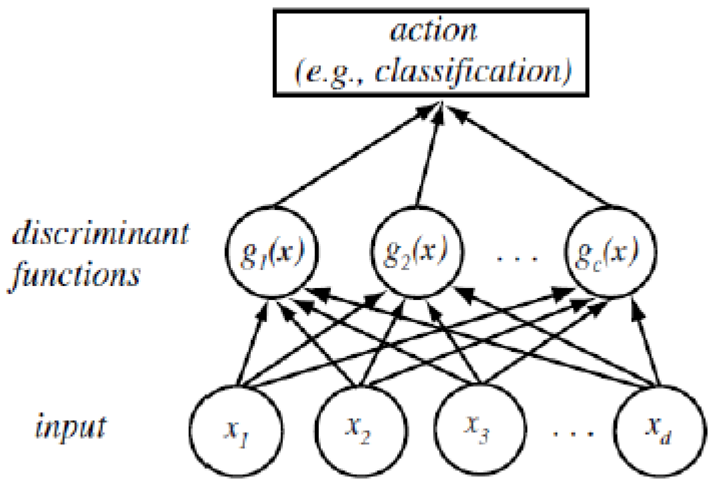
$$g_i : R^d \rightarrow R(\mathbf{x}) \qquad (1 \le i \le c)$$

- Useful way to represent classifier
- One function per category
- Decide ω_i, if

$$g_i(x) > g_j(x) \quad \textit{for all } j \neq i$$



Linear Discriminant Functions

$$g_i(\mathbf{x}) = \underline{\mathbf{w}_i^T}\mathbf{x} + \underline{w_{i0}}$$

Weight vector

Bias/threshold

- Easy for *computing*, *analysis* and *learning*.
- Linear classifiers are attractive candidates for *initial, trial classifier*.
- Learning by minimizing a *criterion function*, e.g., training error.

Difficulty: a small training error does not guarantee a small test error.

Linear Discriminant Functions

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- Two-category case

$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 \Rightarrow \begin{cases} \text{Decide } \omega_1 \text{ if } g(\mathbf{x}) > 0 \\ \text{Decide } \omega_2 \text{ if } g(\mathbf{x}) < 0 \end{cases}$$

$$\Updownarrow$$

$$\begin{cases} g_1(\mathbf{x}) = \mathbf{w}_1^T\mathbf{x} + w_{10} \\ g_2(\mathbf{x}) = \mathbf{w}_2^T\mathbf{x} + w_{20} \end{cases}$$

Thus, it is suffices to consider only d+1 parameters (w and d) instead of 2(d+1) parameters under two-category case.

Linear Discriminant Functions

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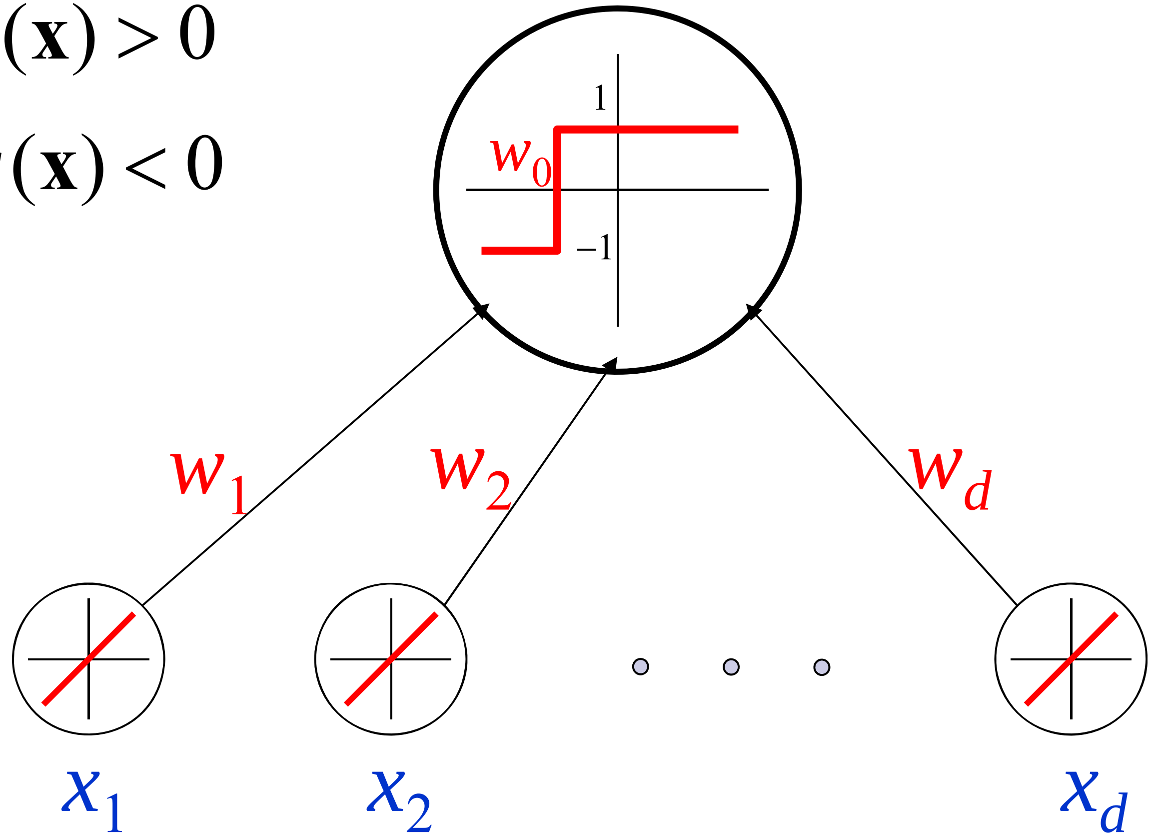
- Two-category case: Implementation

$$\begin{cases} \text{Decide } \omega_1 \text{ if } g(\mathbf{x}) > 0 \\ \text{Decide } \omega_2 \text{ if } g(\mathbf{x}) < 0 \end{cases}$$



Linear Discriminant Functions

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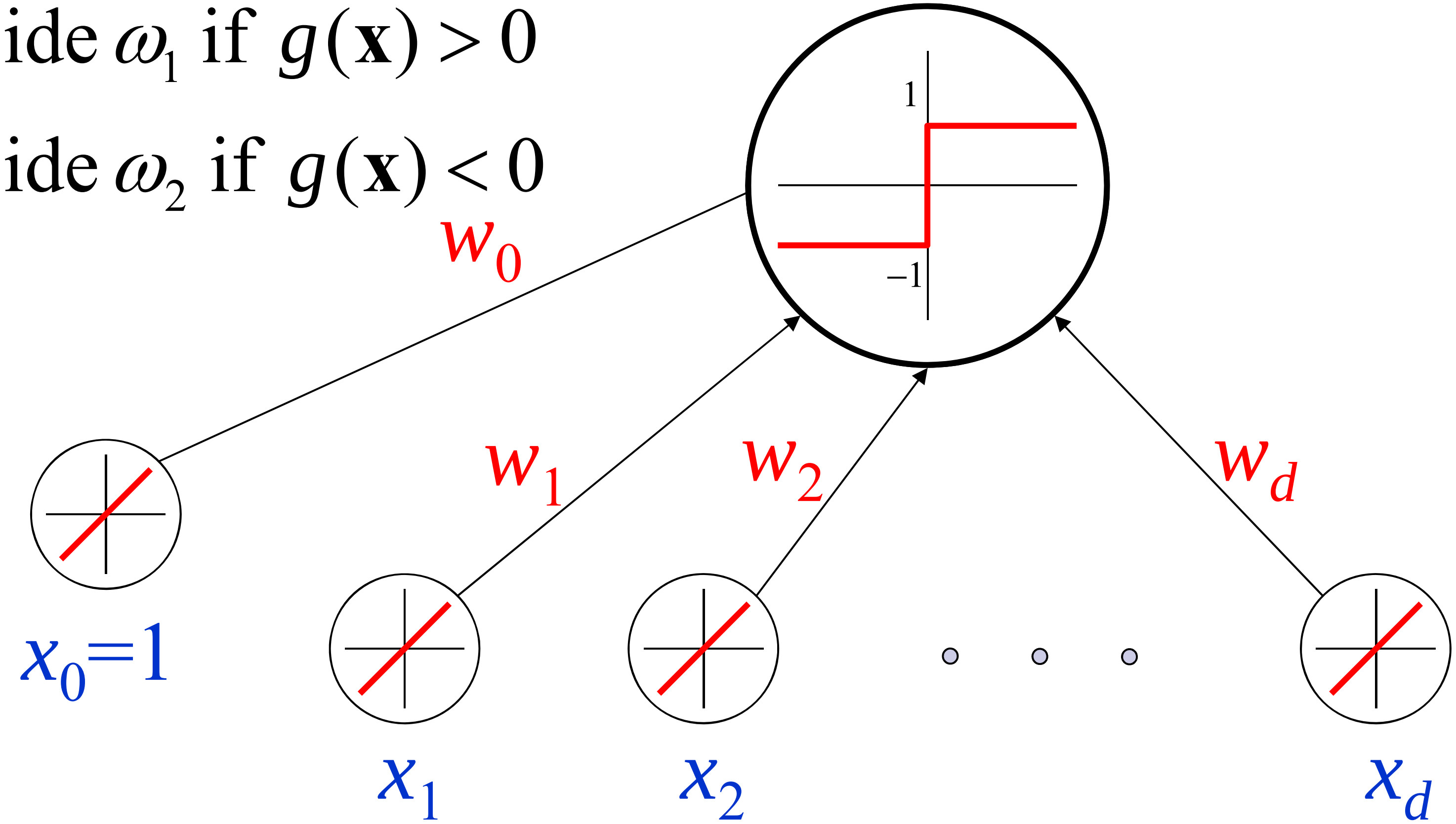
- Two-category case: Implementation

$$\begin{cases} \text{Decide } \omega_1 \text{ if } g(\mathbf{x}) > 0 \\ \text{Decide } \omega_2 \text{ if } g(\mathbf{x}) < 0 \end{cases}$$



Decision Surface

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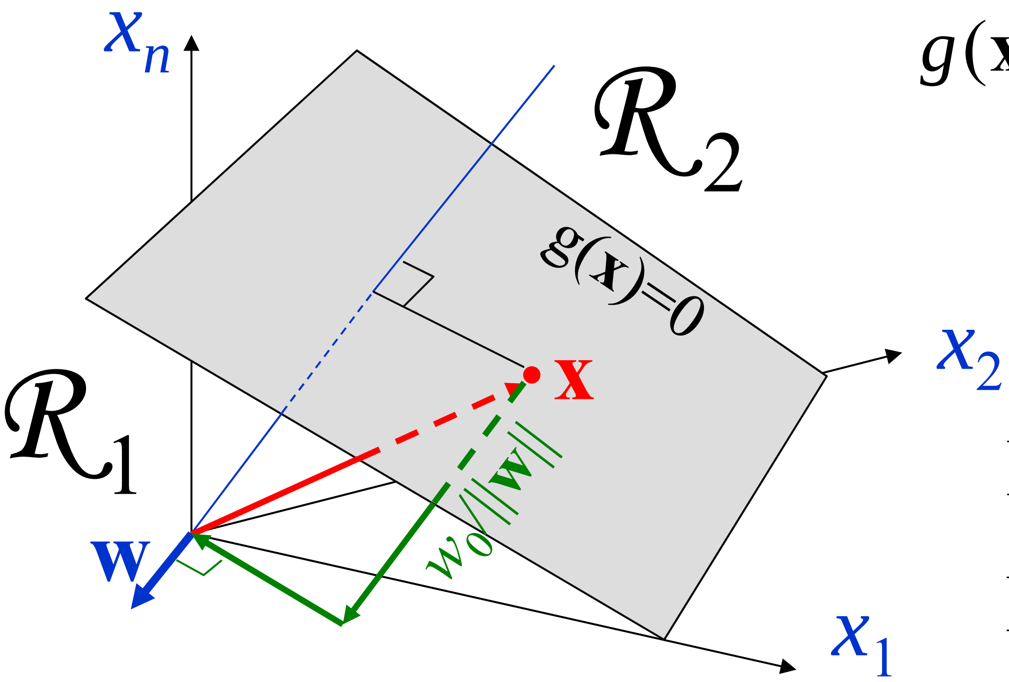
$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$$

$$g(\mathbf{x}) = 0$$



$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + \frac{\mathbf{w}^T\mathbf{w}}{||\mathbf{w}||^2} w_0 = 0$$

$$\mathbf{w}^T\left(\mathbf{x} + \frac{w_0}{||\mathbf{w}||}\frac{\mathbf{w}}{||\mathbf{w}||}\right) = 0$$

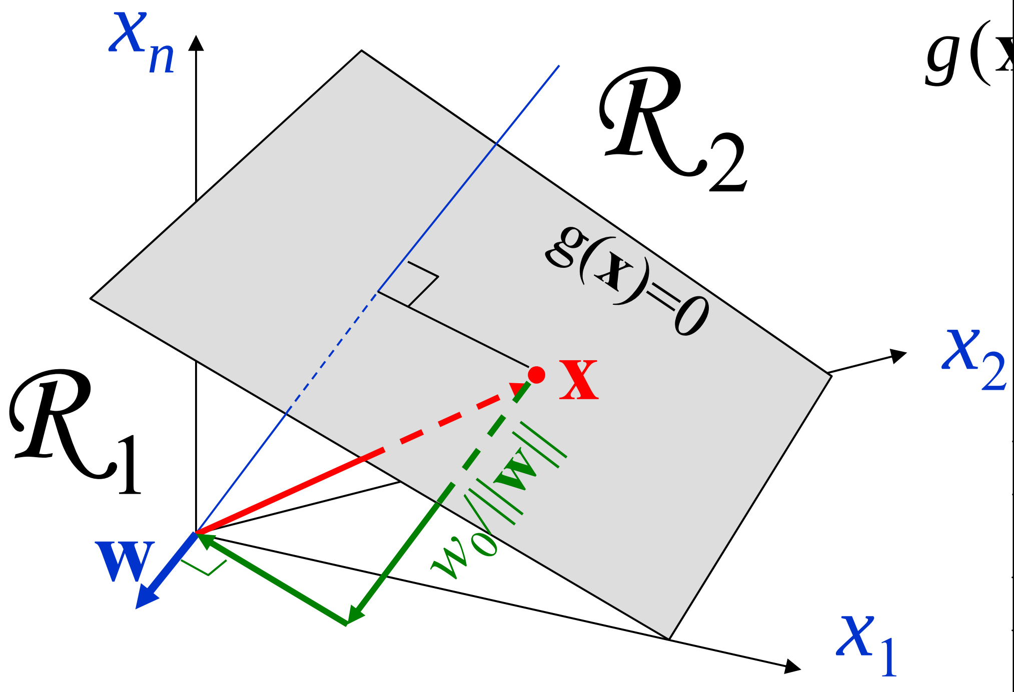
Decide ω_1 if $g(\mathbf{x}) > 0$

Decide ω_2 if $g(\mathbf{x}) < 0$

Decision Surface

MIMA

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



1. A linear discriminant function divides the feature space by a *hyperplane*.

2. The orientation of the surface is determined by the normal vector **w**.

3. The location of the surface is determined by the bias w_0.

Augmented Space

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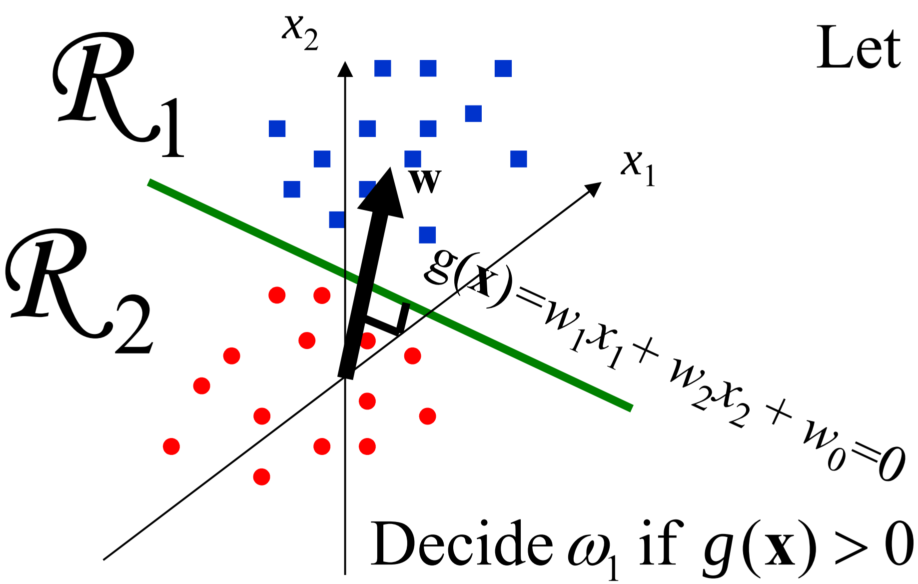
$$g(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0$$

d-dimension

Let $\mathbf{a} = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix} = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_d \end{bmatrix}$ $\quad \mathbf{y} = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_d \end{bmatrix}$

$(d+1)$-dimension



Decision surface: $\mathbf{a}^T\mathbf{y} = 0$

Decide ω_1 if $g(\mathbf{x}) > 0$

Decide ω_2 if $g(\mathbf{x}) < 0$

Decide ω_1 if $\mathbf{a}^T\mathbf{y} > 0$

Decide ω_2 if $\mathbf{a}^T\mathbf{y} < 0$

Augmented Space

$g(\mathbf{x}) = \mathbf{w}$ ...

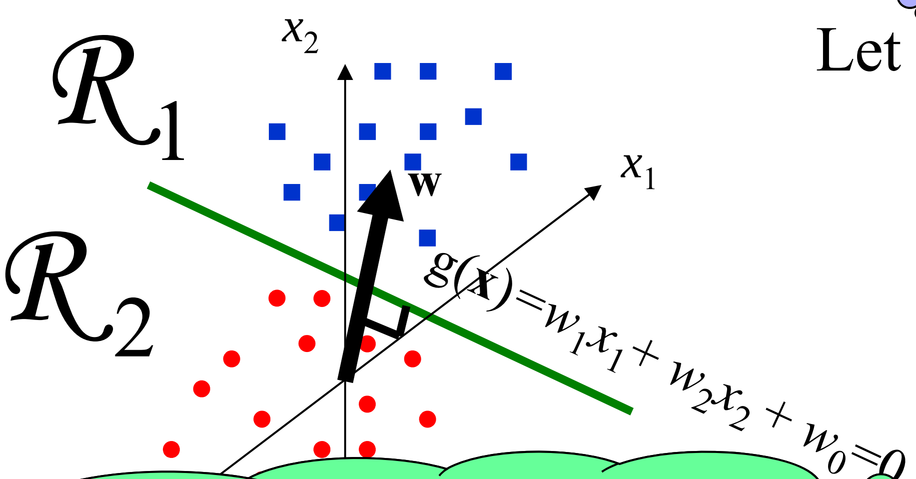
Augmented weight vector

Augmented feature vector

...dimension

Let $\mathbf{a} = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix} = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_d \end{bmatrix}$ $\quad \mathbf{y} = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_d \end{bmatrix}$

$(d+1)$-dimension



Pass through the origin of augmented space

... ω_2 if $g(\mathbf{x}) < 0$

Decision surface: $\mathbf{a}^T \mathbf{y} = 0$

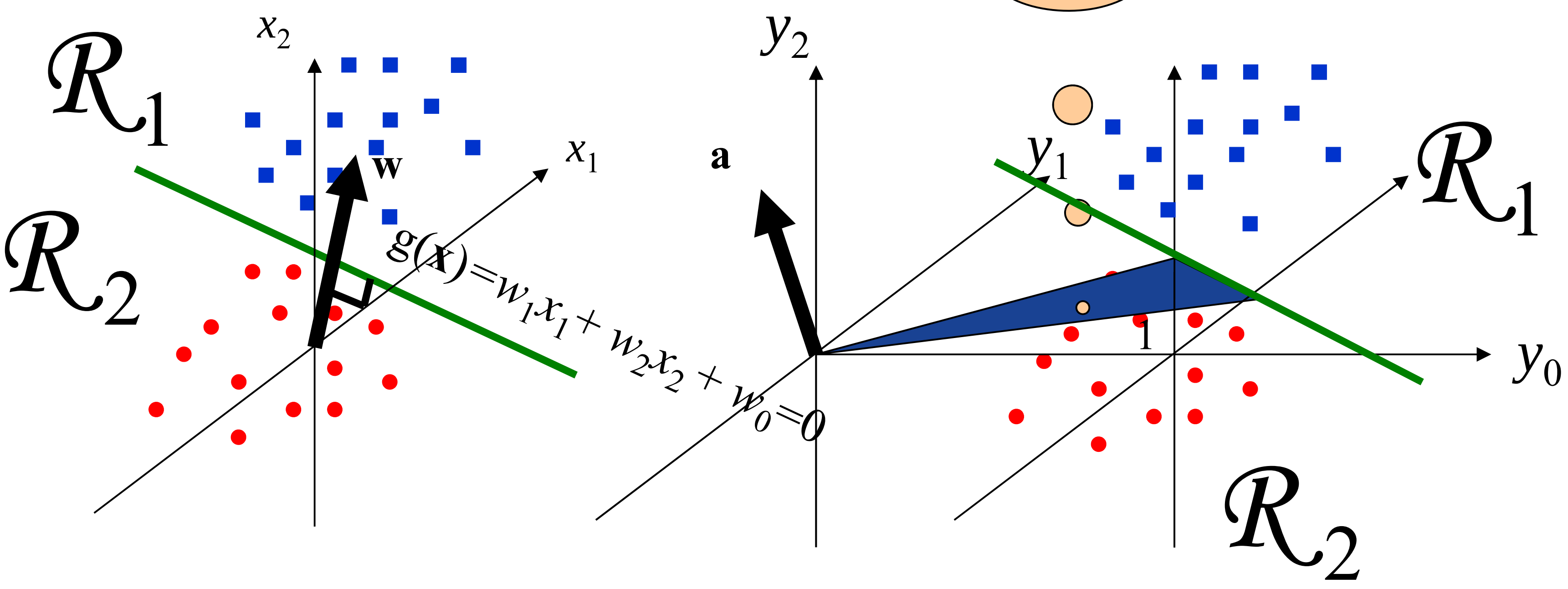
Decide ω_1 if $\mathbf{a}^T \mathbf{y} > 0$

Decide ω_2 if $\mathbf{a}^T \mathbf{y} < 0$

Augmented Space

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

$$\mathbf{a}\mathbf{y} = 0$$



Augmented Space

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- Decision surface in feature space:

$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0 = 0$$

Pass through the origin only when $w_0=0$.

- Decision surface in augmented space:

$$g(\mathbf{x}) = \mathbf{a}^T \mathbf{y} = 0$$

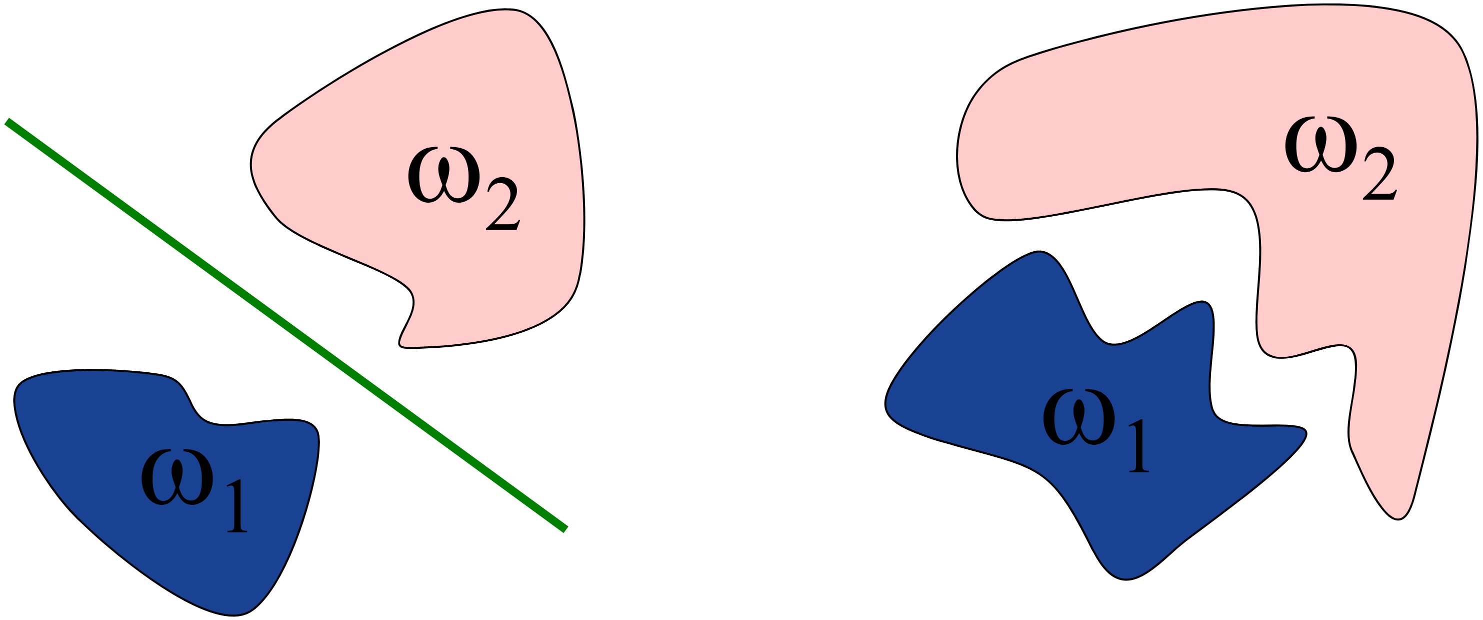
Always pass through the origin.

$$\mathbf{a} = \begin{bmatrix} w_0 \\ \mathbf{w} \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}$$

By using this mapping, the problem of finding weight wector w and threshold w0 is reduced to finding a single vector a.

Linear Separability

- Two-Category Case



Linearly Separable　　　　*Not Linearly Separable*

Linear Separability

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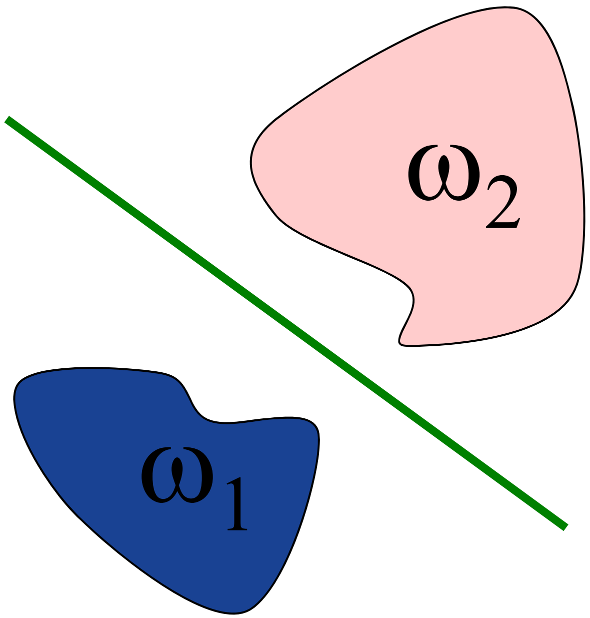
- Two-Category Case



Linearly Separable

Given a set of samples $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n$, some labeled ω_1 and some labeled ω_2,

if there exists a vector $\mathbf{a}$ such that

$$\mathbf{a}^T\mathbf{y}_i > 0 \quad \text{if } \mathbf{y}_i \text{ is labeled } \omega_1$$

$$\mathbf{a}^T\mathbf{y}_i < 0 \quad \text{if } \mathbf{y}_i \text{ is labeled } \omega_2$$

then the samples are said to be

Linearly Separable

Linear Separability

MIMA

- Two-Category Case

Withdrawing all labels of samples and replacing the ones labeled ω_2 by their *negatives*, it is equivalent to find a vector $\mathbf{a}$ such that

$$\mathbf{a}^T \mathbf{y}_i > 0 \quad \forall i$$

Given a set of samples $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n$, some labeled ω_1 and some labeled ω_2,

if there exists a vector $\mathbf{a}$ such that

$$\mathbf{a}^T \mathbf{y}_i > 0 \qquad \text{if } \mathbf{y}_i \text{ is labeled } \omega_1$$

$$\mathbf{a}^T \mathbf{y}_i < 0 \qquad \text{if } \mathbf{y}_i \text{ is labeled } \omega_2$$

then the samples are said to be

Linearly Separable

Solution Region in Feature Space

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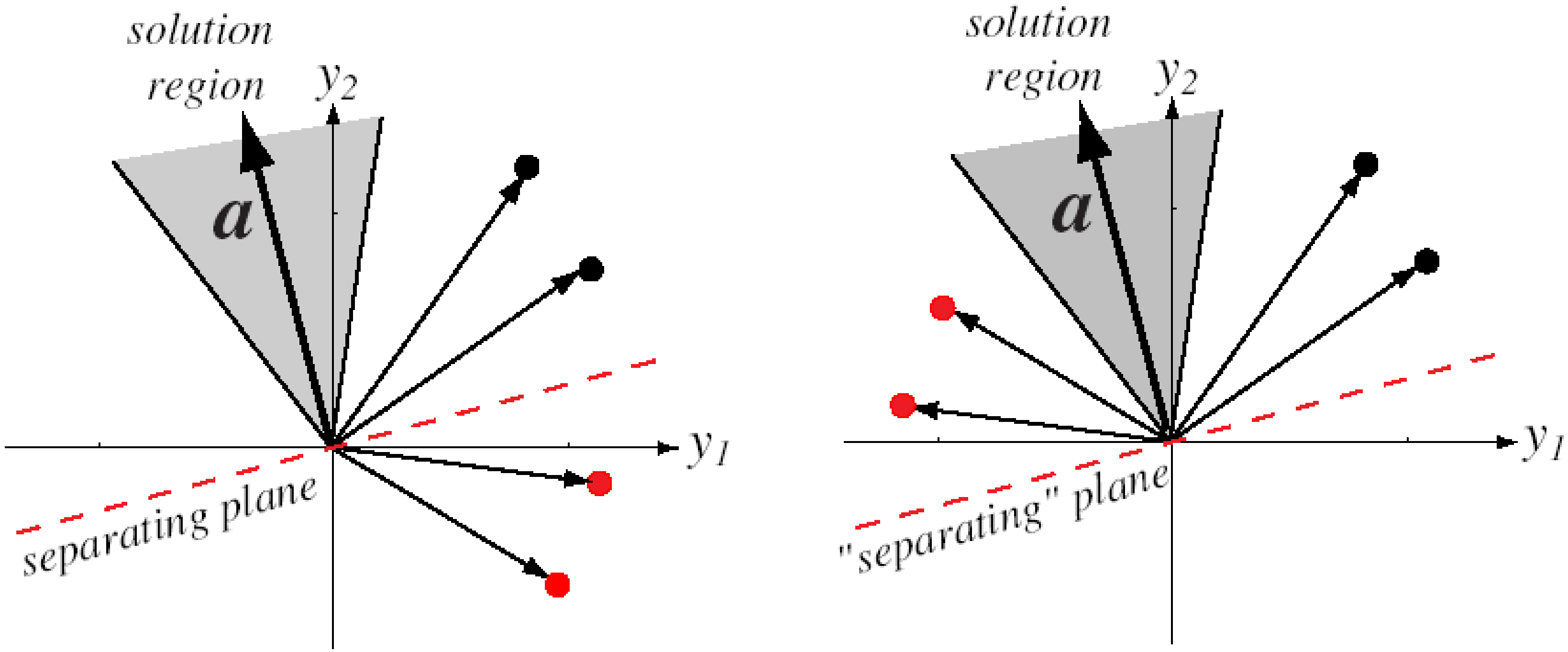
Separating Plane: $a_1 y_1 + a_2 y_2 + \Lambda + a_n y_n = 0$

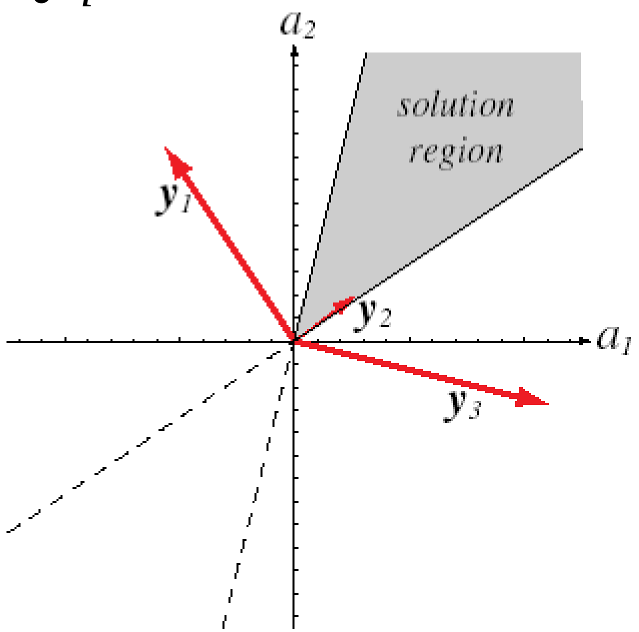


Normalized Case

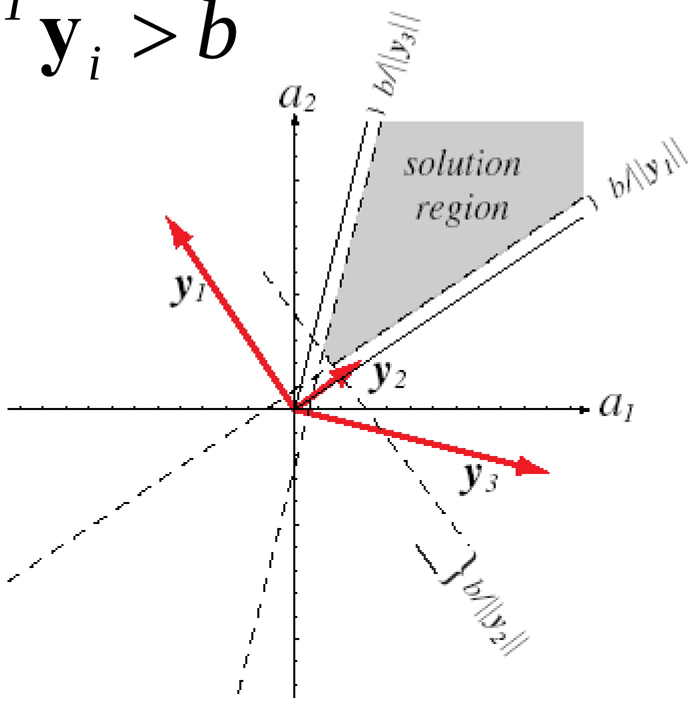
Solution Region in Weight Space

- Solution Region in Weight Space

$\mathbf{a}^T \mathbf{y}_i > 0$



$\mathbf{a}^T \mathbf{y}_i > b$



Shrink solution region by margin $b / \|\mathbf{y}_i\|, \quad b > 0$

Linear Discriminant Functions

How to learn the weights?

Criterion Function

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- To facilitate learning, we usually define a scalar *criterion function*.
- It usually represents the *penalty* or *cost* of a solution.
- Our goal is to *minimize* its value.
- *Function optimization*.

$$J(\mathbf{w}, b) = -\sum_{i=1}^{n} \mathtt{sign}[\omega_i \cdot g(\mathbf{x}_i)]$$

$$J(\mathbf{w}, b) = -\sum_{i=1}^{n} \omega_i \cdot g(\mathbf{x}_i)$$

$$J(\mathbf{w}, b) = \sum_{i=1}^{n} (g(\mathbf{x}_i) - \omega_i)^2$$

......

How to minimize the criterion function?

Gradient Decent Algorithm

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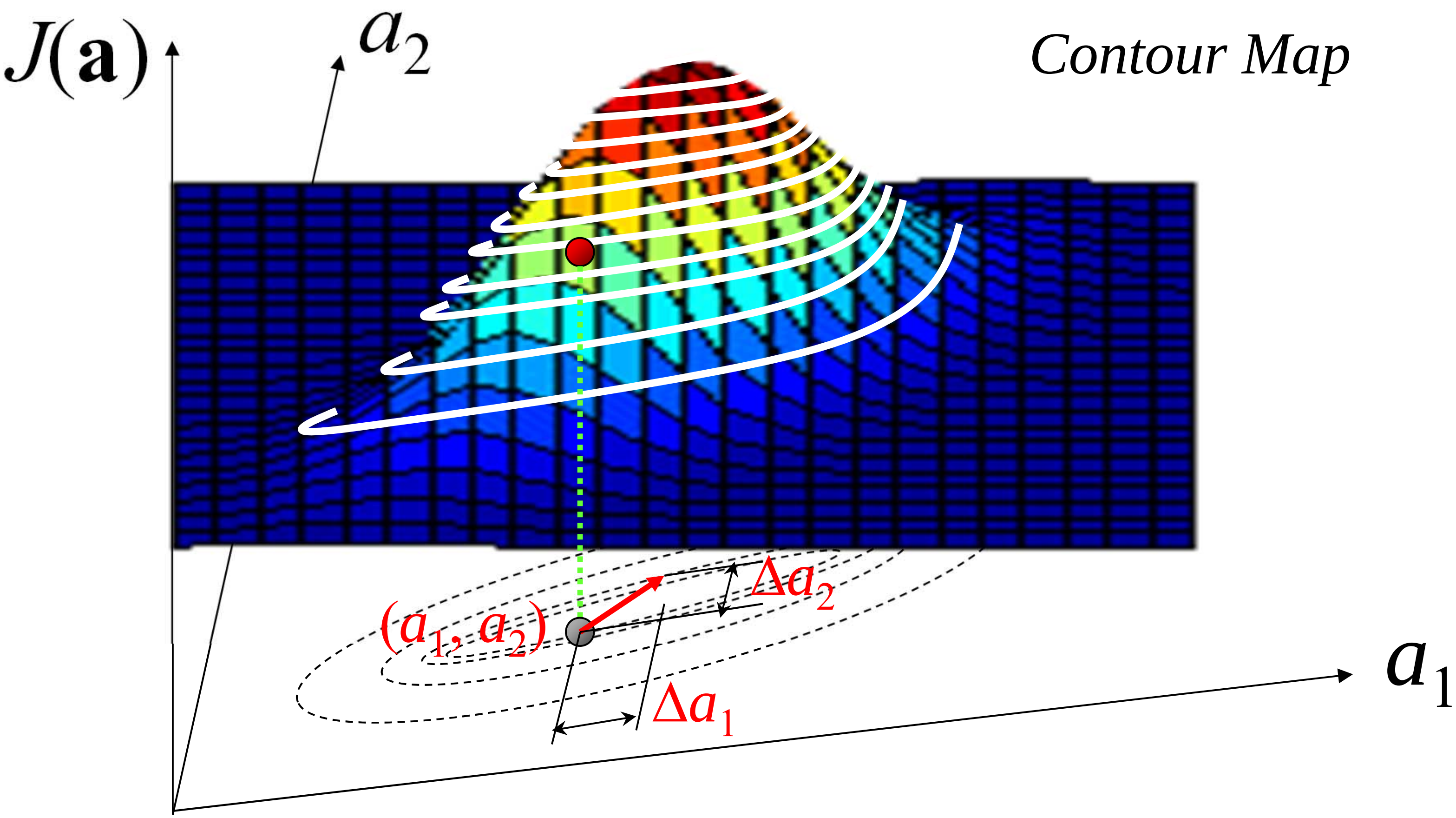
- Our goal is to go *downhill*



Gradient Decent Algorithm

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- Taylor Expansion

$$f(x+\Delta x) = f(x) + \nabla f(x)^{\mathrm{T}} \cdot \Delta x + O(\Delta x^{\mathrm{T}} \cdot \Delta x)$$

$f: R^d \to R:$	A real-valued *d*-variate function
$x \in R^d:$	A point in the *d*-dimensional Euclidean space
$\Delta x \in R^d:$	A small shift in the *d*-dimensional Euclidean space
$\nabla f(x):$	gradient of *f*(.) at *x*
$O(\Delta x^T \cdot \Delta x):$	The big oh order of $\Delta x^T \cdot \Delta x$

Gradient Decent Algorithm

MIMA

- Taylor Expansion

$$f(x+\Delta x) = f(x) + \nabla f(x)^{\mathrm{T}} \cdot \Delta x + O(\Delta x^{\mathrm{T}} \cdot \Delta x)$$

What happens if we set Δx to be negatively proportional to the gradient at x, i.e.,

$$\Delta x = -\eta \cdot \nabla f(x) \quad (\eta \text{ being a small positive scalar})$$

$$f(x+\Delta x) = f(x) - \eta \underline{\nabla f(x)^t \cdot \nabla f(x)} + \underline{O(\Delta x^t \cdot \Delta x)}$$

Being non-negative

Ignored when it is small

There, we have f(x+Δx)<=f(x)

Gradient Decent Algorithm

MIMA

- Basic strategy
  - To minimize some function f(.), the general gradient descent techniques work in the following iterative way:

1. Set learning rate >0, and a small threshold >0.
2. Randomly initialize $x_0 \in R^d$ as the starting point; set k=0.
3. do *k=k+1*
4. $$x_k = x_{k-1} - \eta \cdot \nabla f(x_{k-1})$$
5. until
6. Return x_k and $f(x_k)$

Gradient Decent Algorithm

MIMA

Why the negative gradient direction?

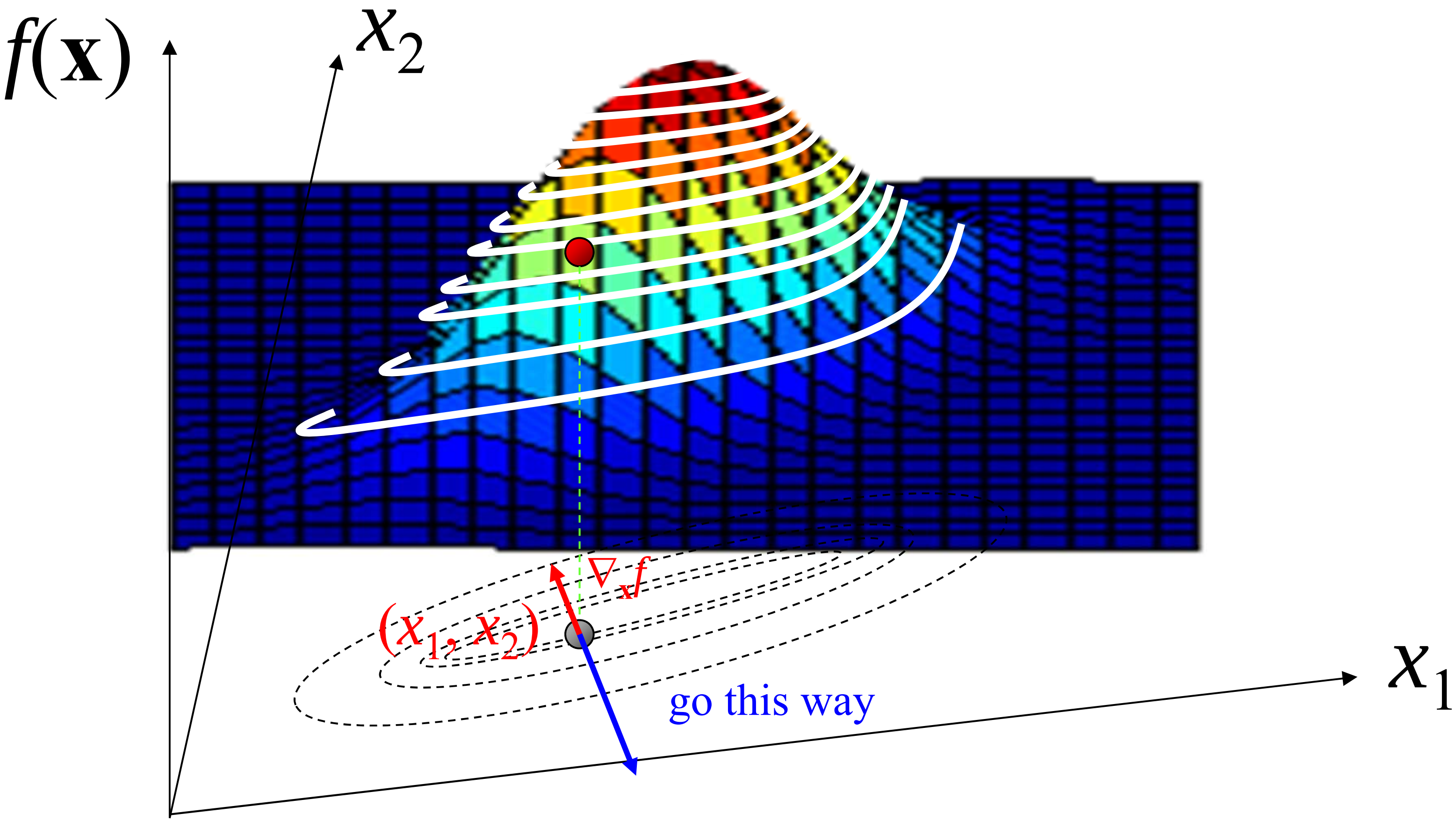
$$\nabla_x = \left(\frac{\partial}{\partial x_1} \quad \frac{\partial}{\partial x_2} \quad \Lambda \quad \frac{\partial}{\partial x_d} \right)^T$$

$$df = (\nabla_x f)^T dx \begin{cases} \text{steepest if } \overrightarrow{dx} = \overrightarrow{\nabla_x f} \\ = 0 \text{ if } \overrightarrow{dx} \perp \overrightarrow{\nabla_x f} \\ \text{steepest decent if } \overrightarrow{dx} = -\overrightarrow{\nabla_x f} \end{cases}$$

Gradient Decent Algorithm

MIMA

How long a step shall we take?



Gradient Decent Algorithm

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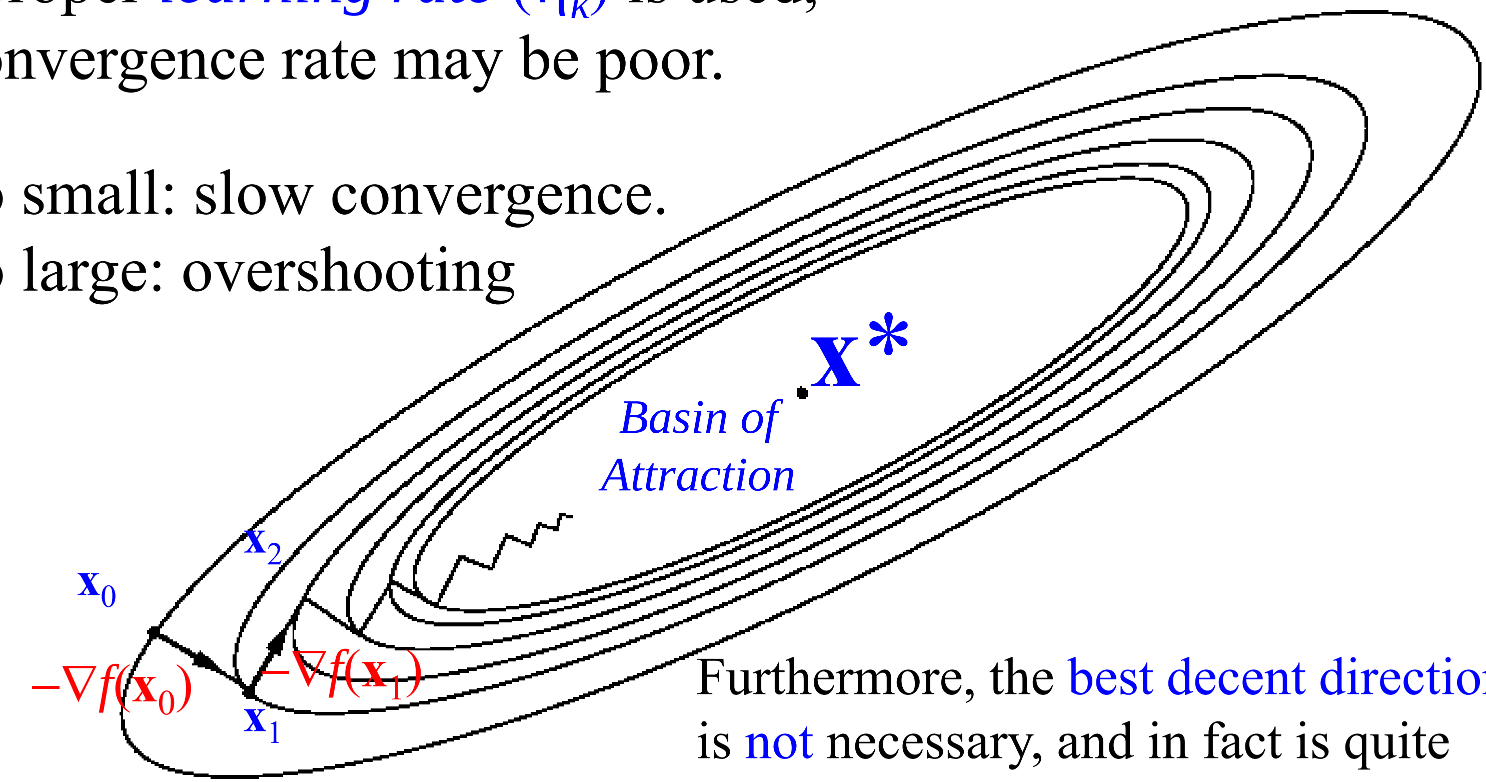
If improper *learning rate* (η_k) is used, the convergence rate may be poor.

1. Too small: slow convergence.
2. Too large: overshooting



Furthermore, the best decent direction is not necessary, and in fact is quite rarely, the direction of steepest decent.

Newton's Method

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- Global minimum of a Paraboloid

Paraboloid $f(\mathbf{x}) = c + \mathbf{a}^T\mathbf{x} + \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}$

We can find the global minimum of a paraboloid by setting its gradient to zero.

$$\nabla_{\mathbf{x}} f(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_k} = \mathbf{a} + \mathbf{Q}\mathbf{x}_k = 0$$

$$\mathbf{x}^* = -\mathbf{Q}^{-1}\mathbf{a}$$

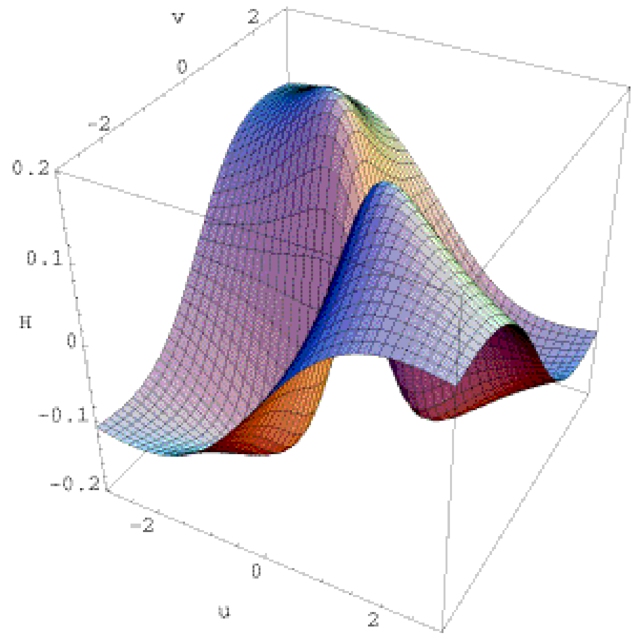
Newton's Method

MIMA

$$f(\mathbf{x}_k + \Delta\mathbf{x}) \approx f(\mathbf{x}_k) + \mathbf{g}_k^T \Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}^T \mathbf{Q}_k \Delta\mathbf{x}$$

Taylor Series Expansion

All smooth functions can be approximated by paraboloids in a sufficiently small neighborhood of any point.



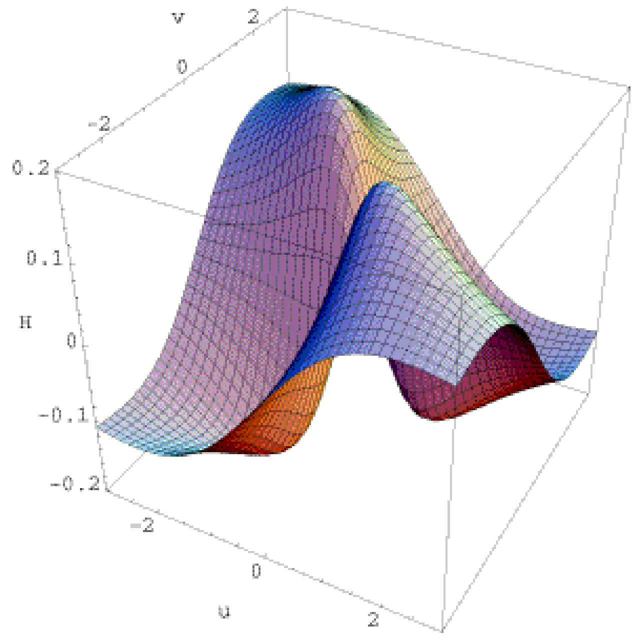
Newton's Method

$$f(\mathbf{x}_k + \Delta\mathbf{x}) \approx f(\mathbf{x}_k) + \mathbf{g}_k^T \Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}^T \mathbf{Q}_k \Delta\mathbf{x}$$

$$\mathbf{g}_k = \nabla_{\mathbf{x}} f(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}_k}$$

Hessian Matrix

$$\mathbf{Q}_k = \frac{\partial^2 f}{\partial\mathbf{x}\partial\mathbf{x}^T}\Bigg|_{\mathbf{x}=\mathbf{x}_k} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d x_1} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}_{\mathbf{x}=\mathbf{x}_k}$$



Newton's Method

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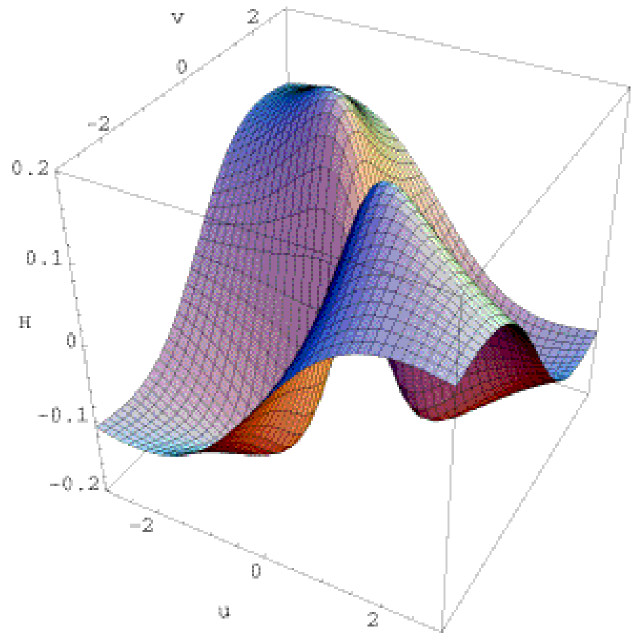
$$f(\mathbf{x}_k + \Delta\mathbf{x}) \approx f(\mathbf{x}_k) + \mathbf{g}_k^T \Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}^T \mathbf{Q}_k \Delta\mathbf{x}$$

$$\text{Set } \nabla_{\Delta\mathbf{x}} f = \mathbf{g}_k + \mathbf{Q}_k \Delta\mathbf{x} = 0$$

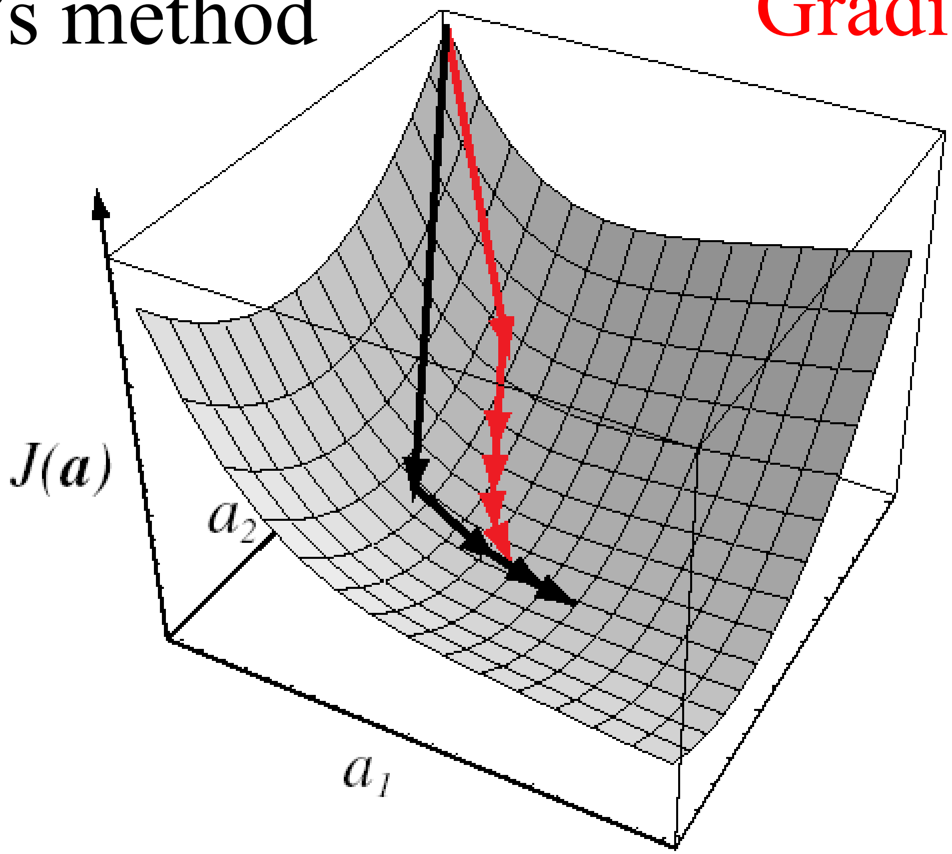
$$\Rightarrow \mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{Q}_k^{-1}\mathbf{g}_k = 0$$



Comparison

Newton's method

Gradient Decent



Comparison

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- *Newton's Method* will usually give a greater improvement *per step* than the *simple gradient decent algorithm*, even with optimal value of η_k.
- However, Newton's Method is not applicable if the Hessian matrix **Q** is *singular*.
- Even when **Q** is nonsingular, compute **Q** is time consuming $O(d^3)$.
- It often takes less time to set η_k to a constant (small than necessary) than it is to compute the optimum η_k at each step.

Summary

MIMA

- Discriminant functions
- Linear Discriminant Functions and Decision Surface
  - The general setting, one function for each class
  - The two-category case
  - Minimization of criterion/objection function
- Linear Separability

Summary

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- Learning
  - Gradient descent

$$x_k = x_{k-1} - \eta \cdot \nabla f(x_{k-1})$$

  - Newton's method

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{Q}_k^{-1}\mathbf{g}_k = 0$$

【 Thank You ! 】

Any question?