Support Vector Machines

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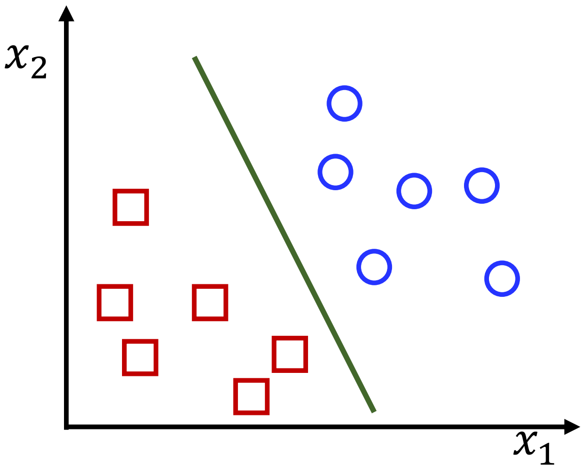
Outline

- Decision Boundaries of Linear Classifiers
- Linear Maximum-Margin Classifier
- Soft Linear Maximum-Margin Classifier
- Support Vector Machine
- Relation to Logistic Regression

Decision Boundaries in Linear Classifiers

- In linear classifiers, the decision boundary is always a hyperplane. The goal is to find the hyperplane that can separate different types of samples

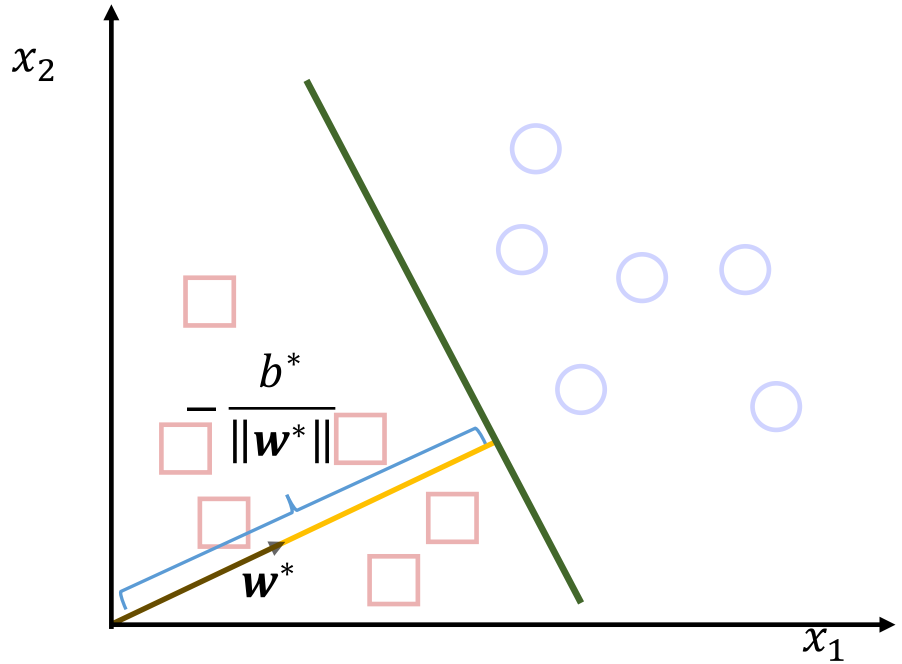


- Logistic regression
  - The decision-boundary hyperplane is found by minimizing the cross-entropy loss

$$L(\boldsymbol{w}, b) = -y \log\left(\sigma(\boldsymbol{w}^T \boldsymbol{x} + b)\right) - (1 - y) \log\left(1 - \sigma(\boldsymbol{w}^T \boldsymbol{x} + b)\right)$$

- With the optimal $\boldsymbol{w}^*$ and b^*, the hyperplane is composed of $\boldsymbol{x}$ in

$$\{\boldsymbol{x} | \boldsymbol{w}^{*T}\boldsymbol{x} + b^* = 0\}$$



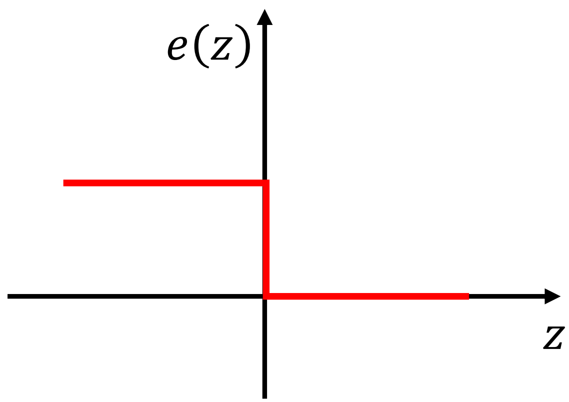
1) The hyperplane is *perpendicular* to the vector $\boldsymbol{w}^*$
2) The distance from the original point to the plane is $-\frac{b^*}{\|\boldsymbol{w}^*\|}$

- Ideal classifier
  - The hyperplane is determined by minimizing the loss

$$L(\boldsymbol{w}, b) = \sum_{\ell=1}^{N} e\left(y^{(\ell)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(\ell)} + b\right)\right)$$

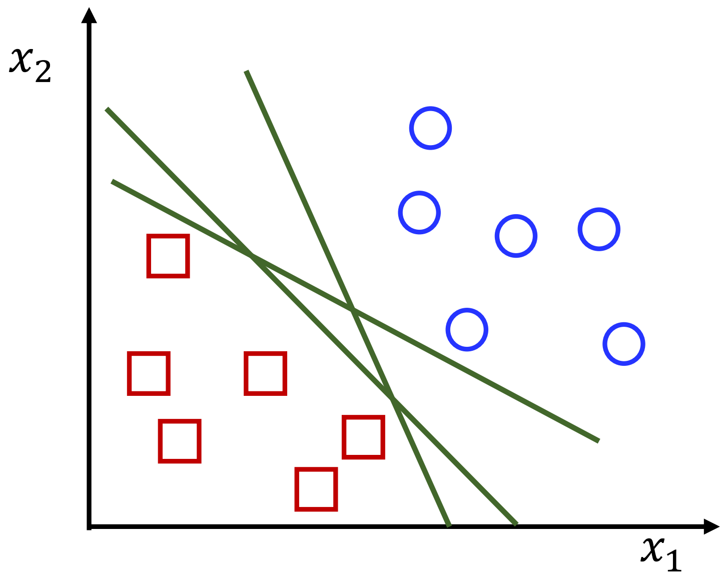
$L(\boldsymbol{w}, b)$ represents the number of misclassified samples

- $y \in \{-1, 1\}$
- $e(z) = 0$ *if* $z \geq 0$; $E[z] = 1$ *otherwise*



- If the samples are linearly separable, there will be numerous ideal classifiers, which are determined by $\boldsymbol{w}^*$ and b^*

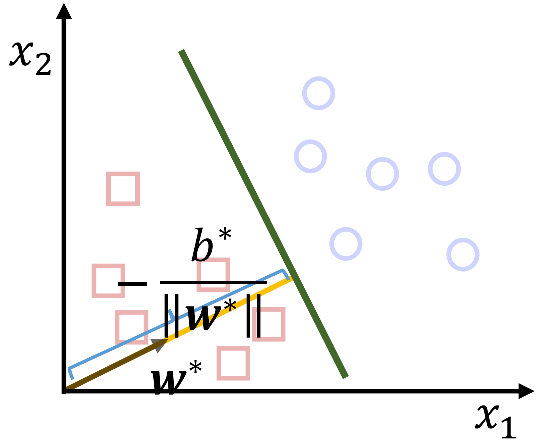
- Every $\boldsymbol{w}^*$ and b^* corresponds to a hyperplane



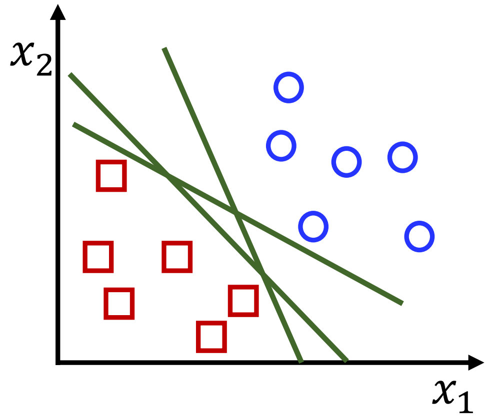
All of hyperplanes above can have the loss reduced to zero

Which Hyperplane is the Best?

- The hyperplane below is optimal from the perspective of *minimizing the cross-entropy loss*

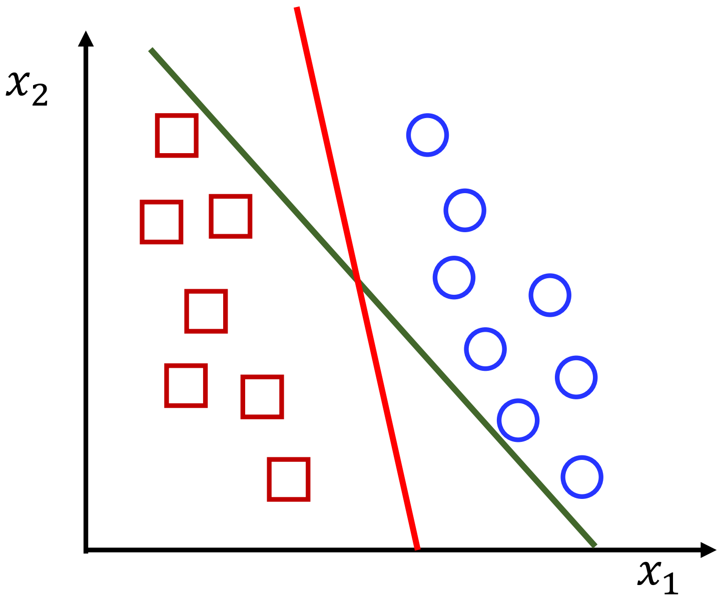


- The hyperplanes below are optimal from the perspective of *minimizing the number of misclassified samples*



- These hyperplanes are all evaluated on the *training samples*
- But what we need is the performance on the (unseen) test data

According to our intuitions, which hyperplane below would more likely produce better results on test data?



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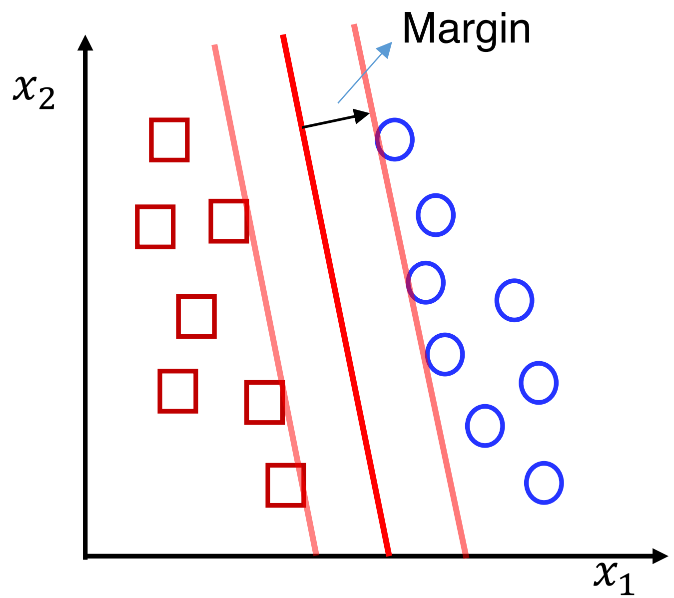
The Maximum-Margin Objective

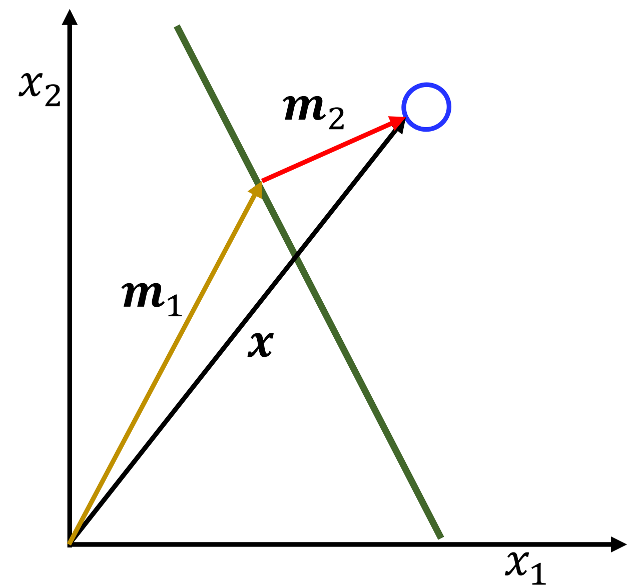
- To perform well on unseen data, the intuition is to find a hyperplane that makes the margin as large as possible



When the margin is large, *we can expect that an unseen sample has a larger chance to be categorized correctly*

How to Represent the Margin?

- The distance from the sample $\boldsymbol{x}$ to the hyperplane $\mathcal{H}$. Denote $\boldsymbol{w}^T\boldsymbol{x} + b = h(\boldsymbol{x})$



  - Every $\boldsymbol{x}$ can be decomposed as

$$\boldsymbol{x} = \boldsymbol{m}_1 + \boldsymbol{m}_2$$

    - $\boldsymbol{m}_1$ is on the $\mathcal{H}$, *i.e.*, $\boldsymbol{w}^T\boldsymbol{m}_1 + b = 0$
    - $\boldsymbol{m}_2 \perp \mathcal{H}$ *and* $\boldsymbol{m}_2 \parallel \boldsymbol{w}$

  - Thus, we have

$$\boldsymbol{w}^T\boldsymbol{x} + b = \boldsymbol{w}^T(\boldsymbol{m}_1 + \boldsymbol{m}_2) + b = \boldsymbol{w}^T\boldsymbol{m}_2 = h(\boldsymbol{x})$$

  - Due to $\boldsymbol{m}_2 \parallel \boldsymbol{w}$, we can write

$$\boldsymbol{m}_2 = \gamma \cdot \frac{\boldsymbol{w}}{\|\boldsymbol{w}\|},$$

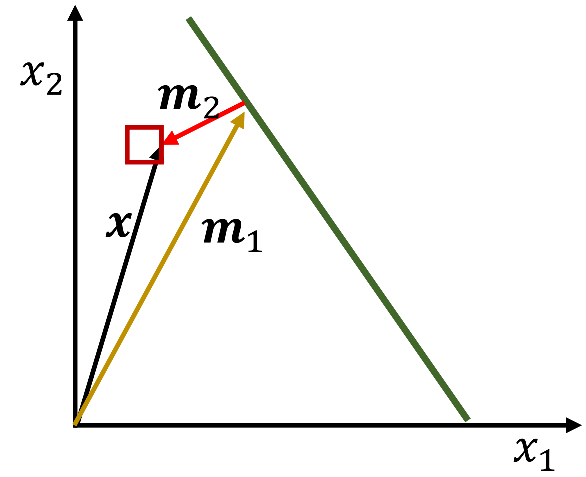
with $|\gamma|$ *representing the length of* $\boldsymbol{m}_2$

- Substituting $\boldsymbol{m}_2 = \gamma \cdot \frac{\boldsymbol{w}}{||\boldsymbol{w}||}$ into $h(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{m}_2$ gives

$$h(\boldsymbol{x}) = \gamma \cdot \frac{\boldsymbol{w}^T \boldsymbol{w}}{||\boldsymbol{w}||} \quad \Longrightarrow \quad \gamma = \frac{h(\boldsymbol{x})}{||\boldsymbol{w}||}$$

- The distance of a sample on the other side of the hyperplane is

$$\gamma = -\frac{h(\boldsymbol{x})}{||\boldsymbol{w}||}$$

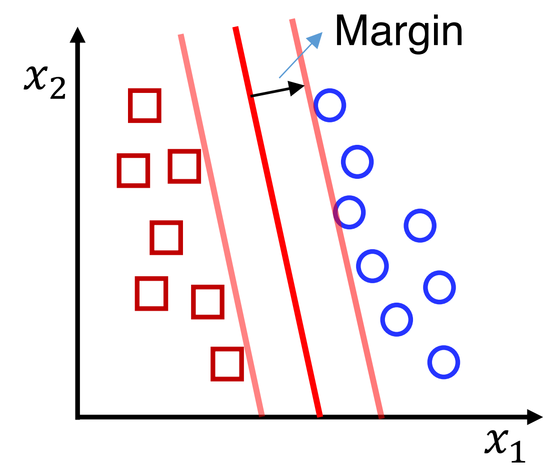


- The distance of a sample $(\boldsymbol{x}, y)$ to the hyperplane is given by

$$\frac{y \cdot h(\boldsymbol{x})}{||\boldsymbol{w}||} = \frac{y \cdot (\boldsymbol{w}^T \boldsymbol{x} + b)}{||\boldsymbol{w}||}$$

where $y \in \{-1, 1\}$

- The margin of a hyperplane under a dataset is given by the minimum distance, *i.e.*,



$$Margin = \min_{\ell} \frac{y^{(\ell)} \cdot \left(\boldsymbol{w}^T \boldsymbol{x}^{(\ell)} + b\right)}{\|\boldsymbol{w}\|}$$

- Thus, the maximum-margin classifier is to find the $\boldsymbol{w}^*$ and b^* that maximize the margin, *i.e.*,

$$\boldsymbol{w}^*, b^* = \arg\max_{\boldsymbol{w},b} \left\{ \frac{1}{\|\boldsymbol{w}\|} \min_{\ell} \left[y^{(\ell)} \cdot \left(\boldsymbol{w}^T \boldsymbol{x}^{(\ell)} + b\right) \right] \right\}$$

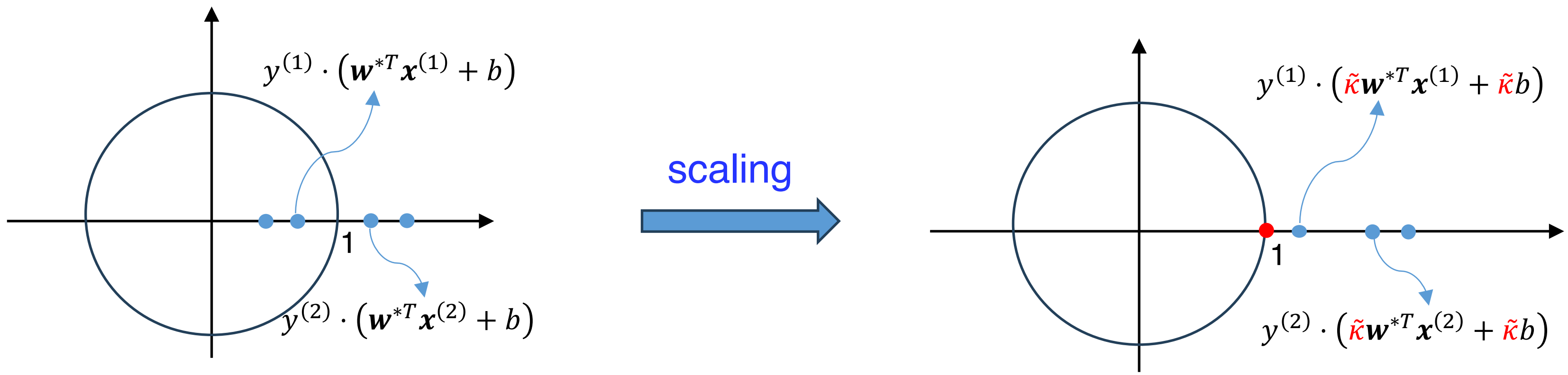
But how to optimize is unknown

The Transformed Objective Function

- Optimizing another objective function that shares the same optima as the original problem
  - Suppose $\boldsymbol{w}^*$ and b^* is an optima of $\frac{1}{\|\boldsymbol{w}\|}\min_{\ell}\left[y^{(\ell)}\cdot\left(\boldsymbol{w}^T\boldsymbol{x}^{(\ell)}+b\right)\right]$.
    Then, $\kappa\boldsymbol{w}^*$ and κb^* must also be an optima for all $\kappa \neq 0$
  - Moreover, there always exists a specific $\tilde{\kappa}$ such that

$$\boxed{y^{(\ell)}\cdot\left(\tilde{\kappa}\boldsymbol{w}^{*T}\boldsymbol{x}^{(\ell)}+\tilde{\kappa}b^*\right)\geq 1 \text{ for all } \ell = 1,2,\cdots,n}$$

and at least one '=' must hold



- Therefore, the maxima of $\frac{1}{\|\boldsymbol{w}\|}\min_{\ell}\left[y^{(\ell)}\cdot\left(\boldsymbol{w}^T\boldsymbol{x}^{(\ell)}+b\right)\right]$ can be found by solving the constraint-free optimization problem

$$\max_{\boldsymbol{w},b}\left[\frac{1}{\|\boldsymbol{w}\|}\min_{\ell}\left[y^{(\ell)}\cdot\left(\boldsymbol{w}^T\boldsymbol{x}^{(\ell)}+b\right)\right]\right]$$

or by solving the constrained optimization problem

$$\max_{\widetilde{\boldsymbol{w}},\tilde{b}}\left[\frac{1}{\|\widetilde{\boldsymbol{w}}\|}\min_{\ell}\left[y^{(\ell)}\cdot\left(\widetilde{\boldsymbol{w}}^T\boldsymbol{x}^{(\ell)}+\tilde{b}\right)\right]\right]$$

$$s.t.\quad y^{(\ell)}\cdot\left(\widetilde{\boldsymbol{w}}^T\boldsymbol{x}^{(\ell)}+\tilde{b}\right)\geq 1 \;\text{ for all } \ell=1,2,\cdots,n$$

at least one '=' must hold

  - The optimal solution $\boldsymbol{w}^*$ and $\widetilde{\boldsymbol{w}}^*$ may not be idential, but their induced values $\frac{1}{\|\boldsymbol{w}^*\|}\min_{\ell}\left[y^{(\ell)}\cdot\left(\boldsymbol{w}^{*T}\boldsymbol{x}^{(\ell)}+b^*\right)\right]$ and $\frac{1}{\|\widetilde{\boldsymbol{w}}^*\|}\min_{\ell}\left[y^{(\ell)}\cdot\left(\widetilde{\boldsymbol{w}}^{*T}\boldsymbol{x}^{(\ell)}+\tilde{b}^*\right)\right]$ must be equal

- In the second optimization problem, since $y^{(\ell)} \cdot \left(\widetilde{\boldsymbol{w}}^T \boldsymbol{x}^{(\ell)} + \tilde{b}\right) \geq 1$ for all $\ell = 1,2,\cdots,n$ and there exists at least one '=' holding, we can easily see that

$$\min_{\ell}\left[y^{(\ell)} \cdot \left(\widetilde{\boldsymbol{w}}^T \boldsymbol{x}^{(\ell)} + \tilde{b}\right)\right] = 1$$

Thus, the objective of second optimization problem is reduced to $\frac{1}{||\widetilde{\boldsymbol{w}}||}$

- Maximizing $\frac{1}{||\widetilde{\boldsymbol{w}}||}$ can be replaced by minimizing $||\widetilde{\boldsymbol{w}}||^2$. Hence, the optimization problem can be equivalently written as

$$\min_{\widetilde{\boldsymbol{w}},\tilde{b}} \ ||\widetilde{\boldsymbol{w}}||^2$$

$$s.t. \quad y^{(\ell)} \cdot \left(\widetilde{\boldsymbol{w}}^T \boldsymbol{x}^{(\ell)} + \tilde{b}\right) \geq 1 \ \text{ for all } \ell = 1,2,\cdots,n$$

at least one '=' holds

- When minimizing $||\widetilde{\boldsymbol{w}}||^2$, the constraint 'at least one '=' holds' will be satisfied automatically (why??). Thus, it can be dropped without influencing the result

- Therefore, the maximum-margin hyperplane can be found by solving the optimization problem below

$$\boxed{\begin{aligned} &\min_{\boldsymbol{w},b} \frac{1}{2}\|\boldsymbol{w}\|^2 \\ &\qquad s.t.: y^{(\ell)} \cdot \left(\boldsymbol{w}^T \boldsymbol{x}^{(\ell)} + b\right) \geq 1, \quad \text{for } \ell = 1, 2, \cdots, N \end{aligned}}$$

- This is a quadratic optimization problem. Its optimal solution can be found by *numerical methods* efficiently

- With the optimal $\boldsymbol{w}^*$ and b^*, an unseen data $\boldsymbol{x}$ can be classified as

$$\hat{y}(\boldsymbol{x}) = sign(\boldsymbol{w}^{*T}\boldsymbol{x} + b^*)$$

The Equivalent Dual Formulation

- Every convex optimization problem corresponds to an equivalent dual formulation

All contents in this section are extracted from the subject of convex optimization

- The Lagrangian function of the original optimization problem

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{a}) = \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_{\ell=1}^{N} a_\ell \left(y^{(\ell)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(\ell)} + b\right) - 1\right),$$

where the Lagrange multiplier a_ℓ is required to satisfy $a_\ell \geq 0$

- The *Lagrange dual function*

$$g(\boldsymbol{a}) = \min_{\boldsymbol{w}, b} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{a})$$

- The dual formulation of the original optimization problem

$$\boxed{\begin{aligned} &\max_{\boldsymbol{a}} \; g(\boldsymbol{a}) \\ &\quad s.t.: \boldsymbol{a} \geq \boldsymbol{0} \end{aligned}}$$

- Deriving the close-form expression of function $g(\boldsymbol{a})$
  - Setting the gradient $\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = \mathbf{0}$ and $\frac{\partial \mathcal{L}}{\partial b} = 0$ gives

$$\boldsymbol{w} = \sum_{\ell=1}^{N} a_\ell y^{(\ell)} \boldsymbol{x}^{(\ell)} \qquad \sum_{\ell=1}^{N} a_\ell y^{(\ell)} = 0$$

$$\mathcal{L} = \frac{1}{2}\|\boldsymbol{w}\|^2 - \sum_{\ell=1}^{N} a_\ell \left(y^{(\ell)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(\ell)} + b\right) - 1\right)$$

  - Substituting them into $\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{a})$ gives $g(\boldsymbol{a}) = \min_{\boldsymbol{w},b} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{a})$ as

$$g(\boldsymbol{a}) = \underbrace{\sum_{\ell=1}^{N} a_\ell - \frac{1}{2}\sum_{\ell=1}^{N}\sum_{j=1}^{N} a_\ell a_j y^{(\ell)} y^{(j)} \boldsymbol{x}^{(\ell)T} \boldsymbol{x}^{(j)}}_{=\mathbf{1}^T\boldsymbol{a} - \frac{1}{2}\boldsymbol{a}^T \boldsymbol{M} \boldsymbol{a}}$$

where $[\boldsymbol{M}]_{\ell j} \triangleq y^{(\ell)} y^{(j)} \boldsymbol{x}^{(\ell)T} \boldsymbol{x}^{(j)}$

- Then, the dual optimization becomes

$$\boxed{\begin{aligned}&\max_{\boldsymbol{a}}\ g(\boldsymbol{a})\\ &\qquad\quad s.t.:\boldsymbol{a}\geq\mathbf{0}\ \text{and}\ \sum_{\ell=1}^{N}a_\ell y^{(\ell)}=0\end{aligned}}$$

$$\text{where } g(\boldsymbol{a})=\underbrace{\sum_{\ell=1}^{N}a_\ell-\frac{1}{2}\sum_{\ell=1}^{N}\sum_{j=1}^{N}a_\ell a_j y^{(\ell)}y^{(j)}\boldsymbol{x}^{(\ell)T}\boldsymbol{x}^{(j)}}_{=\mathbf{1}^T\boldsymbol{a}-\frac{1}{2}\boldsymbol{a}^T\boldsymbol{M}\boldsymbol{a}}$$

It is also a quadratic optimization, which can be efficiently solved by *numerical methods*

- Relation between optima $\boldsymbol{w}^*$, b^* and optima $\boldsymbol{a}^*$

  - Given the optima $\boldsymbol{a}^*$, according to $\boldsymbol{w} = \sum_{\ell=1}^{N} a_\ell y^{(\ell)} \boldsymbol{x}^{(\ell)}$, the optimal $\boldsymbol{w}^*$ can be equivalently represented as

$$\boldsymbol{w}^* = \sum_{\ell=1}^{N} a_\ell^* y^{(\ell)} \boldsymbol{x}^{(\ell)}$$

  - Due to $y^{(\ell)}\left(\boldsymbol{w}^{*T} \boldsymbol{x}^{(\ell)} + b\right) = 1$ for all samples $\left(\boldsymbol{x}^{(\ell)}, y^{(\ell)}\right)$ that are on the margin, we can derive that

$$b^* = \frac{1}{N_S} \sum_{n \in S}^{N} \left(y^{(n)} - \sum_{m} a_m^* y^{(m)} \boldsymbol{x}^{(n)T} \boldsymbol{x}^{(m)} \right)$$

- Maximum-margin classifiers
  - Primal version

$$\boxed{\hat{y}(\boldsymbol{x}) = sign(\boldsymbol{w}^{*T}\boldsymbol{x} + b^*)}$$

  - Dual version

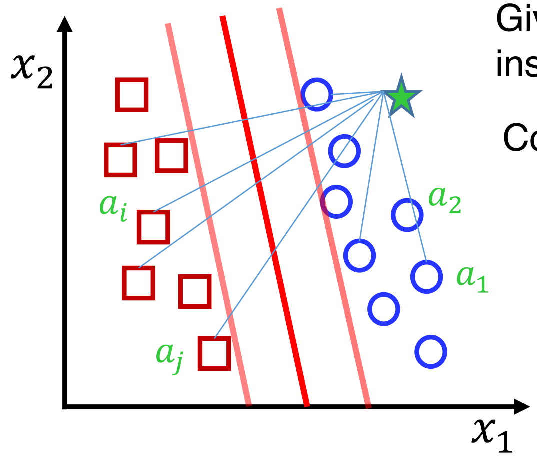
    Substituting $\boldsymbol{w}^* = \sum_{n=1}^{N} a_n^* y^{(n)} \boldsymbol{x}^{(n)}$ into the primal version gives

$$\boxed{\hat{y}(\boldsymbol{x}) = sign\left(\sum_{n=1}^{N} a_n^* y^{(n)} \boldsymbol{x}^{(n)T} \boldsymbol{x} + b^*\right)}$$

The two classifiers are *equivalent*

$$\hat{y}(\boldsymbol{x}) = sign\left(\sum_{n=1}^{N} a_n^* \cdot \left(\boldsymbol{x}^{(n)T}\boldsymbol{x}\right) \cdot y^{(n)} + b^*\right)$$

- How to understand the dual maximum-margin classifier?
  - For a test $\boldsymbol{x}$, computing its similarity with all the training samples $\boldsymbol{x}^{(n)}$ for $n = 1, \cdots, N$ by $\boldsymbol{x}^{(n)T}\boldsymbol{x}$
  - Summing all the labels $y^{(n)}$ weighted by the sample similarity $\boldsymbol{x}^{(n)T}\boldsymbol{x}$ and the multiplier a_n^*



Giving weights to different data instance a_i

Computing the similarity $\boldsymbol{x}^{(n)T}\boldsymbol{x}$

Comparisons on the Primal and Dual Results

- Optimization complexity

Primal

$$\min_{\boldsymbol{w},b} \frac{1}{2}||\boldsymbol{w}||^2$$

$$s.t.: y^{(\ell)} \cdot \left(\boldsymbol{w}^T \boldsymbol{x}^{(\ell)} + b\right) \geq 1,$$

$$\text{for } \ell = 1, 2, \cdots, N$$

# of parameters to optimize:
dimension of features

Dual

$$\max_{\boldsymbol{a}} g(\boldsymbol{a})$$

$$s.t.: \quad \boldsymbol{a} \geq \boldsymbol{0}$$

$$\sum_{\ell=1}^{N} a_\ell y^{(\ell)} = 0$$

# of parameters to optimize:
# of training samples

In *high-dimensional feature case*, solving the dual problem is more efficient

- Testing complexity

Primal	Dual
$\hat{y}(\boldsymbol{x}) = sign(\boldsymbol{w}^{*T}\boldsymbol{x} + b^*)$	$\hat{y}(\boldsymbol{x}) = sign\left(\sum_{n=1}^{N} a_n^* \left(\boldsymbol{x}^{(n)T}\boldsymbol{x}\right) y^{(n)} + b^*\right)$
Just need one inner-product operation $\boldsymbol{w}^{*T}\boldsymbol{x}$	Need N inner-product operations $\boldsymbol{x}^{(n)T}\boldsymbol{x}$ for $n = 1, 2, \cdots, N$

At the first glance, the dual classifier looks much more expensive than the primal one

- Fortunately, it can be proved that most of a_n^* are 0

Sparsity in the Lagrange Multiplier a^*

- For any convex optimization problem, the optima satisfies the *KKT conditions*, which, for our problem, are

$$a_n^* \geq 0$$

$$y^{(n)}\left(\boldsymbol{w}^{*T}\boldsymbol{x}^{(n)} + b^*\right) - 1 \geq 0$$

$$\boxed{a_n^*\left[y^{(n)}\left(\boldsymbol{w}^{*T}\boldsymbol{x}^{(n)} + b^*\right) - 1\right] = 0}$$

The first two conditions come from the original primal and dual problems

- From the last condition, we can see that $a_n^* \neq 0$ only when $y^{(n)}\left(\boldsymbol{w}^{*T}\boldsymbol{x}^{(n)} + b^*\right) = 1$

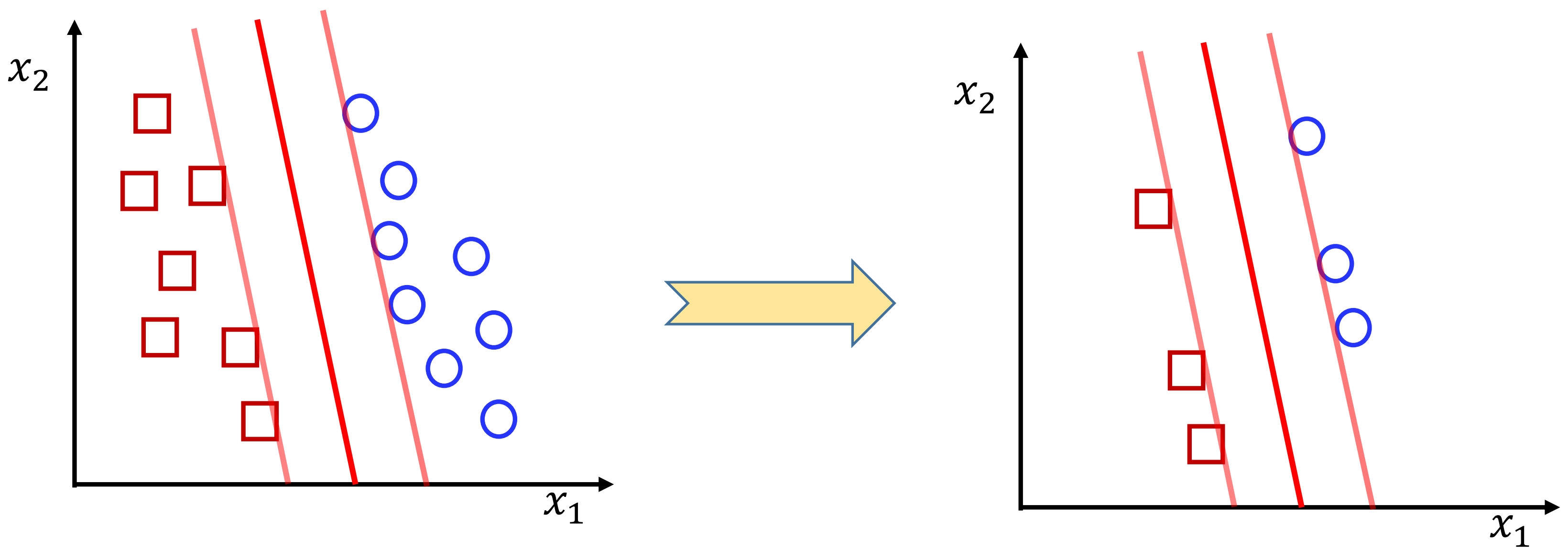
- If $\boldsymbol{x}^{(n)}$ staisfies $y^{(n)}\left(\boldsymbol{w}^{*T}\boldsymbol{x}^{(n)} + b^*\right) = 1$, it means that it lies on the margin

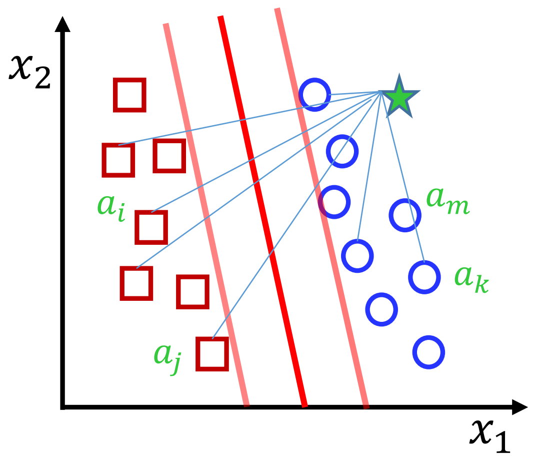
This kind of samples are called *support vectors*

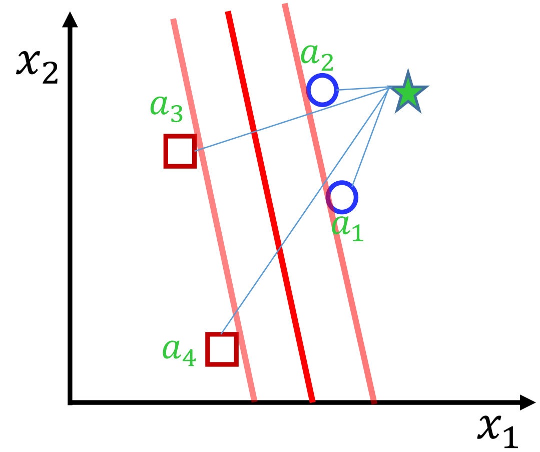
- Thus, when we classify an unseen sample $\boldsymbol{x}$ as

$$\hat{y}(\boldsymbol{x}) = sign\left(\sum_{n} a_n^* y^{(n)} \boldsymbol{x}^{(n)T} \boldsymbol{x} + b^*\right),$$

we only need to evaluate the similarity $\boldsymbol{x}^{(n)T}\boldsymbol{x}$ between $\boldsymbol{x}$ and the support vectors (samples)







$$\hat{y}(\boldsymbol{x}) = sign\left(\sum_{n=1}^{N}\left(a_n^*\left(\boldsymbol{x}^{(n)T}\boldsymbol{x}\right)\right)\cdot y^{(n)} + b^*\right)$$

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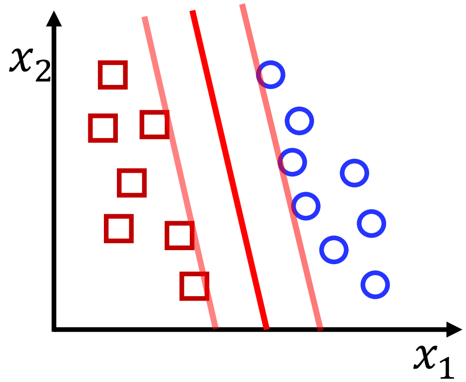
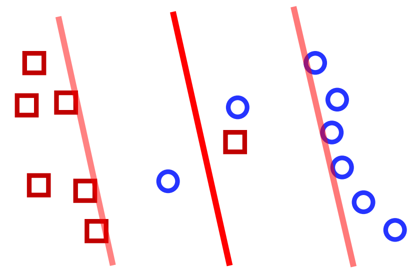
Non-separable Classes

- The implicit assumption in the previous maximum-margin classifier

The training samples are linearly separable!!!





- What happens to the optimization problem under such circumstances?

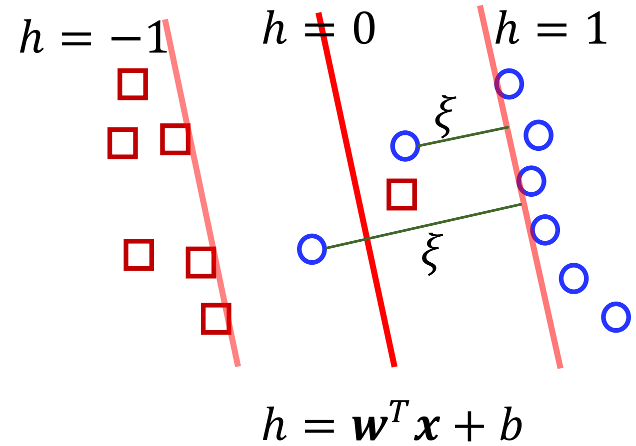
$$\min_{\boldsymbol{w},b} \frac{1}{2}\|\boldsymbol{w}\|^2$$

$$s.t.: \; y^{(n)} \cdot \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + b\right) \geq 1, \quad \text{for } n = 1, 2, \cdots, N$$

- There is no feasible solution to the optimization problem. That is, *no such hyperplane exist*

Soft Maximum Margin

- To address the issue, instead of requiring $y^{(n)} \cdot \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + b\right) \geq 1$ for all $n = 1, \cdots, N$, we only require



$$y^{(n)} \cdot \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} + b\right) \geq 1 - \xi_n$$

where ξ_n is *slack variable* with $\xi_n \geq 0$

- The objective is not just to minimize $\frac{1}{2}\|\boldsymbol{w}\|^2$, but also need to minimize the sum of ξ_n, which leads to the objective

$$\frac{1}{2}\|\boldsymbol{w}\|^2 + C \sum_{n=1}^{N} \xi_n$$

where C is used to control the relative importance

- The optimization problem now becomes

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

$$s.t.: \ y^{(n)} \cdot \left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} + b\right) \geq 1 - \xi_n,$$

$$\xi_n \geq 0, \qquad \text{for } n = 1, 2, \cdots, N$$

- Using the same method as before, the *dual formulation* can be derived as

$$\max_{\boldsymbol{a}} \ g(\boldsymbol{a})$$

$$s.t.: \quad a_n \geq 0, \quad a_n \leq C$$

$$\sum_{n=1}^{N} a_n y^{(n)} = 0$$

When $a_n > C$, it can be shown that $g(\boldsymbol{a}) = -\infty$

where $g(\boldsymbol{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m y^{(n)} y^{(m)} \boldsymbol{x}^{(n)T}\boldsymbol{x}^{(m)}$

- With the optima $\boldsymbol{w}^*$ and b^*, a sample $\boldsymbol{x}$ is classified as

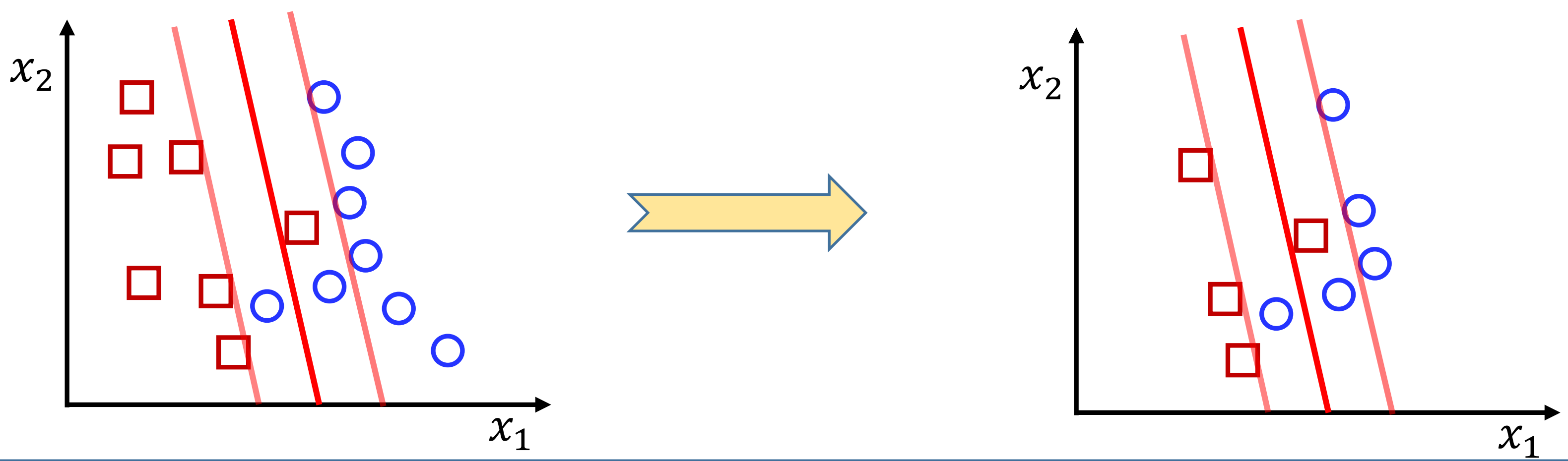
$$\hat{y}(\boldsymbol{x}) = sign(\boldsymbol{w}^{*T}\boldsymbol{x} + b^*)$$

- With the optima $\boldsymbol{a}^*$, a sample $\boldsymbol{x}$ is classified as

$$\hat{y}(\boldsymbol{x}) = sign\left(\sum_{n=1}^{N} a_n^* y^{(n)} \boldsymbol{x}^{(n)T}\boldsymbol{x} + b^*\right)$$

Also, the two classifiers above are *equivalent*

- The optima $\boldsymbol{a}^*$ is sparse, with only elements within the margin being nonzero



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Non-linearization

- The maximum-margin classifiers so far are still linear

- To non-linearize the model, we can transform the original data $\boldsymbol{x}$ to the feature space via the basis function

$$\boldsymbol{\phi}\colon\ \boldsymbol{x} \longrightarrow \boldsymbol{\phi}(\boldsymbol{x})$$

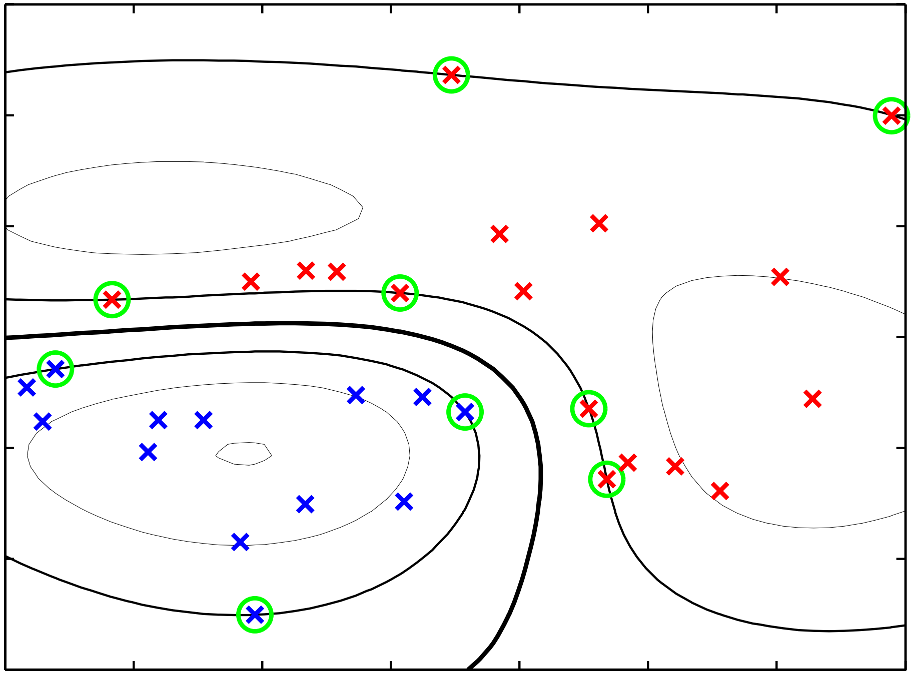
- The primal maximum-margin optimization problem becomes

$$\min_{\boldsymbol{w},b,\xi} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

$$s.t.:\ y^{(n)} \cdot \left(\boldsymbol{w}^T \boldsymbol{\phi}\left(\boldsymbol{x}^{(n)}\right) + b\right) \geq 1 - \xi_n,$$

$$\xi_n \geq 0, \qquad \text{for } n = 1, 2, \cdots, N$$

Classifier: $\hat{y}(\boldsymbol{x}) = sign\left(\boldsymbol{w}^{*T}\boldsymbol{\phi}\left(\boldsymbol{x}^{(n)}\right) + b^*\right)$



- Intuitively, data is easier to be separated in high-dimensional space

- To achieve better performance, we prefer to set the dimension of transformed feature space $\boldsymbol{\phi}\left(\boldsymbol{x}^{(n)}\right)$ *to be as high as possible*

- However, the dimension of basis function $\boldsymbol{\phi}(\boldsymbol{x})$ *cannot be set too high* since the primal problem would become very expensive

$$\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{n=1}^{N}\xi_n$$

$$s.t.: \; y^{(n)} \cdot \left(\boldsymbol{w}^T\boldsymbol{\phi}\left(\boldsymbol{x}^{(n)}\right) + b\right) \geq 1 - \xi_n,$$

$$\xi_n \geq 0, \qquad \text{for } n = 1, 2, \cdots, N$$

- The problem can be solved via its dual form

$$\max_{\boldsymbol{a}} \; g(\boldsymbol{a})$$

$$s.t.: \quad a_n \geq 0, \quad a_n \leq C$$

$$\sum_{n=1}^{N} a_n y^{(n)} = 0$$

where $g(\boldsymbol{a}) = \underbrace{\sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m y^{(n)} y^{(m)} \boldsymbol{\phi}\left(\boldsymbol{x}^{(n)}\right)^T \boldsymbol{\phi}\left(\boldsymbol{x}^{(m)}\right)}_{=\mathbf{1}^T\boldsymbol{a}-\frac{1}{2}\boldsymbol{a}^T\boldsymbol{M}\boldsymbol{a}}$

Classifier: $\hat{y}(\boldsymbol{x}) = sign\left(\sum_{n=1}^{N} a_n^* y^{(n)} \boldsymbol{\phi}\left(\boldsymbol{x}^{(n)}\right)^T \boldsymbol{\phi}(\boldsymbol{x}) + b^*\right)$

- The dimension of $\boldsymbol{a}$ is *independent of the dimension of $\boldsymbol{\phi}(\cdot)$*, thus the dual form is able to work in a very large feature space $\boldsymbol{\phi}(\cdot)$

The dual formulation requires to evaluate the inner product

$$\boldsymbol{\phi}\left(\boldsymbol{x}^{(n)}\right)^T \boldsymbol{\phi}(\boldsymbol{x}),$$

which is expensive in high-dimensional case

The issue can be addressed by using the *kernel trick*

Kernel Function

- A kernel function is a two-variable function $k(\boldsymbol{x}, \boldsymbol{x}')$ that can be expressed as an inner product of some function $\boldsymbol{\phi}(\cdot)$

$$k(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{x}')$$

Obviously, $\boldsymbol{x}^T \boldsymbol{x}'$ and $\boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{x}')$ are kernel functions

- Mercer Theorem: If a function $k(\boldsymbol{x}, \boldsymbol{x}')$ is symmetric positive definite, *i.e.*,

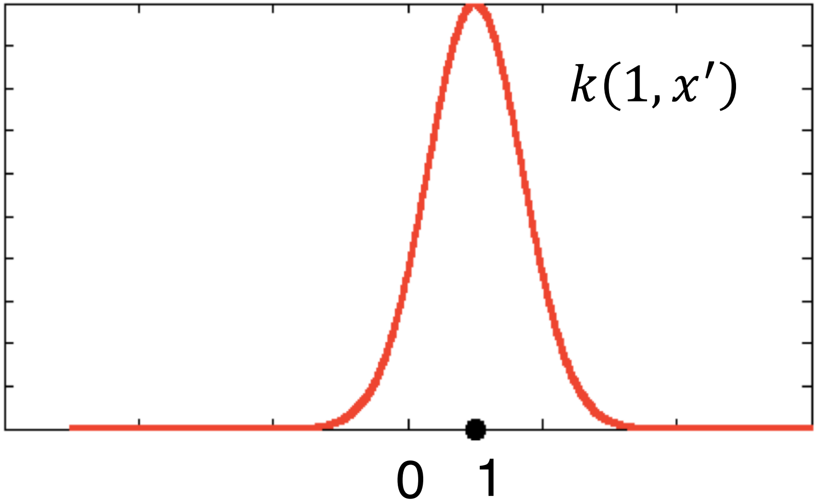
$$\int \int g(\boldsymbol{x}) k(\boldsymbol{x}, \boldsymbol{y}) g(\boldsymbol{y}) d\boldsymbol{x} d\boldsymbol{y} \geq 0, \qquad \forall\, g(\cdot) \in L^2,$$

there must exist a function $\boldsymbol{\phi}(\cdot)$ such that $k(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{x}')$

If a function $k(\boldsymbol{x}, \boldsymbol{x}')$ satisfies the symmetric positive definite condition, it must be a kernel function

- One of the most widely used kernel is the Gaussian kernel, which takes the form

$$k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left\{-\frac{1}{2\sigma^2}\|\boldsymbol{x} - \boldsymbol{x}'\|^2\right\}$$



➢ The function $\boldsymbol{\phi}(\cdot)$ of Gaussian kernel has infinite dimensions

$$\boldsymbol{\phi}(x) = e^{-x^2/2\sigma^2}\left[1, \sqrt{\frac{1}{1!\sigma^2}}x, \sqrt{\frac{1}{2!\sigma^4}}x^2, \sqrt{\frac{1}{3!\sigma^6}}x^3, \cdots\right]^T$$

Kernel Trick

- With the kernel function, the dual maximum-margin classifier can be equivalently rewritten as

$$\max_{\boldsymbol{a}} \; g(\boldsymbol{a})$$

$$s.t.: \quad a_n \geq 0, \quad a_n \leq C$$

$$\sum_{n=1}^{N} a_n y^{(n)} = 0$$

where $g(\boldsymbol{a}) = \underbrace{\sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m y^{(n)} y^{(m)} k\left(\boldsymbol{x}^{(n)}, \boldsymbol{x}^{(m)}\right)}_{= \boldsymbol{1}^T \boldsymbol{a} - \frac{1}{2} \boldsymbol{a}^T \boldsymbol{M} \boldsymbol{a}}$

- The induced classifier

$$\hat{y}(\boldsymbol{x}) = sign\left(\sum_{n=1}^{N} a_n^* y^{(n)} k\left(\boldsymbol{x}^{(n)}, \boldsymbol{x}\right) + b^*\right)$$

Kernel trick: replacing the $\boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{x}')$ with the kernel function $k(\boldsymbol{x}, \boldsymbol{x}')$

- The conclusions can be summarized as
  - If $k(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^T \boldsymbol{x}'$, it is a linear maximum-margin classifier
  - If $k(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{\phi}(\boldsymbol{x})^T \boldsymbol{\phi}(\boldsymbol{x}')$, it is a *finite-dimensional* nonlinear maximum-margin classifier based on basis functions
  - If $k(\boldsymbol{x}, \boldsymbol{x}') = \exp\left\{-\frac{1}{2\sigma^2} \|\boldsymbol{x} - \boldsymbol{x}'\|^2\right\}$, it is an *infinite-dimensional* nonlinear maximum-margin classifier

Outline

- Decision Boundaries of Linear Classifiers
- Linear Maximum-Margin Classifier
- Soft Linear Maximum-Margin Classifier
- Support Vector Machine
- Relation to Logistic Regression

- In the logistic regression, we minimize the loss

$$L(\boldsymbol{w}, b) = -\sum_{n=1}^{N} \left[\tilde{y}^{(n)} \log \sigma\left(h^{(n)}\right) + \left(1 - \tilde{y}^{(n)}\right) \log\left(1 - \sigma\left(h^{(n)}\right)\right)\right] + \lambda\|\boldsymbol{w}\|^2$$

$$= \sum_{n=1}^{N} \log\left(1 + \exp\left(-y^{(n)} h^{(n)}\right)\right) + \lambda\|\boldsymbol{w}\|^2$$

$$= \sum_{n=1}^{N} E_{LR}\left(y^{(n)} h^{(n)}\right) + \lambda\|\boldsymbol{w}\|^2$$

Note:
$\tilde{y} \in \{0, 1\}$, $y \in \{-1, 1\}$

where $E_{LR}(z) = \log(1 + \exp(-z))$

- In the ideal classifier, we minimize the loss

$$L(\boldsymbol{w}, b) = \sum_{n=1}^{N} E_{Ideal}\left(y^{(n)} h^{(n)}\right) + \lambda\|\boldsymbol{w}\|^2$$

where $E_{Ideal}(z) = 0$ *if* $z \geq 0$; 1 *otherwise*

- In the linear maximum-margin classifier, we are equivalently minimizing the loss

$$L(\boldsymbol{w}, b) = \sum_{n=1}^{N} E_{\infty}\left(y^{(n)} h^{(n)} - 1\right) + \frac{1}{2}\|\boldsymbol{w}\|^2$$

where $E_{\infty}(z) = 0$ *if* $z \geq 0$*;* $+\infty$ *otherwise*

- In the soft linear maximum-margin classifier, we are equivalently minimizing the loss

$$L(\boldsymbol{w}, b) = C \sum_{n=1}^{N} E_{SV}\left(y^{(n)} h^{(n)}\right) + \frac{1}{2}\|\boldsymbol{w}\|^2$$

$$= \sum_{n=1}^{N} E_{SV}\left(y^{(n)} h^{(n)}\right) + \lambda\|\boldsymbol{w}\|^2$$

where $E_{SV}(z) = \max(0, 1 - z)$, which is called the *hinge loss*

- We can see that the four classifiers can be formulated under the same framework, with the only difference coming from the chosen error function

- The plot of the four error functions