Model

Two kinds of models: deterministic models and probabilistic models

Deterministic model: Given an input, produces an output

- Example: $\hat{y} = \vec{w}^{\top}\vec{x}$

Probabilistic model: Given an input, produces a distribution over possible outputs.

- Example: $y|\vec{x}, \vec{w}, \sigma \sim \mathcal{N}\left(\vec{w}^{\top}\vec{x}, \sigma^2\right)$

Loss Function

For a deterministic model: Can be any function that assigns high values to incorrect outputs and low values to correct outputs.

For a probabilistic model:

- Maximum likelihood (MLE): Loss function is the negative log-likelihood
$$\log p\left(\mathcal{D}\middle|\vec{\theta}\right)$$

- Maximum a posteriori (MAP): Loss function is the negative log-posterior
$$\log p\left(\vec{\theta}\middle|\mathcal{D}\right) = \log\left(\frac{p(\vec{\theta})p(\mathcal{D}|\vec{\theta})}{p(\mathcal{D})}\right)$$

Training

Training involves finding the model parameters that minimize the loss. Several approaches:

- Set the gradient to zero and solve for the optimal parameters analytically.
- If there is no closed-form solution for the optimal parameters:
  - If optimization problem is unconstrained: use iterative gradient-based optimization methods.
  - **Next: constrained optimization**

Machine Learning

CMPT 726

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SFU School of Computing Science

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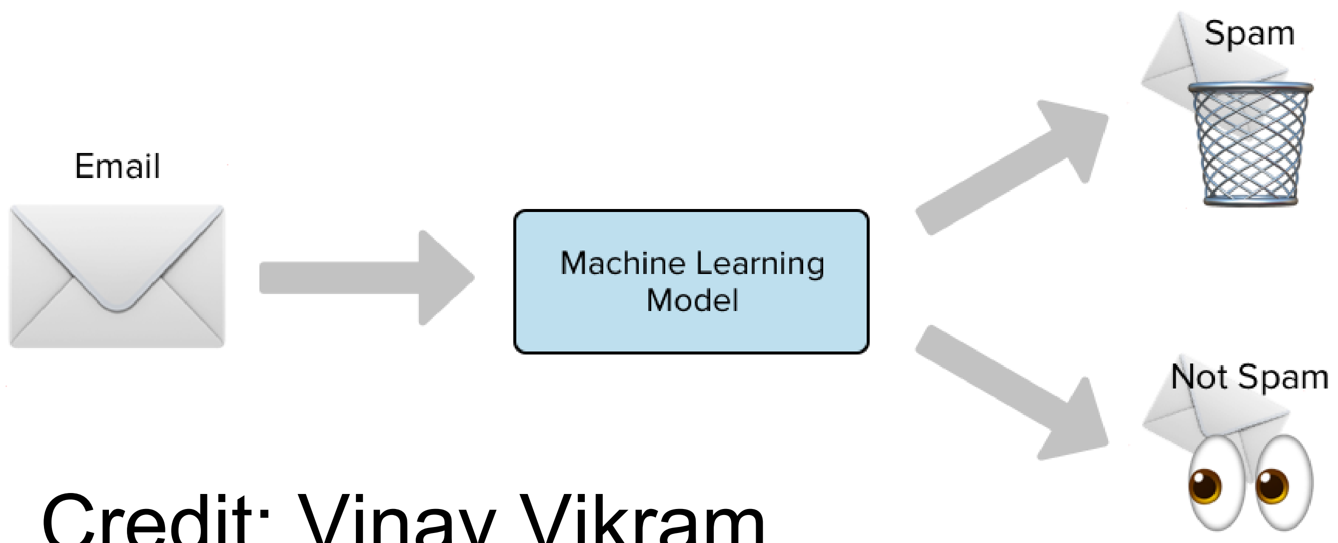
Classification

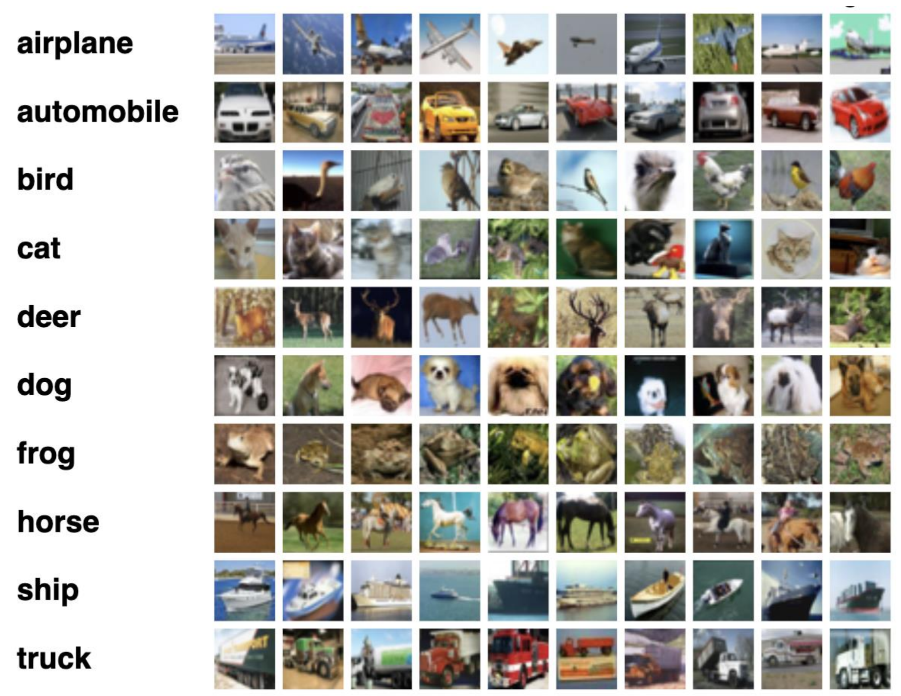
Motivation

In many problems, we would like to categorize an observation:

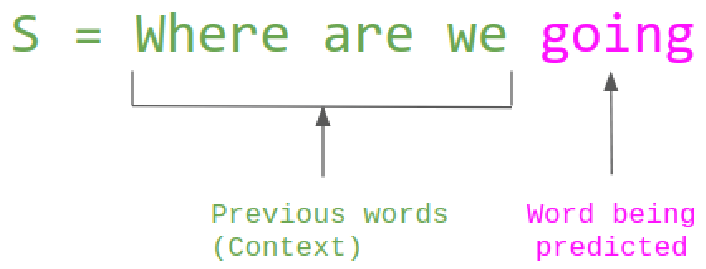
- Is an email spam?
- What object is depicted in an image?
- What will be the next word?



Credit: Vinay Vikram



Credit: Alex Krizhevsky



P(S) = P(Where) x P(are | Where) x P(we | Where are) x P(going | Where are we)

Credit: The Gradient

Binary Classification

Unlike regression, the goal of classification is to classify the input into one of multiple discrete classes.

A regression model produces a real number or in the case of multiple output regression, a real vector.

A classification model produces a class prediction.

Such a model is known as a **classifier**.

In binary classification, the goal is to classify into one of **two** discrete classes.

A binary classification model is known as a **binary classifier**.

Without loss of generality, we call one class the **positive class** and the other the **negative class**.

Data points whose labels are positive are known as **positive examples** and data points whose labels are negative are known as **negative examples**.

Support Vector Machines

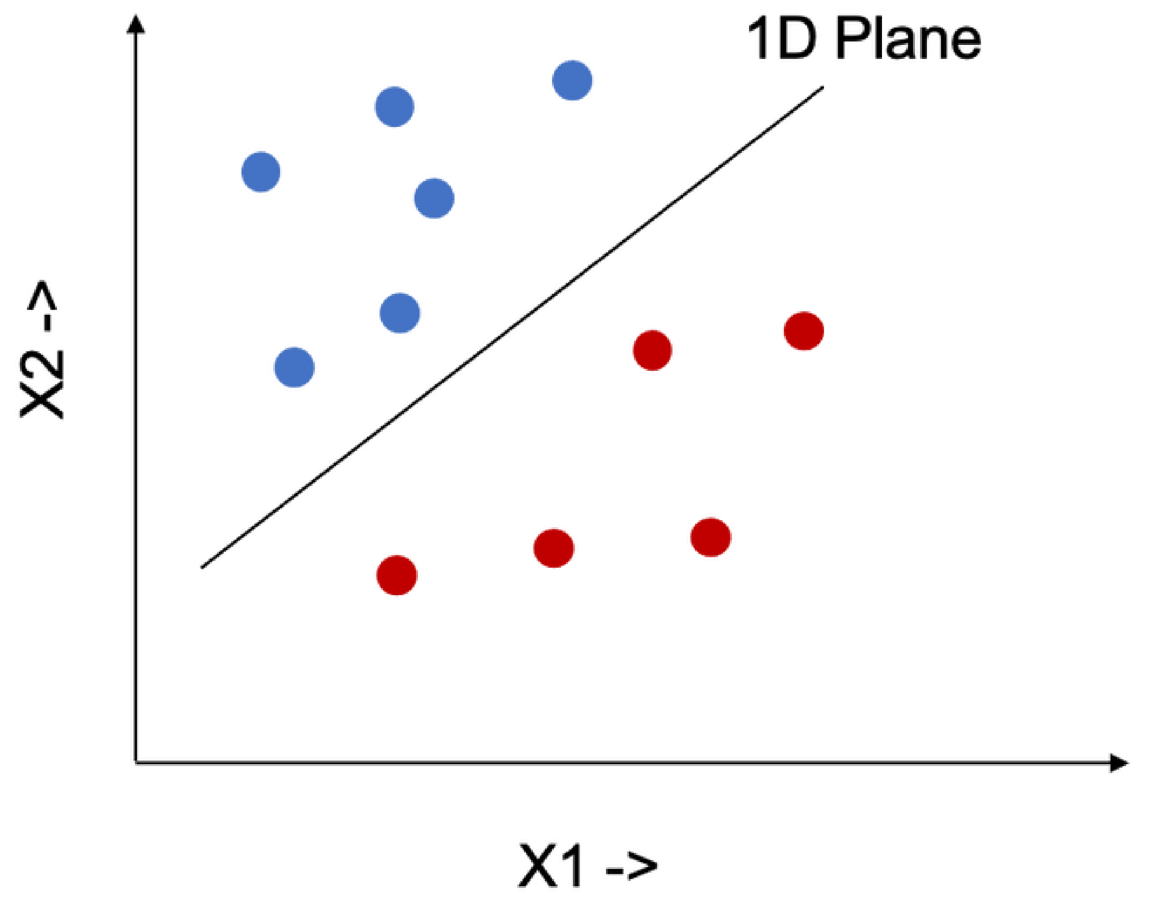
Given a dataset of input-output pairs (a.k.a. "observations"), $\{(\vec{x}_i, y_i)\}_{i=1}^{N}$, where $\vec{x}_i \in \mathbb{R}^{n-1}$ and $y_i \in \{-1,1\}$

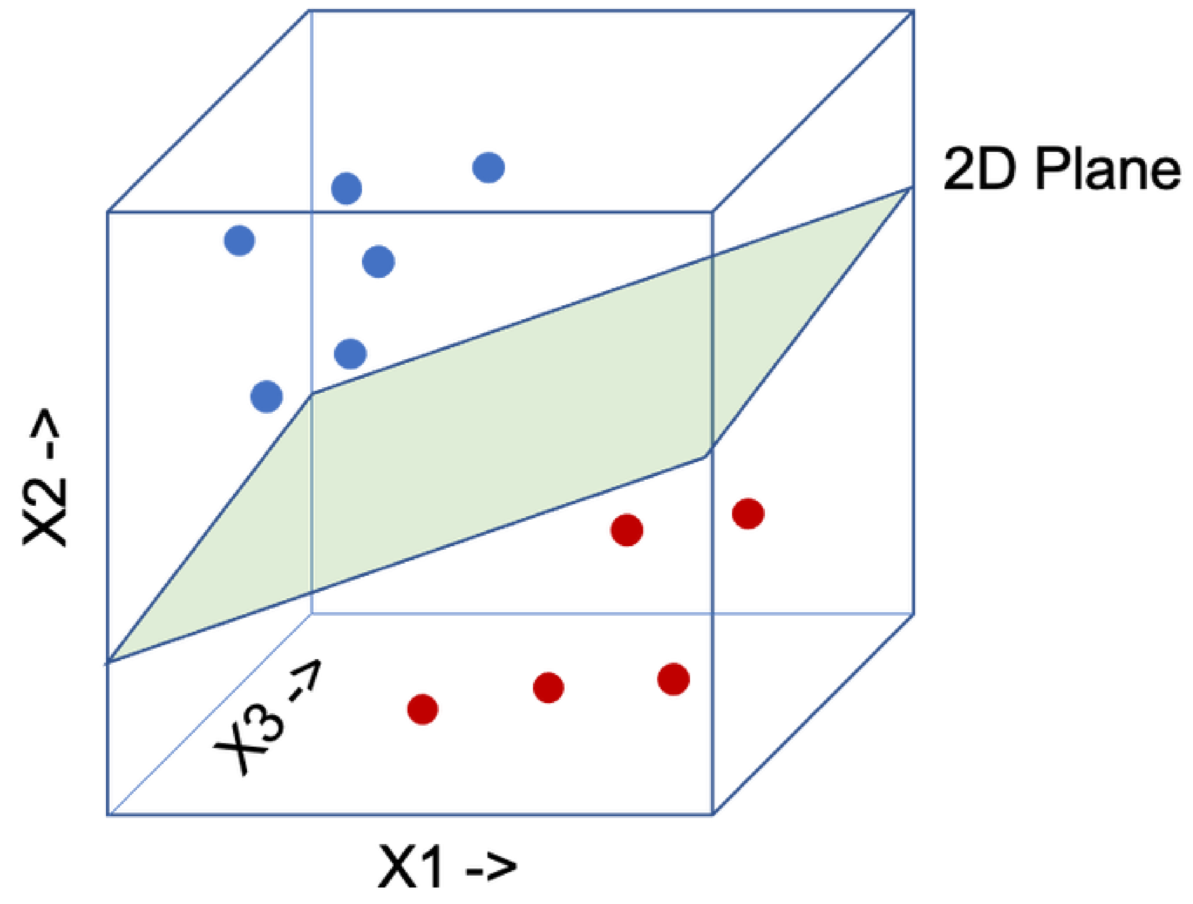
We will construct a model called the support vector machine (SVM) to predict the label y from the data point $\vec{x}$.

The model is simply a line (in the case of 2D data), a plane (in the case of 3D data) or more generally, a hyperplane (in the case of higher dimensional data) that separates the data points.

For a new data point on one side, we predict the positive label.

For a new data point on the other side, we predict the negative label.





Credit: Abhisek Jana

Support Vector Machines

The **decision boundary** is the boundary that separates the region where the model generates positive predictions from the region where the model generates negative predictions.

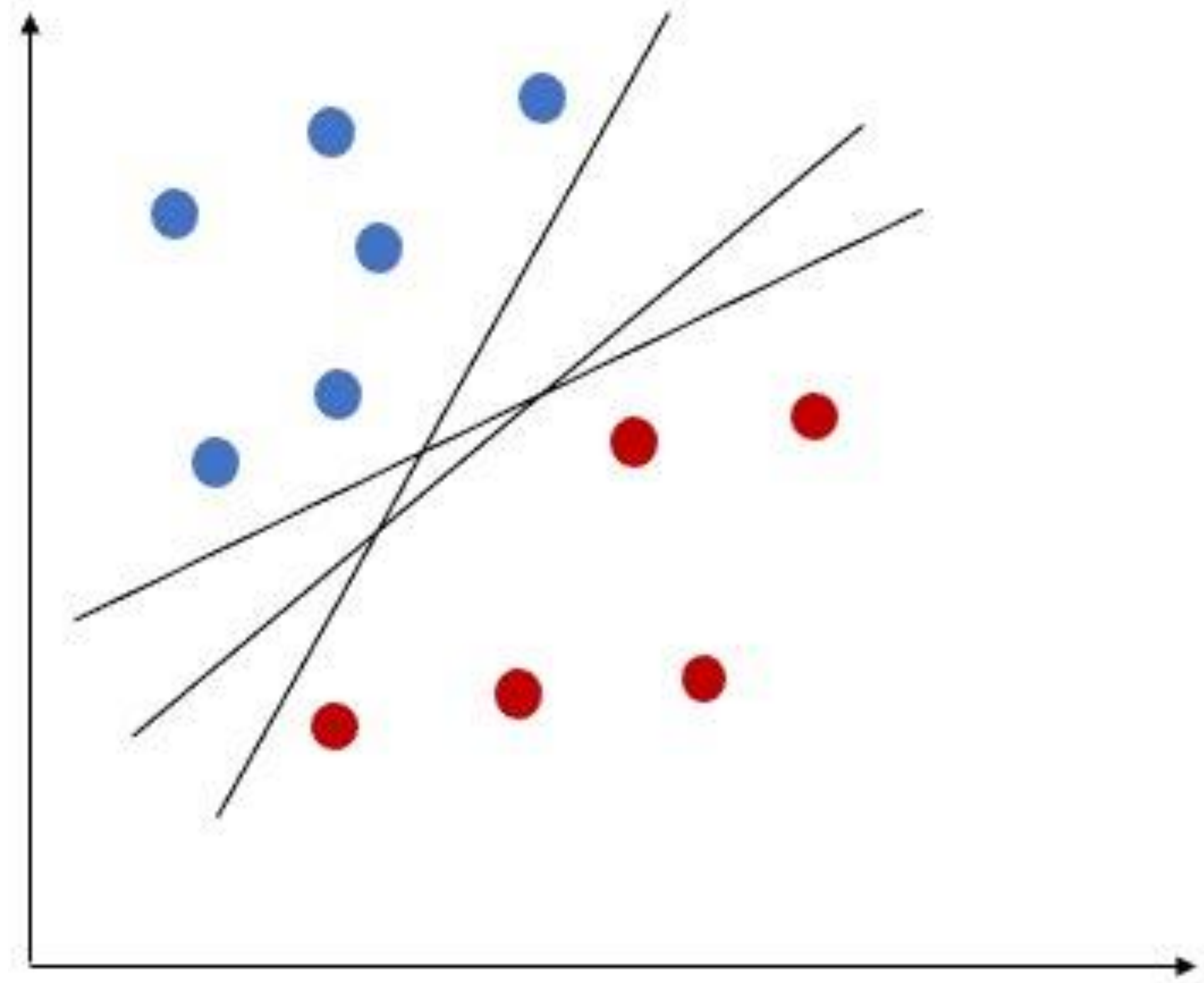
A **linear classifier** whose decision boundary is a hyperplane.

The support vector machine is an example of a linear classifier.

Support Vector Machines

There are many hyperplanes that would classify a training dataset perfectly.

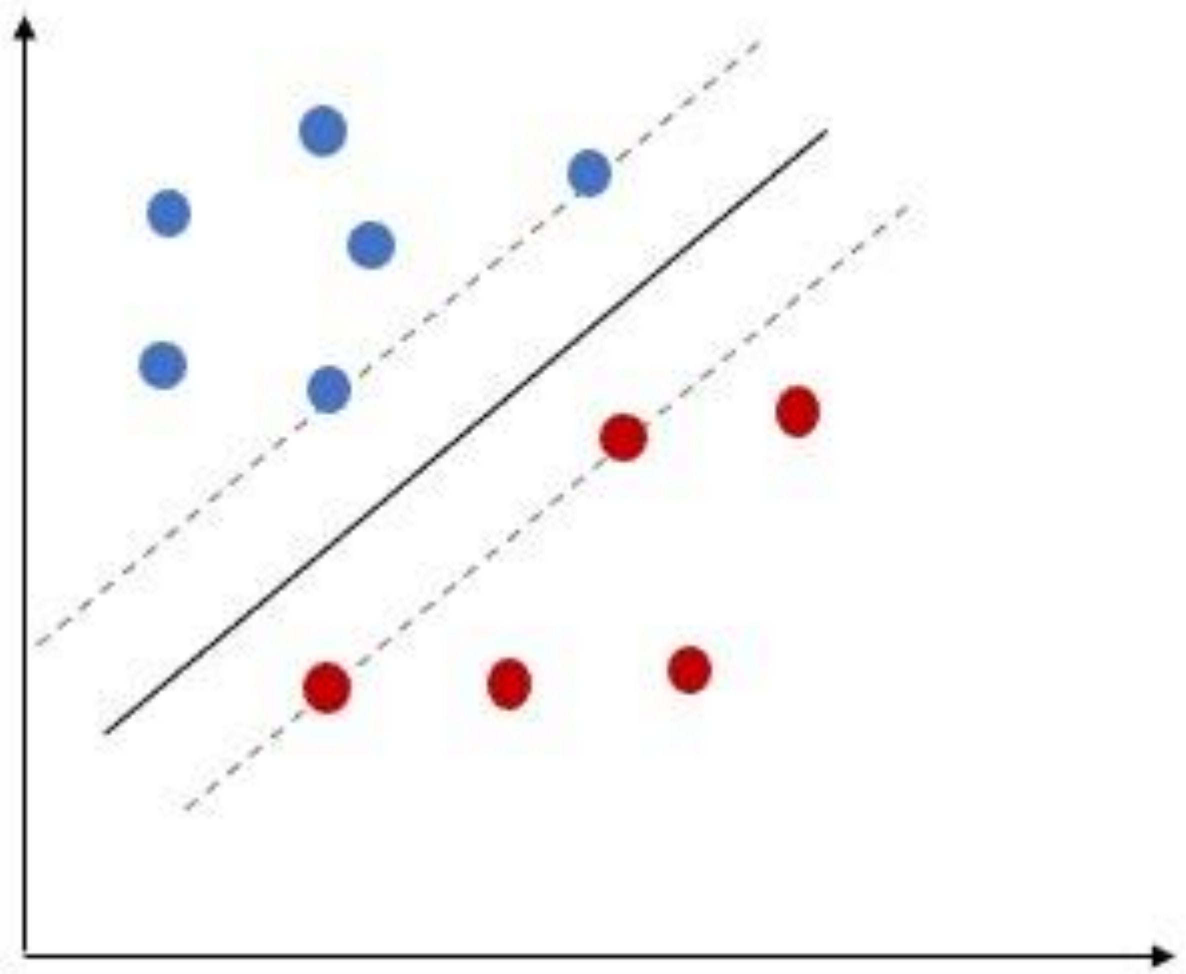
Which one should we choose?



Support Vector Machines

A boundary that is as far away from data points as possible is more robust to perturbations to the data points.

Intuitively, such a boundary is less prone to overfitting.



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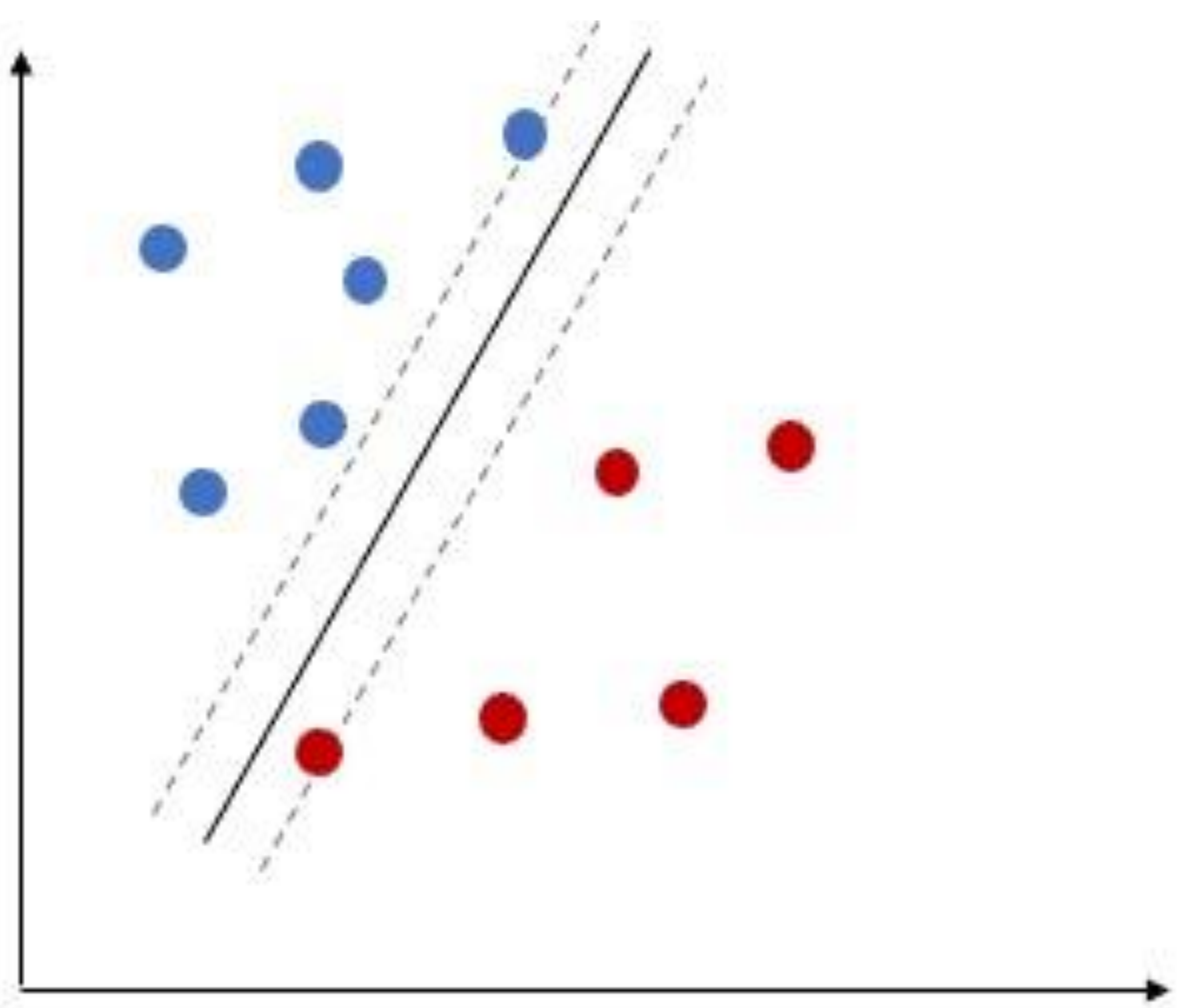


Less Preferred

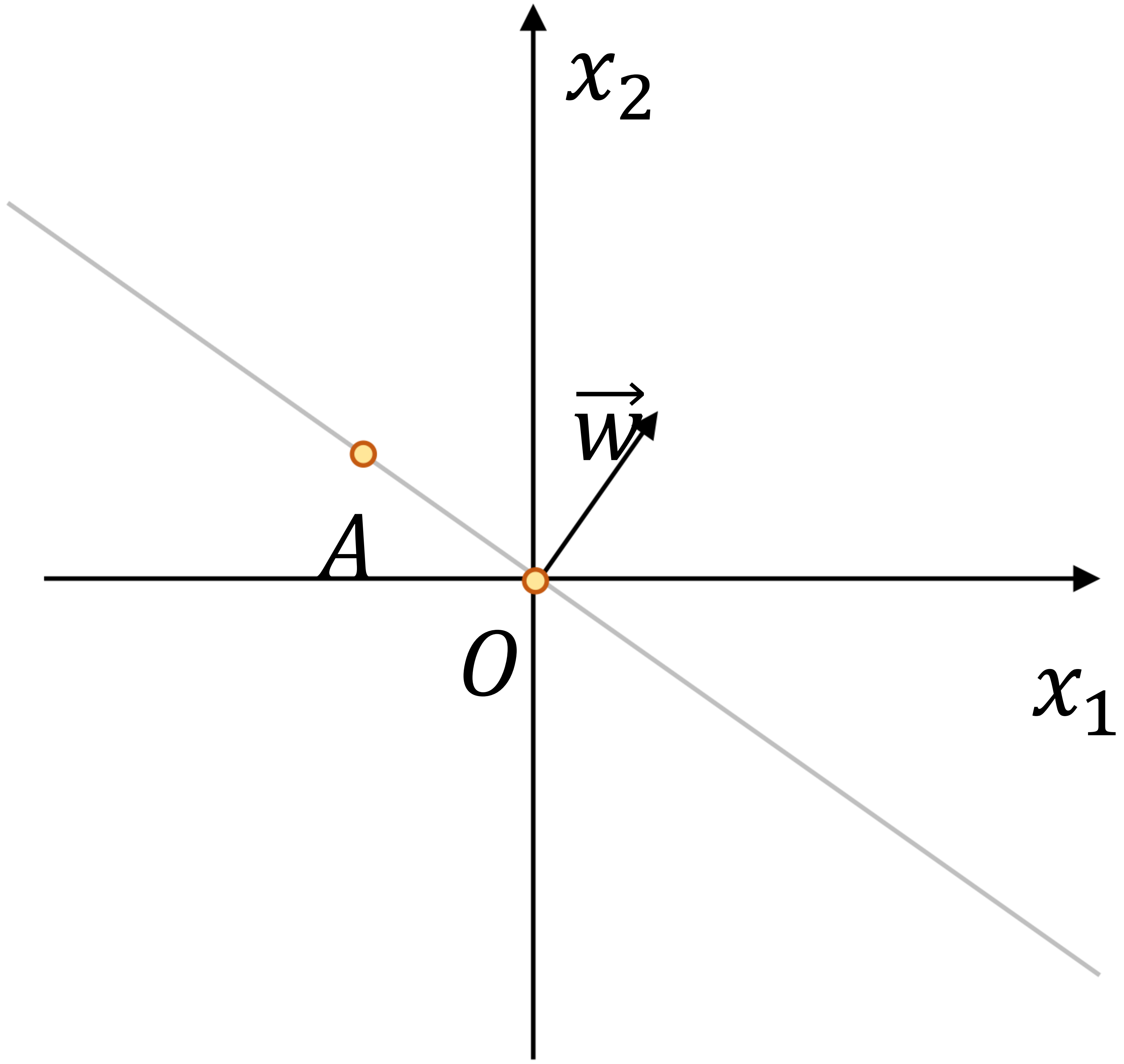
Let’s formulate an optimization problem to find such a boundary.

Hyperplanes

Consider a vector $\vec{w}$, and a hyperplane that is perpendicular to it (shown on the right).

For any A on the hyperplane, $\overrightarrow{OA}$ is perpendicular to $\vec{w}$.

Hence, $\vec{w}^{\top}(\overrightarrow{OA}) = 0$. So, this hyperplane corresponds to the set $\{\vec{x} | \vec{w}^{\top}\vec{x} = 0\}$.



Special case when $b = 0$

Hyperplanes

We shift the hyperplane in parallel (as shown on the right).

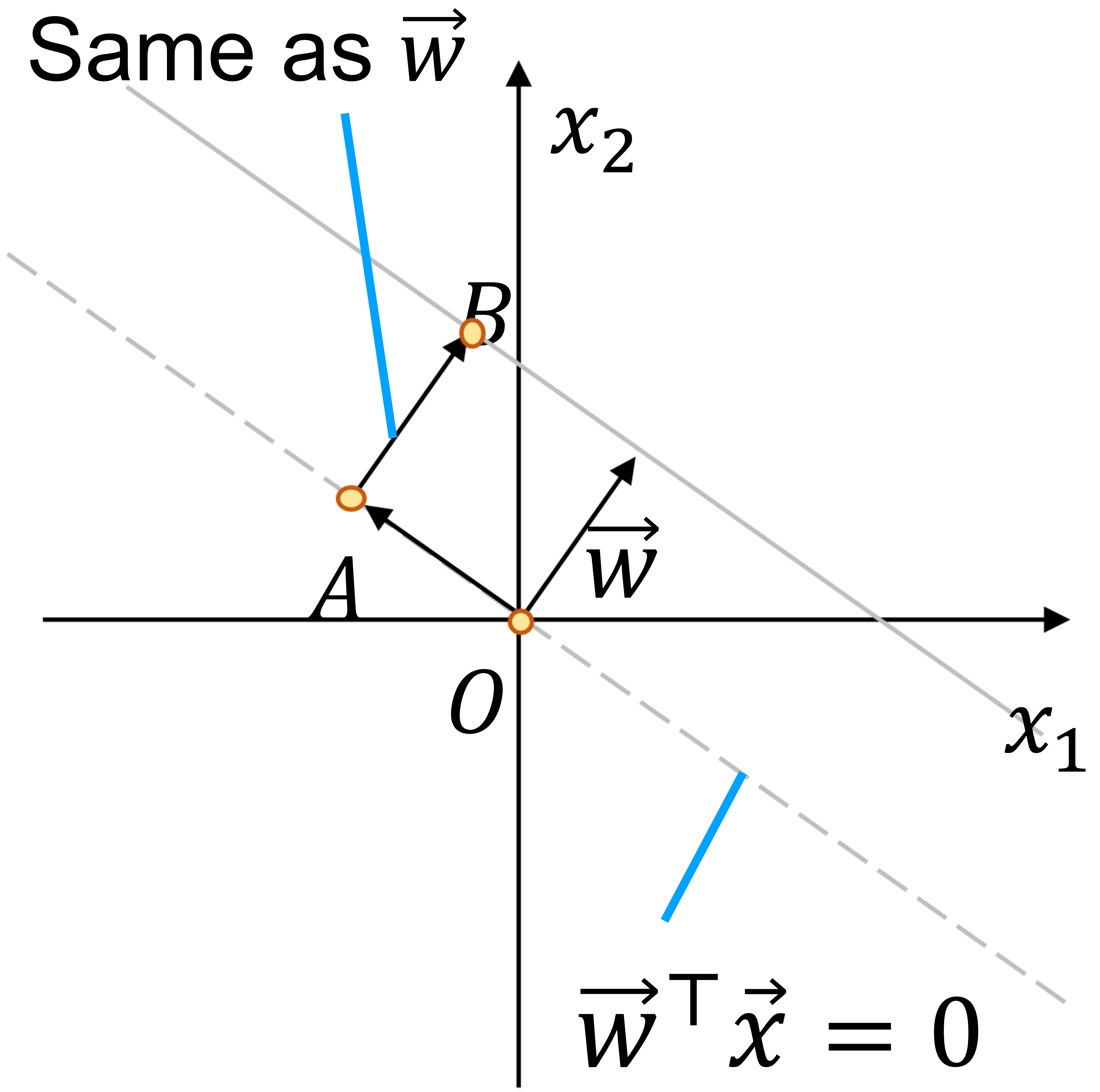
Consider any point B on the hyperplane and the vector $\overrightarrow{OB}$.

$$\vec{w}^\top\left(\overrightarrow{OB}\right) = \vec{w}^\top\left(\overrightarrow{OA} + \overrightarrow{AB}\right)$$
$$= \vec{w}^\top\left(\overrightarrow{OA}\right) + \vec{w}^\top\left(\overrightarrow{AB}\right)$$
$$= 0 + \vec{w}^\top\vec{w}$$
$$= \|\vec{w}\|_2^2$$

So, for any B on the hyperplane, $\vec{w}^\top(\overrightarrow{OB}) = \|\vec{w}\|_2^2$.

Hence, the hyperplane corresponds to the following set:

$$\{\vec{x} \mid \vec{w}^\top\vec{x} = \|\vec{w}\|_2^2\}$$

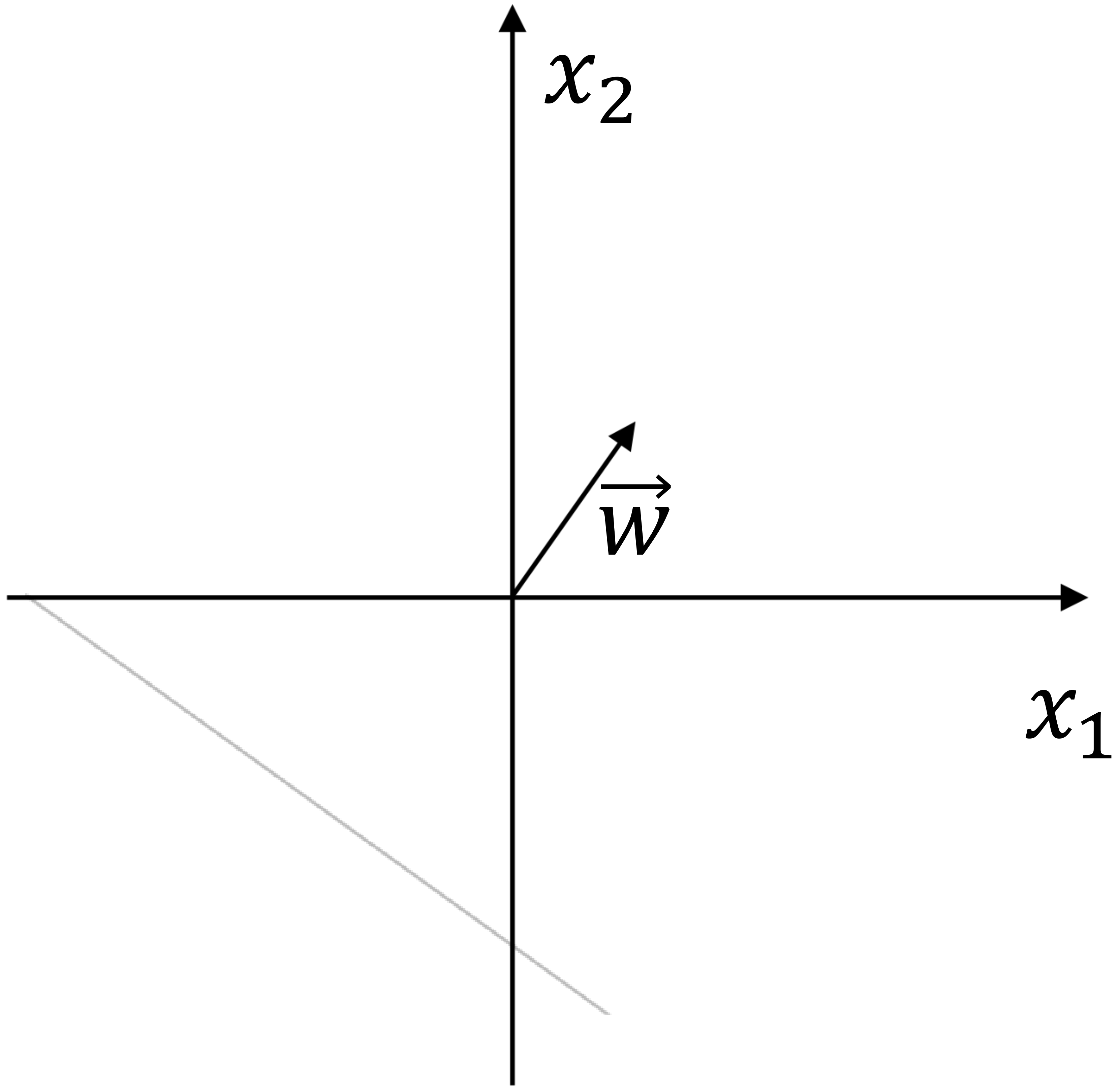


Special case when $b = \|\vec{w}\|_2^2$

Hyperplanes

So, in general:

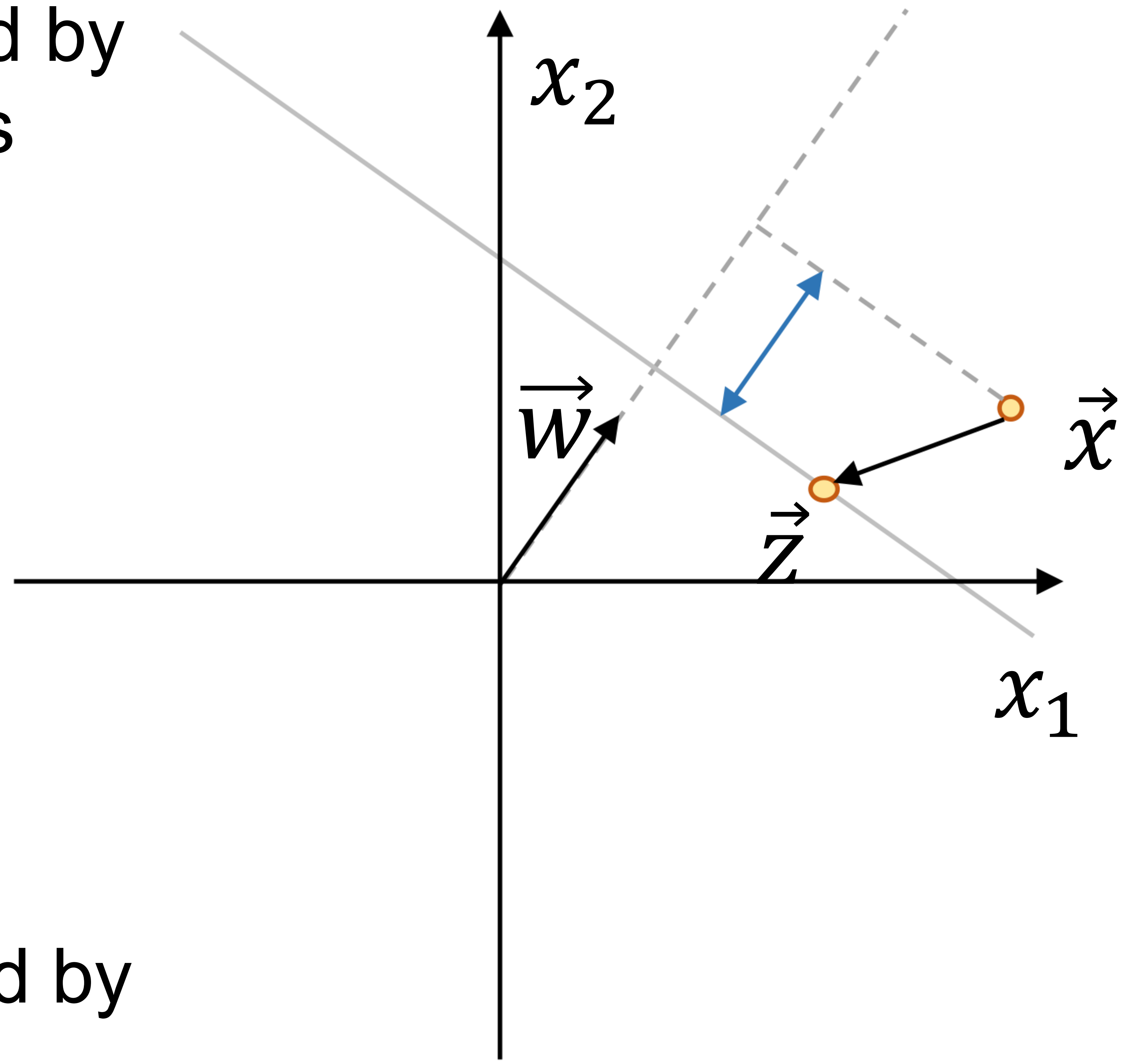
As b changes, $\{\vec{x} | \vec{w}^\top \vec{x} = b\}$ corresponds to shifting the hyperplane in parallel.



Distance to the Hyperplane

Consider an arbitrary points on the hyperplane, $\vec{z}$.

The distance to the hyperplane from $\vec{x}$ can be obtained by projecting the vector $\vec{x} - \vec{z}$ along the vector $\vec{w}$) which is orthogonal to the hyperplane).



The length of the projection is given by:

$$\left|\left\langle \vec{x} - \vec{z}, \frac{\vec{w}}{\|\vec{w}\|_2} \right\rangle\right| = \frac{1}{\|\vec{w}\|_2} |\langle \vec{x} - \vec{z}, \vec{w} \rangle|$$

$$= \frac{1}{\|\vec{w}\|_2} \left| \vec{w}^\top \vec{x} - \vec{w}^\top \vec{z} \right|$$

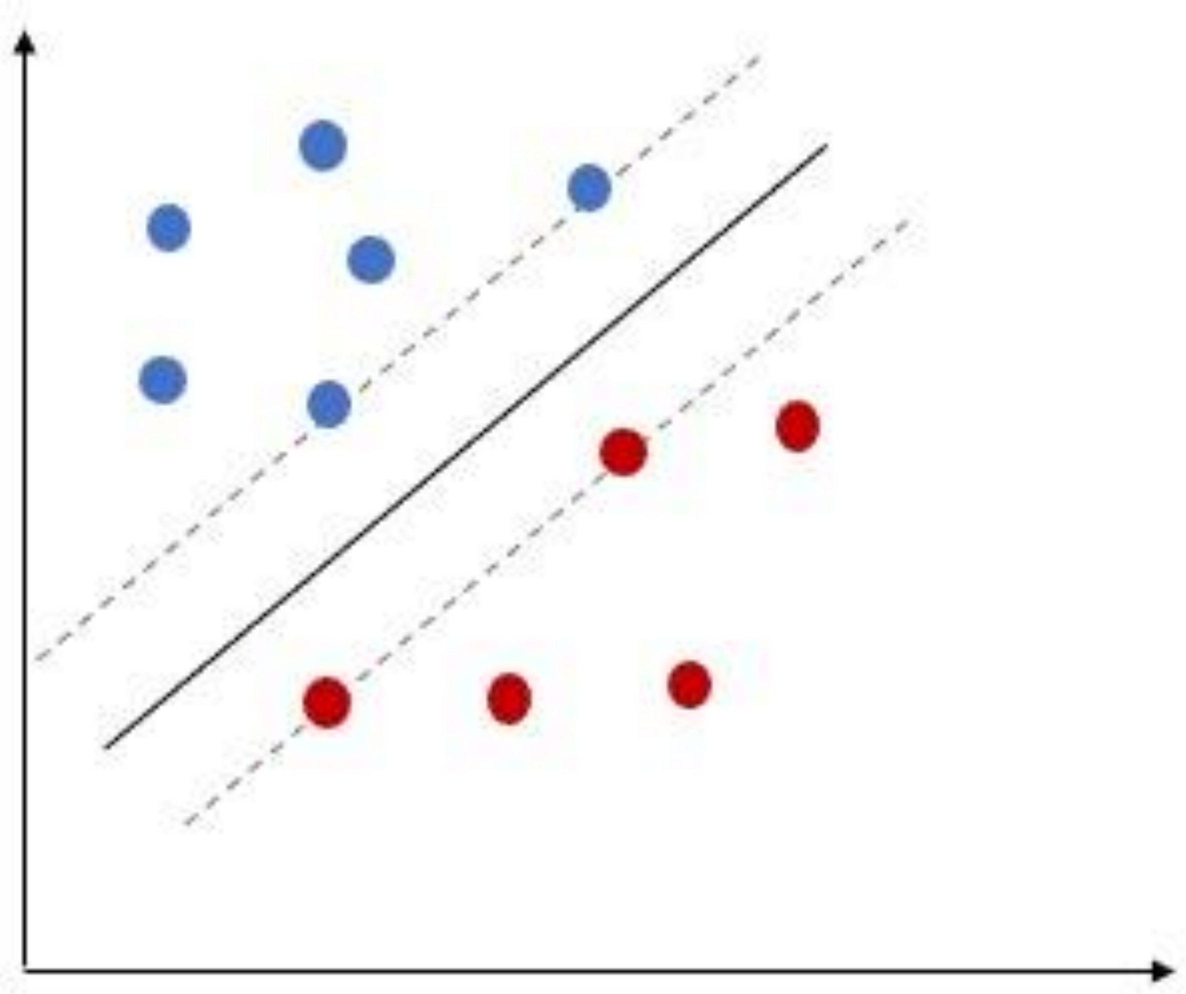
Because $\vec{z}$ is on the hyperplane, which is characterized by $\{\vec{x} | \vec{w}^\top \vec{x} = b\}$, $\vec{w}^\top \vec{z} = b$.

So, the distance to the hyperplane from $\vec{x}$ is $\frac{1}{\|\vec{w}\|_2} \left| \vec{w}^\top \vec{x} - b \right|$.

Goals of SVM

Recall: We would like to find a hyperplane that:

(1) Separates the positive data points from the negative data points
(2) Is as far away from the data points as possible



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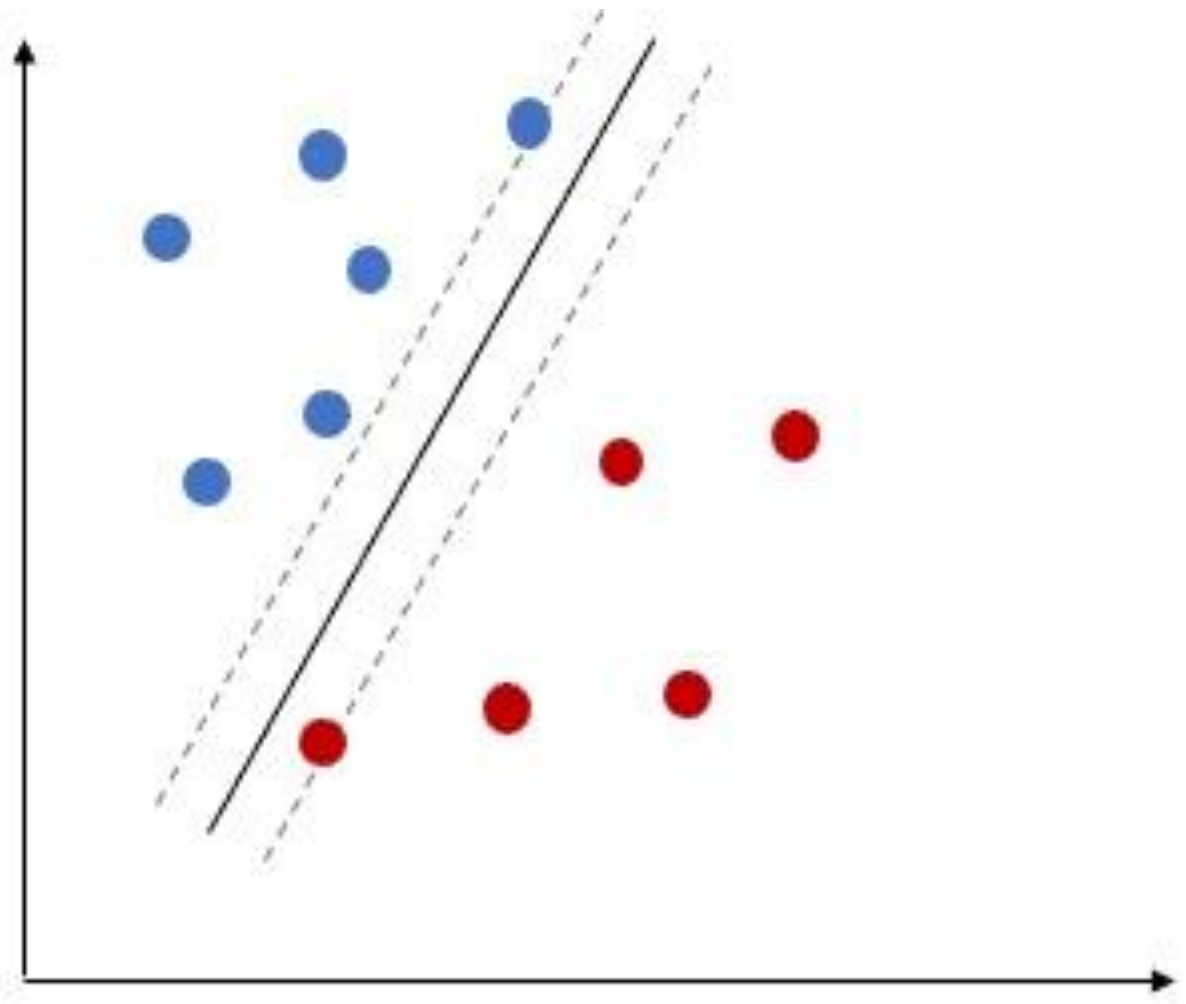

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Margin

We define the width of the buffer on each side of the hyperplane as the margin.

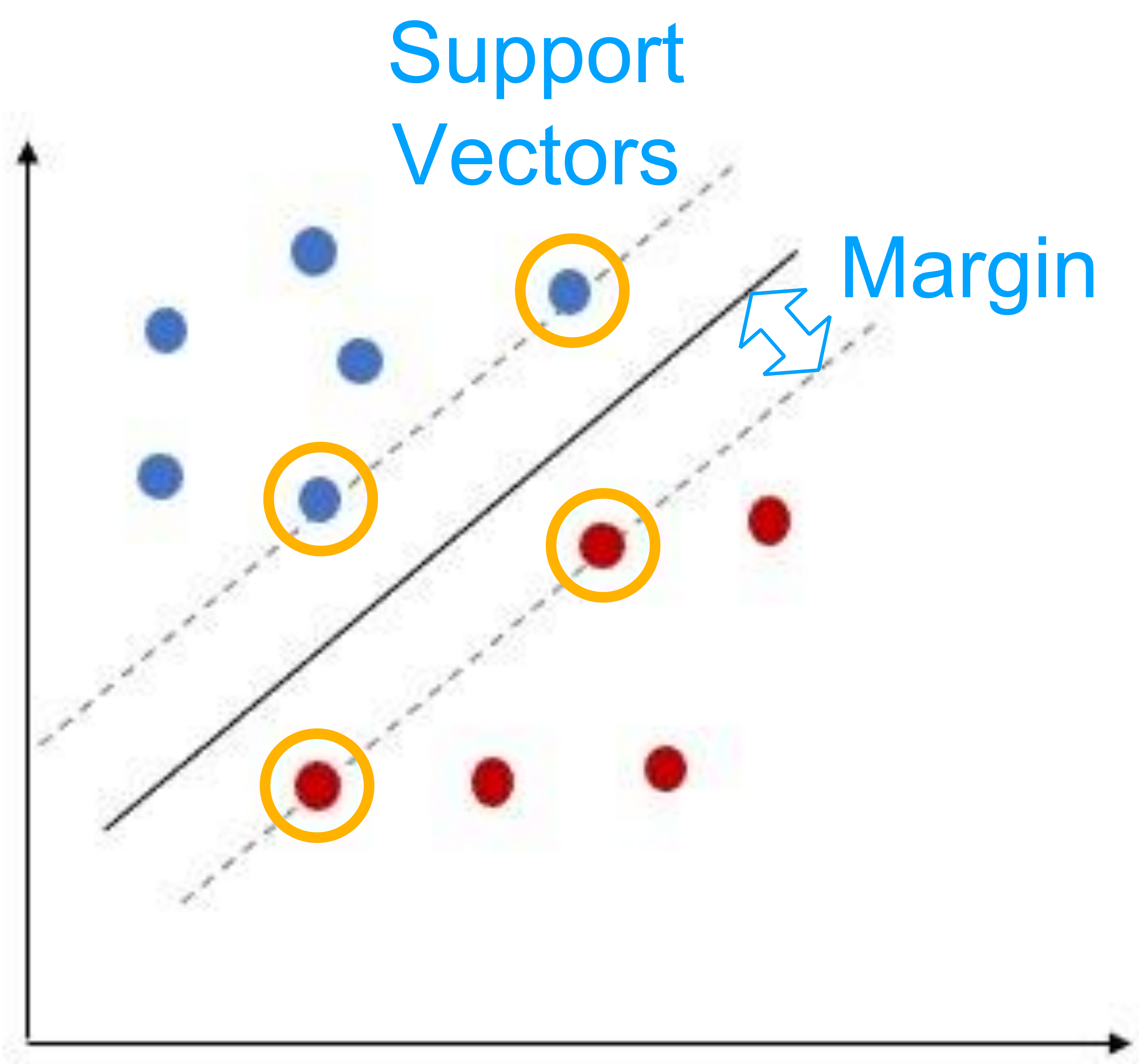
Let's derive a mathematical expression for the margin.

The margin is determined by the data points closest to the hyperplane.

These data points are known as **support vectors**.

The margin is the distance from support vectors to the hyperplane:

$$m = \min_i \left\{ \frac{1}{\|\vec{w}\|_2} \left| \vec{w}^\top \vec{x}_i - b \right| \right\}$$



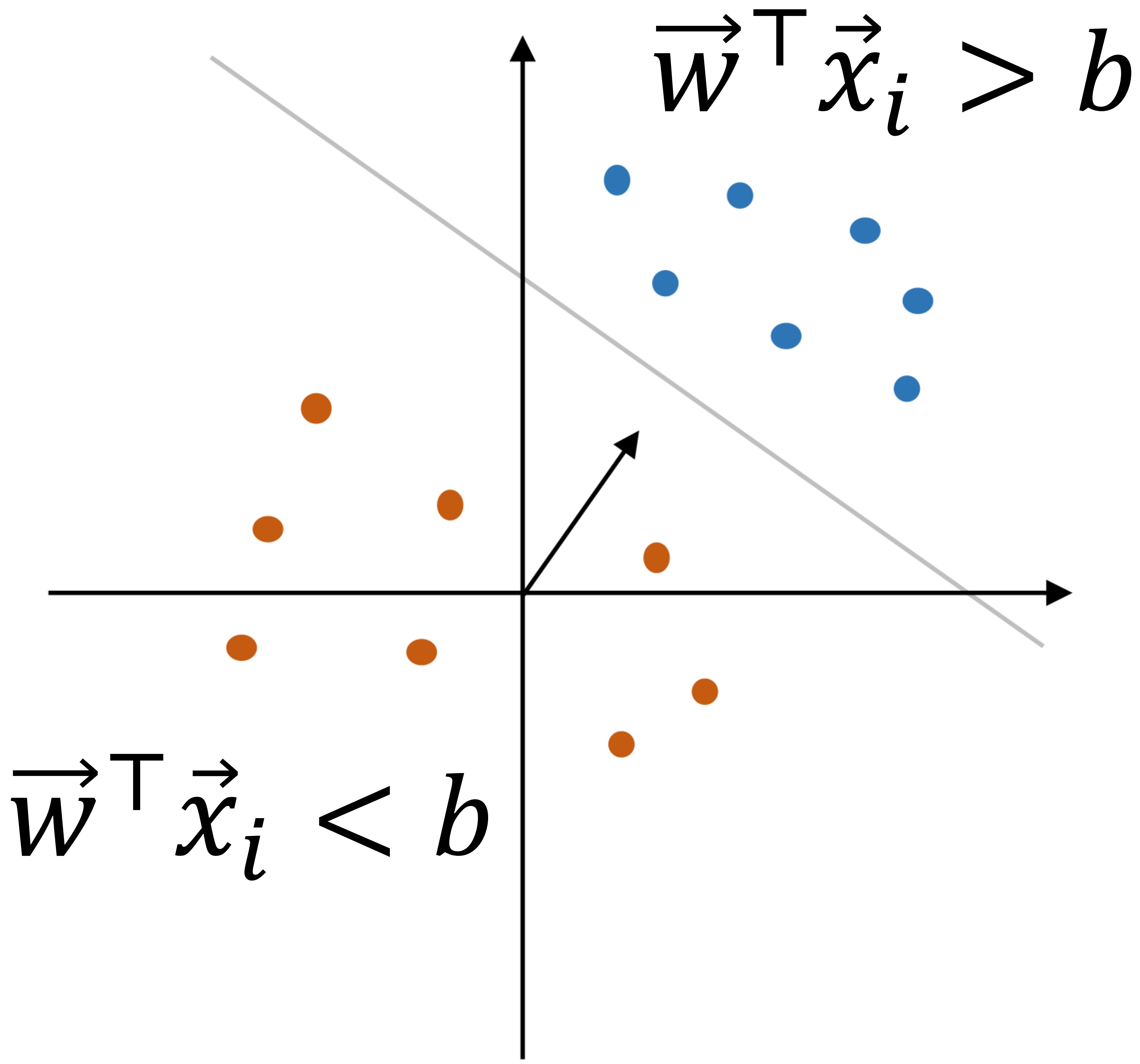
Formulation

Recall: We would like to find a hyperplane that:

(1) Separates the positive data points from the negative data points
$\vec{w}^\top \vec{x}_i > b$ for all i such that $y_i = 1$
$\vec{w}^\top \vec{x}_i < b$ for all i such that $y_i = -1$

(2) Is as far away from the data points as possible

Maximize the margin $m = \min_i \left\{ \frac{1}{\|\vec{w}\|_2} \left| \vec{w}^\top \vec{x}_i - b \right| \right\}$



Formulation

$$\max_{m,\vec{w},b} m$$

Maximize margin

subject to

$$\vec{w}^\top \vec{x}_i > b \text{ for all } i \text{ such that } y_i = 1,$$

For positive examples, should lie on one side of the hyperplane

$$\vec{w}^\top \vec{x}_i < b \text{ for all } i \text{ such that } y_i = -1,$$

For negative examples, should lie on one side of the hyperplane

$$m = \min_i \left\{ \frac{1}{\|\vec{w}\|_2} \left| \vec{w}^\top \vec{x}_i - b \right| \right\}$$

The definition of margin

Formulation

$$\max_{m,\vec{w},b} m$$

Maximize margin

subject to

$$\vec{w}^\top \vec{x}_i - b > 0 \text{ for all } i \text{ such that } y_i = 1,$$

For positive examples, should lie on one side of the hyperplane

$$\vec{w}^\top \vec{x}_i - b < 0 \text{ for all } i \text{ such that } y_i = -1,$$

For negative examples, should lie on one side of the hyperplane

$$m = \min_i \left\{ \frac{1}{\|\vec{w}\|_2} \left| \vec{w}^\top \vec{x}_i - b \right| \right\}$$

The definition of margin

Formulation

$$\max_{m,\vec{w},b} m$$

Maximize margin

subject to

$$\vec{w}^\top \vec{x}_i - b > 0 \ \forall i \text{ such that } y_i = 1,$$

For positive examples, should lie on one side of the hyperplane

$$\vec{w}^\top \vec{x}_i - b < 0 \ \forall i \text{ such that } y_i = -1,$$

For negative examples, should lie on one side of the hyperplane

$$\frac{1}{\|\vec{w}\|_2} \left| \vec{w}^\top \vec{x}_i - b \right| \geq m$$

The margin is by definition less than or equal to the distance from any data point to the hyperplane

$$m \geq 0$$

Formulation

$$\max_{m,\vec{w},b} m$$

Maximize margin

subject to

$$\vec{w}^\top \vec{x}_i - b > 0 \ \forall i \text{ such that } y_i = 1,$$

For positive examples, should lie on one side of the hyperplane

$$\vec{w}^\top \vec{x}_i - b < 0 \ \forall i \text{ such that } y_i = -1,$$

For negative examples, should lie on one side of the hyperplane

$$\left|\vec{w}^\top \vec{x}_i - b\right| \geq m \|\vec{w}\|_2 \ \forall i$$

$$m \geq 0$$

The margin is by definition less than or equal to the distance from any data point to the hyperplane

Formulation

$$\max_{m,\vec{w},b} m$$

Maximize margin

subject to

$$\vec{w}^\top \vec{x}_i - b > 0 \ \forall i \text{ such that } y_i = 1,$$

For positive examples, should lie on one side of the hyperplane

$$\vec{w}^\top \vec{x}_i - b < 0 \ \forall i \text{ such that } y_i = -1,$$

For negative examples, should lie on one side of the hyperplane

$$\vec{w}^\top \vec{x}_i - b \geq m\|\vec{w}\|_2 \text{ or } \vec{w}^\top \vec{x}_i - b \leq -m\|\vec{w}\|_2 \ \forall i$$

$$m \geq 0$$

Formulation

$$\max_{m,\vec{w},b} m$$

Maximize margin

subject to

$$\vec{w}^\top \vec{x}_i - b > 0 \ \forall i \text{ such that } y_i = 1,$$

For positive examples, should lie on one side of the hyperplane

$$\vec{w}^\top \vec{x}_i - b < 0 \ \forall i \text{ such that } y_i = -1,$$

For negative examples, should lie on one side of the hyperplane

$$\vec{w}^\top \vec{x}_i - b \geq m \|\vec{w}\|_2 \ \forall i \text{ such that } y_i = 1,$$

$$\vec{w}^\top \vec{x}_i - b \leq -m \|\vec{w}\|_2 \ \forall i \text{ such that } y_i = -1,$$

$$m \geq 0$$

Formulation

Maximize margin

$$\max_{m,\vec{w},b} m$$

subject to

$$\vec{w}^{\top}\vec{x}_i - b \geq m\|\vec{w}\|_2 \ \forall i \text{ such that } y_i = 1,$$

$$\vec{w}^{\top}\vec{x}_i - b \leq -m\|\vec{w}\|_2 \ \forall i \text{ such that } y_i = -1,$$

$$m \geq 0$$

Formulation

Maximize margin

$$\max_{m,\vec{w},b} m$$

subject to

$$1 \cdot \left(\vec{w}^\top \vec{x}_i - b\right) \geq m\|\vec{w}\|_2 \ \forall i \text{ such that } y_i = 1,$$

$$-1 \cdot \left(\vec{w}^\top \vec{x}_i - b\right) \geq m\|\vec{w}\|_2 \ \forall i \text{ such that } y_i = -1,$$

$$m \geq 0$$

Formulation

$$\max_{m,\vec{w},b} m$$

Maximize margin

subject to

$$y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq m\|\vec{w}\|_2 \ \forall i \text{ such that } y_i = 1,$$

$$y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq m\|\vec{w}\|_2 \ \forall i \text{ such that } y_i = -1,$$

$$m \geq 0$$

Formulation

$$\max_{m,\vec{w},b} m$$

subject to

$$y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq m\|\vec{w}\|_2$$

$$m \geq 0$$

Formulation

$$\max_{m,\vec{w},b} m$$

subject to

$$y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq m\|\vec{w}\|_2$$

$$m \geq 0$$

$$\max_{m,\vec{w},b} m$$

subject to

$$y_i\left((\alpha\vec{w})^\top \vec{x}_i - (\alpha b)\right) \geq m\|(\alpha\vec{w})\|_2$$

$$m \geq 0$$

It turns out that the scale of $\begin{pmatrix}\vec{w}\\ b\end{pmatrix}$ doesn't matter, in the sense that if $\begin{pmatrix}\vec{w}^*\\ b^*\\ m^*\end{pmatrix}$ is a feasible solution, then $\begin{pmatrix}\alpha\vec{w}^*\\ \alpha b^*\\ m^*\end{pmatrix}$ is feasible and achieves the same objective value as $\begin{pmatrix}\vec{w}^*\\ b^*\\ m^*\end{pmatrix}$ for any $\alpha > 0$.

Formulation

$$\max_{m,\vec{w},b} m$$

subject to

$$y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq m\|\vec{w}\|_2$$

$$m \geq 0$$

$$\max_{m,\vec{w},b} m$$

subject to

$$\alpha y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq m|\alpha|\|\vec{w}\|_2$$

$$m \geq 0$$

It turns out that the scale of $\begin{pmatrix}\vec{w}\\ b\end{pmatrix}$ doesn't matter, in the sense that if $\begin{pmatrix}\vec{w}^*\\ b^*\\ m^*\end{pmatrix}$ is a feasible solution, then $\begin{pmatrix}\alpha\vec{w}^*\\ \alpha b^*\\ m^*\end{pmatrix}$ is feasible and achieves the same objective value as $\begin{pmatrix}\vec{w}^*\\ b^*\\ m^*\end{pmatrix}$ for any $\alpha > 0$.

Formulation

$$\max_{m,\vec{w},b} m$$

subject to

$$y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq m\|\vec{w}\|_2$$

$$m \geq 0$$

Therefore, without loss of generality, we can set the scale of $\vec{w}$.

We set $\|\vec{w}\|_2 = \frac{1}{m}$, so $m = \frac{1}{\|\vec{w}\|_2}$

Formulation

$$\max_{\vec{w},b} \frac{1}{\|\vec{w}\|_2}$$

subject to

$$y_i(\vec{w}^\top \vec{x}_i - b) \geq 1$$

Since $x \mapsto \frac{1}{x}$ is strictly decreasing, we can apply the transformation to the objective and change the max to a min.

Formulation

$$\min_{\vec{w},b} ||\vec{w}||_2$$

subject to

$$y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq 1$$

Want to make the objective function convex. Will see why this is useful later.

Since $x \mapsto \frac{1}{2}x^2$ is strictly increasing for $x \geq 0$, we can apply the transformation to the objective.

Formulation

$$\min_{\vec{w},b} \frac{1}{2} ||\vec{w}||_2^2$$

subject to

$$y_i\left(\vec{w}^\top \vec{x}_i - b\right) \geq 1$$

Since $x \mapsto \frac{1}{2}x^2$ is strictly increasing for $x \geq 0$, we can apply the transformation to the objective.

This is an example of a constrained optimization problem