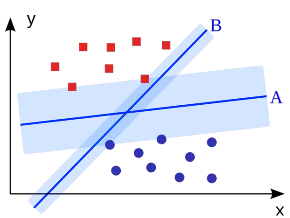
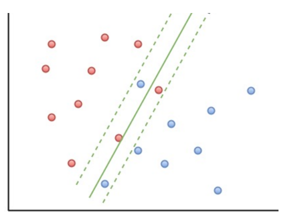
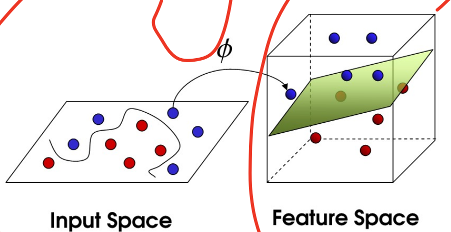
Section 16. Support vector machines and kernel methods

SVM

- Support Vector Machines
- Lagrange multiplier (KKT theorem)
- Regularization
- Kernel Methods







➢ **Support Vector Machines (SVM)**

1963

SVM was Developed at AT&T Bell Laboratories by Vladimir Vapnik with colleagues in 1994.

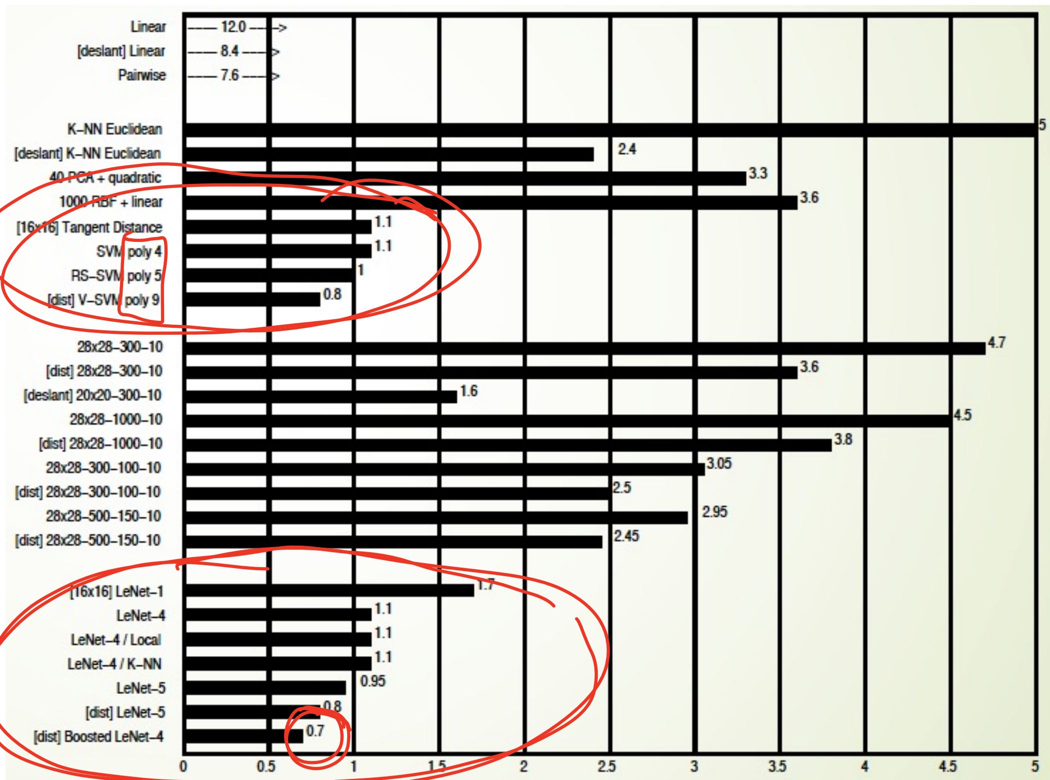
- Support vector machine is one of the most popular machine learning methodologies.
- Empirically successful, with well developed theory.
- One of the best off-the-shelf methods.
- We mainly address classification.

SVM v.s. CNN:

Simple SVM performs as well as Multilayer Convolutional Neural Networks which need careful tuning (LeNets) (Second dark era for NN: 2000s)

MNIST Dataset Test Error: SVM vs. CNN

2010



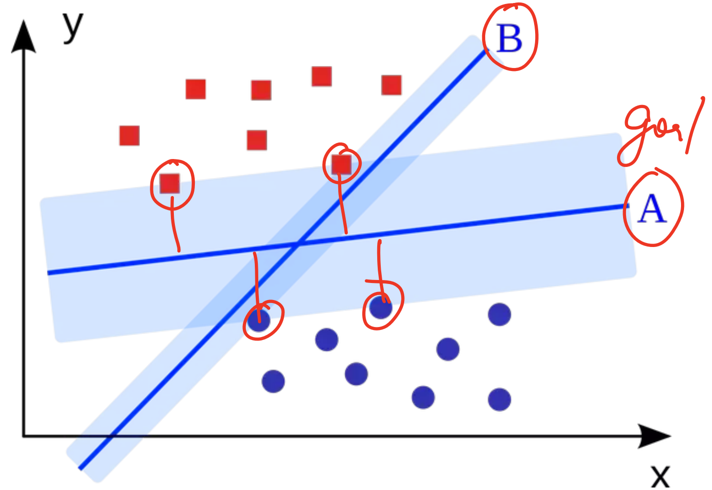
LeCun et al. 1998

➢ **Support Vector Machines (SVM)** for binary classification. (Max-Margin Classifier)

Assume the datasets are ***linearly separable***.

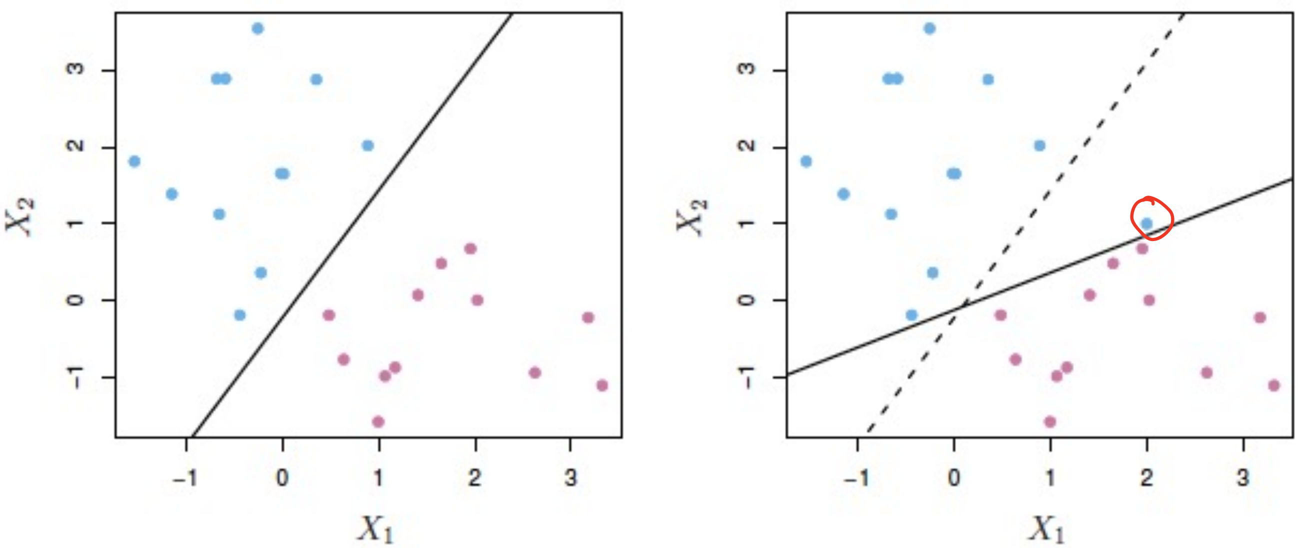
Maximal margin hyperplane:

- The **optimal** separating hyperplane that is **farthest** from the training observations.
- The separating hyperplane such that the **minimum** distance of any training point to the hyperplane is the **largest**.



- Creates the **widest gap** between the two classes.
- Points on the boundary hyperplane, those with smallest distance to the max margin hyperplane, are called **support vectors**. They support the maximal margin hyperplane in the sense vector that if these points were moved slightly then the maximal margin hyperplane would move as well.

- Note that **margin** M > 0 is the **half** of the width of the strip separating the two classes.
- The eventual solution, the **max margin hyperplane** is determined by the **support vectors.**
- If $x^{(i)}$ on the correct side of the trip varies, the solution would remain same.
- The max margin hyperplane may vary a lot when the support vectors vary.



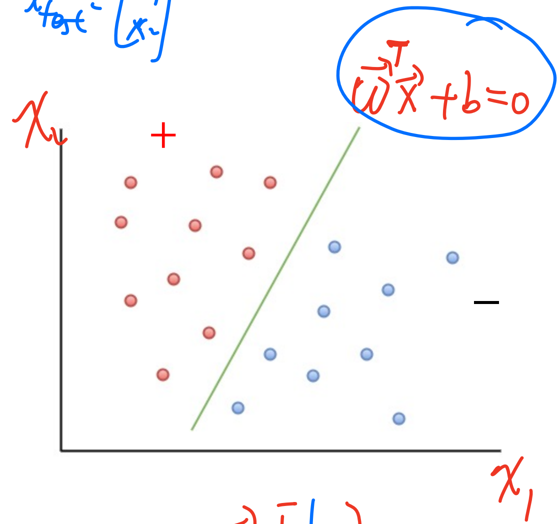
➢ SVM setup:

Binary Classification Data: $D = \{(\vec{x}^{(i)}, y^{(i)}), i = 1, \dots n\}$ $\quad y^{(i)} \in \{-1, 1\}$,

Assume the datasets are ***linearly separable***.

$\vec{x}_{test} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

Goal: Find a **linear classifier**:



$\vec{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}$

$$h(\vec{x}) = \text{sign}\left(\vec{\theta}^T\vec{x}\right) = \text{sign}(\vec{w} \cdot \vec{x} + b)$$

$$h(\vec{x}) = \begin{cases} 1, & if\ \vec{w} \cdot \vec{x} + b \geq 0 \\ -1, & if\ \vec{w} \cdot \vec{x} + b < 0 \end{cases}$$

Notations: $\vec{\theta} = \begin{bmatrix} b \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$ $\quad \vec{x} = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}$ or $\vec{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$

Decision Boundary: Hyperplane H

$H = \{ \vec{x} \mid \vec{\theta}^T \vec{x} = 0 \}$

or: $w_1 x_1 + \cdots w_d x_d + b = 0$

or:

$$\vec{w}^T \vec{x} + b = 0$$

Property:

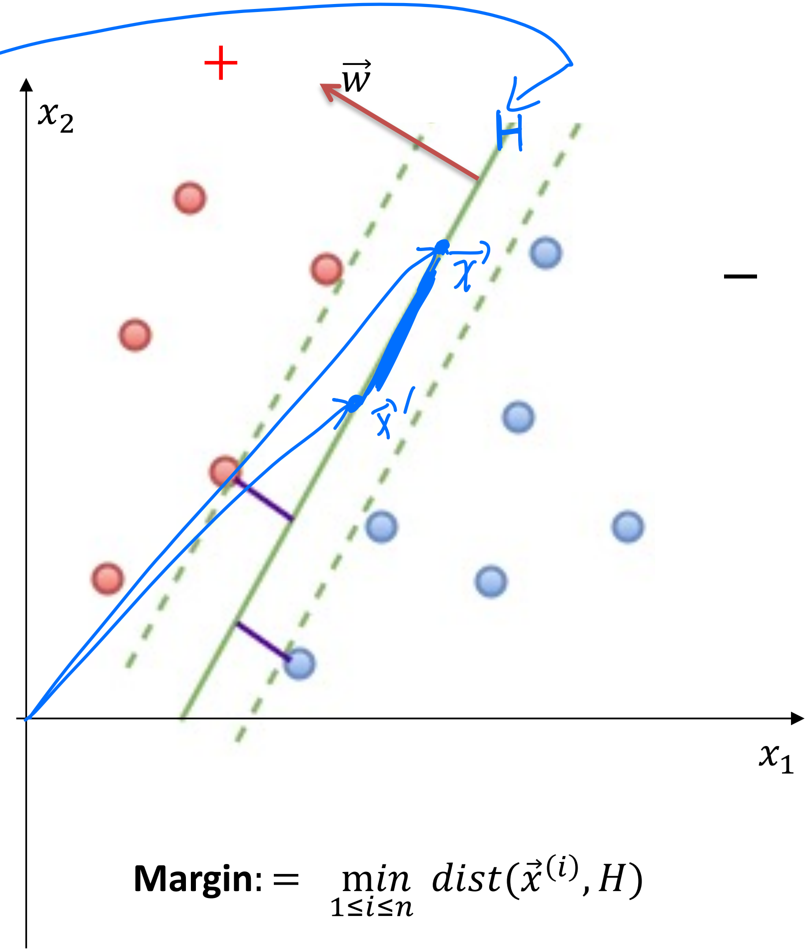
$\vec{w}$ is orthogonal to the hyperplane H.

Reason:
Any two points $\vec{x}$ and $\vec{x}'$ on hyperplane,

$$\vec{w}^T \vec{x} + b = 0$$

$$\vec{w}^T \vec{x}' + b = 0$$

So, $\vec{w} \cdot (\vec{x} - \vec{x}') = 0$.

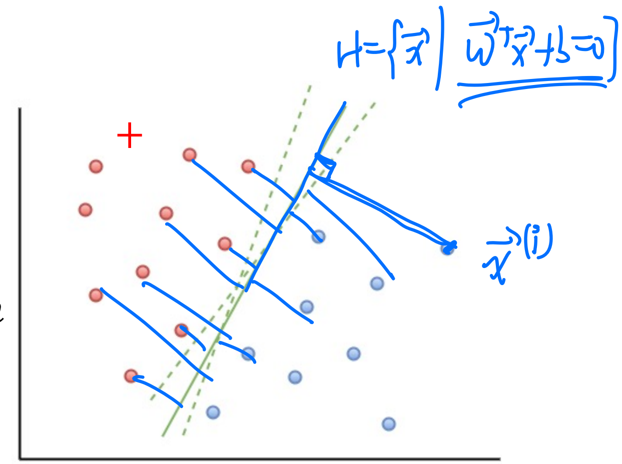


Margin: $= \min_{1 \le i \le n} dist(\vec{x}^{(i)}, H)$

➢ Maximal margin hyperplane (Hard-margin SVM classifier)

Initial Goal: Find hyperplane parameters $\vec{w}$ and b such that for all $1 \leq i \leq n$

$$y^{(i)} = \begin{cases} 1, & if\ \vec{w} \cdot \vec{x}^{(i)} + b \geq 0 \\ -1, & if\ \vec{w} \cdot \vec{x}^{(i)} + b < 0 \end{cases}$$



Equivalently, find $\vec{w}$ and b such that for all $1 \leq i \leq n$

$$y^{(i)}\left(\vec{w} \cdot \vec{x}^{(i)} + b\right) > 0 \qquad \text{(I)}$$

There are many different hyperplanes $H = \{\vec{x} \mid \vec{w}^T \vec{x} + b = 0\}$.

Question: What is the best separating hyperplane?

Updated SVM Goal: Find hyperplane with **largest margin**

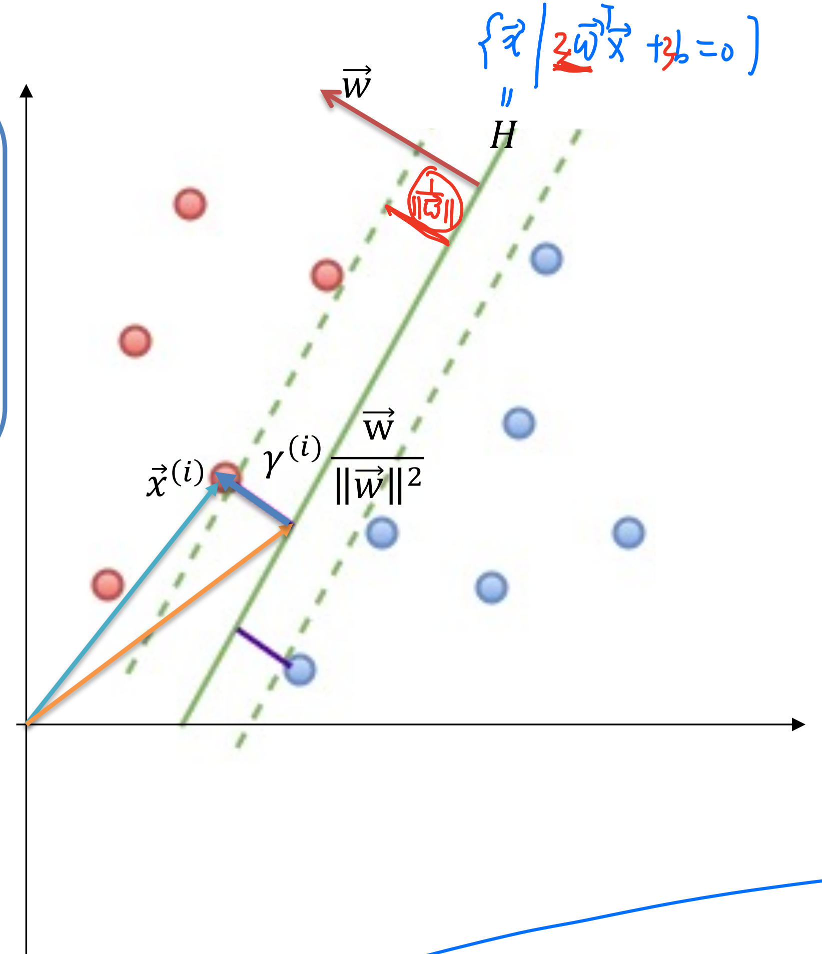
Find $\vec{w}$ and b such that (I) and

$$\max_{\vec{w},b} \text{Margin} := \max_{\vec{w},b} \boxed{\min_{1\leq i\leq n} dist(\vec{x}^{(i)}, H)} \qquad \text{(II)}$$

Property: The **distance** $\gamma^{(i)}$ between $\vec{x}^{(i)}$ and H is

$$\gamma^{(i)} := dist(\vec{x}^{(i)}, H)$$

$$= y^{(i)} \frac{1}{\|\vec{w}\|}(\vec{w} \cdot \vec{x}^{(i)} + b)$$



Proof: For positive point $(\vec{x}^{(i)}, y^{(i)} = 1)$,

$$\vec{w}^T \boxed{\left(\vec{x}^{(i)} - \gamma^{(i)} \frac{\vec{w}}{\|\vec{w}\|^2}\right)} + b = 0$$

Solve $\gamma^{(i)}$ we have

$$\gamma^{(i)} = \frac{1}{\|\vec{w}\|}(\vec{w} \cdot \vec{x}^{(i)} + b)$$

Similarly for negative label points, we have $\gamma^{(i)} = -\frac{1}{\|\vec{w}\|}(\vec{w} \cdot \vec{x}^{(i)} + b)$.

SVM Goal: Find $\vec{w}$ and b such that $y^{(i)}(\vec{w}\cdot\vec{x}^{(i)}+b) > 0$ for all $1 \le i \le n$

1

and $\max\limits_{\vec{w},b}\ \min\limits_{1\le i\le n} dist(\vec{x}^{(i)}, H)$ 2

Equivalently, find $\vec{w}$ and b

$$\max_{\vec{w},b}\ \min_{1\le i\le n} y^{(i)}\frac{1}{\|\vec{w}\|}\left(\vec{w}\cdot\vec{x}^{(i)}+b\right) \text{ such that } y^{(i)}\left(\vec{w}\cdot\vec{x}^{(i)}+b\right) > 0$$

Equivalently, find $\vec{w}$ and b

$$\max_{\vec{w},b}\frac{1}{\|\vec{w}\|}\min_{1\le i\le n} y^{(i)}\left(\vec{w}\cdot\vec{x}^{(i)}+b\right) \text{ such that } y^{(i)}\left(\vec{w}\cdot\vec{x}^{(i)}+b\right) > 0$$

algebraic margin.

Denote $\lambda := \min\limits_{1\le i\le n} y^{(i)}\left(\vec{w}\cdot\vec{x}^{(i)}+b\right)$. Equivalently, find $\vec{w}$ and b

= 1

$$\max_{\vec{w},b}\frac{1}{\|\vec{w}\|}\lambda \text{ such that } y^{(i)}\left(\vec{w}\cdot\vec{x}^{(i)}+b\right) \ge \lambda$$

For the **same** hyperplane $H = \{\vec{x}\ |\vec{w}^T\vec{x}+b=0\}$, we can scale $\vec{w}$ and b anyway we want. So, we choose a 'smart' scale such that $\lambda = 1$, i.e., **margin**$= \frac{1}{\|\vec{w}\|}$

Equivalently, find $\vec{w}$ and b

$$\max_{\vec{w},b} \frac{1}{\|\vec{w}\|} \text{ such that } y^{(i)}(\vec{w}\cdot\vec{x}^{(i)}+b) \geq 1$$

for each $i=1,\ldots,n$

Equivalently, find $\vec{w}$ and b

$$\max_{\vec{w},b} \frac{1}{\|\vec{w}\|^2} \text{ such that } 1 - y^{(i)}(\vec{w}\cdot\vec{x}^{(i)}+b) \geq 0$$

Equivalently, find $\vec{w}$ and b

$= w_1^2 + w_2^2 + \cdots + w_d^2$

$$\min_{\vec{w},b} \vec{w}^T\vec{w} \text{ such that } 1 - y^{(i)}(\vec{w}\cdot\vec{x}^{(i)}+b) \leq 0$$

$i=1,\ldots,n$

quadratic linear

The objective is a *quadratic term,* and the constraints are all *linear, which* is called a quadratic optimization problem. https://en.wikipedia.org/wiki/Quadratic_programming

It has a unique solution whenever a separating hyper plane exists

Remarks: SVM

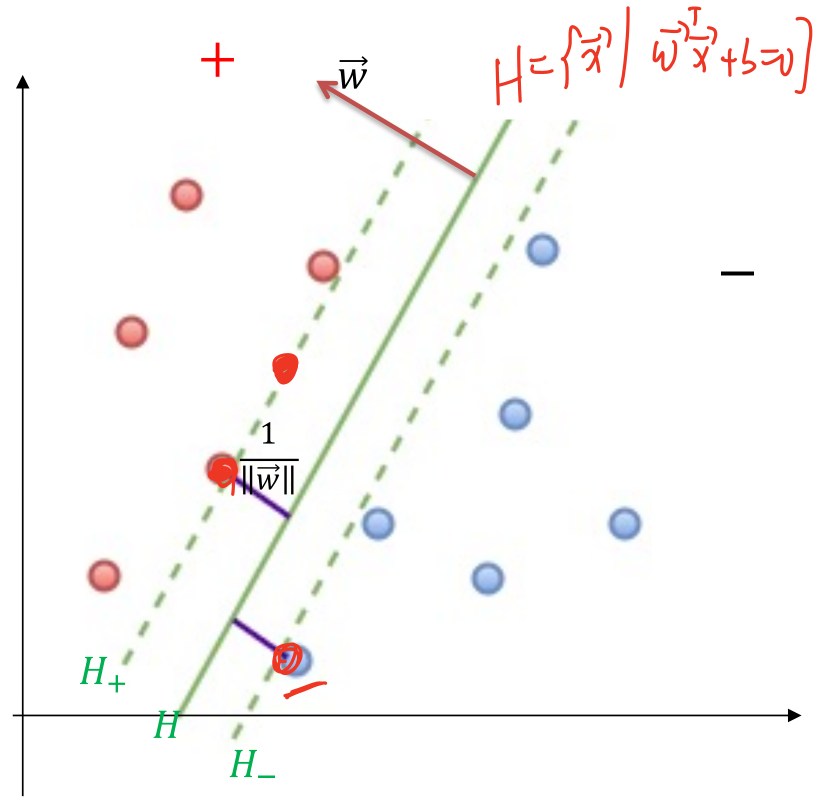
- The constraints $y^{(i)}\left(\vec{w}\cdot\vec{x}^{(i)}+b\right)\geq 1$ for all i are equivalent to **margin**$=\frac{1}{\|\vec{w}\|}$

- The max-margin separating hyperplane, and two margin hyperplanes are:

$$H=\{\vec{x}\mid\vec{w}\cdot\vec{x}+b=0\}$$

$$H_{+}=\{\vec{x}\mid\vec{w}\cdot\vec{x}+b=1\}$$

$$H_{-}=\{\vec{x}\mid\vec{w}\cdot\vec{x}+b=-1\}$$



- For optimal $\vec{w},b$, the support vectors $(\vec{x}^{(i)},y^{(i)})$ satisfy

$$y^{(i)}\left(\vec{w}\cdot\vec{x}^{(i)}+b\right)=1$$

Optimization with Constraints.

Example: Consider the optimization problem

$$\text{Maximize(Minimize) } f(x,y) \text{ subject to } g(x,y) = c$$

sln.

Following J. Lagrange (1736–1813),

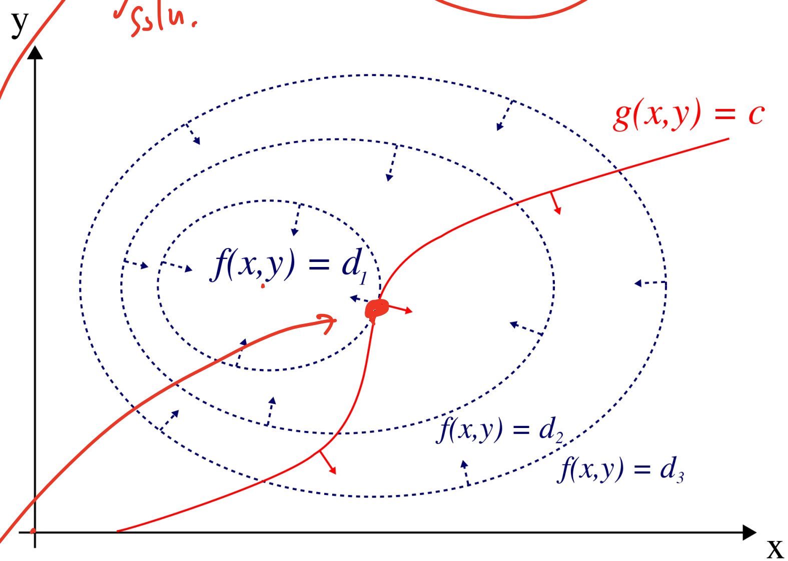
we can to define Lagrangian

$$L(x,y,\lambda) := f(x,y) - \lambda(g(x,y) - c)$$

and calculate gradients

$$\nabla_{x,y,\lambda} L = 0$$

$$\begin{cases} \dfrac{\partial L}{\partial x} = 0 \\ \dfrac{\partial L}{\partial y} = 0 \\ g(x,y) = c \end{cases}$$



➢ Optimization with Constraints.

e.g. $f(\vec{w}) := \vec{w}^T \vec{w}$

Optimization Question (⭐):

or max

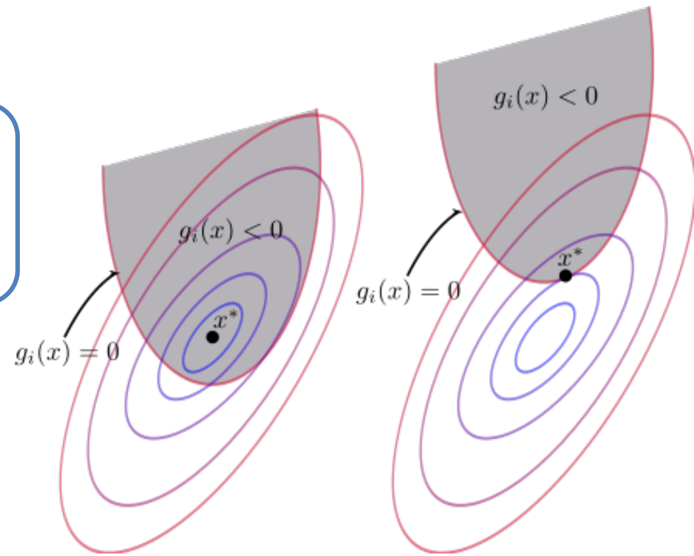
Optimize $\min_{\vec{w}} f(\vec{w})$

such that $g_i(\vec{w}) \le 0$ *and* $h_j(\vec{w}) = 0$ for $1 \le i \le m$ and $1 \le j \le n$

Define **Lagrangian**:

$$L(\vec{w}, \vec{\alpha}, \vec{\beta}) := f(\vec{w}) + \sum_{i=1}^{m} \alpha_i g_i(\vec{w}) + \sum_{j=1}^{n} \beta_j h_j(\vec{w})$$

Here, $\vec{\alpha}$ *and* $\vec{\beta}$ are Lagrange multipliers



➢ Karush(1939)–Kuhn–Tucker (1951) Theorem (KKT)

- Suppose $f(\vec{w})$ and $g_i(\vec{w})$ are **convex.**
- Suppose $h_j(\vec{w})$ are **affine**.
- Suppose there exists $\vec{w}_0$ such that $g_i(\vec{w}_0) < 0$ for all $1 \le i \le n$.

Under the above assumptions, the previous optimization question (⭐) has a solution $\vec{w}^*$ *if and only if* there exist $\vec{w}^*$, $\vec{\alpha}^*$, $\vec{\beta}^*$ satisfying the following

Karush-Kuhn-Tucker **(KKT) conditions**:

$$\nabla_{\vec{w}} L(\vec{w}, \vec{\alpha}^*, \vec{\beta}^*) = 0$$

$$g_i(\vec{w}) \le 0 \text{ for } 1 \le i \le m$$

$$h_j(\vec{w}) = 0 \text{ for } 1 \le j \le n$$

$$\vec{\alpha}_i^{\,*} \ge 0$$

$$\alpha_i^* g_i(\vec{w}^*) = 0 \ \text{ for } \ 1 \le i \le m \qquad \text{(complementary slackness)}$$

Application to SVM optimization: find $\vec{w}$ and b

$$\min_{\vec{w},b} \ \frac{1}{2}\vec{w}^T\vec{w} \text{ such that } 1 - y^{(i)}\left(\vec{w}^T\vec{x}^{(i)} + b\right) \le 0 \quad \text{for } 1 \le i \le n$$

Define **Lagrangian**:

$$L(\vec{w}, b, \vec{\alpha}) := \frac{1}{2}\vec{w}^T\vec{w} + \sum_{i=1}^{n} \alpha_i \left(1 - y^{(i)}\left(\vec{w}^T\vec{x}^{(i)} + b\right)\right)$$

$\vec{w}^T\vec{x} + b = 0$

By **KKT conditions:**

- $\nabla_{\vec{w}} L = 0$ implies $\Rightarrow$ $$\vec{w} = \sum_{i=1}^{n} \alpha_i y^{(i)} \vec{x}^{(i)}$$
- $\nabla_b L = 0$ implies $\Rightarrow$ $$\sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

± 1

- $1 - y^{(i)}(\vec{w}^T\vec{x}^{(i)} + b) \le 0$
- $\alpha_i \ge 0$
- $\alpha_i\left(1 - y^{(i)}(\vec{w}^T\vec{x}^{(i)} + b)\right) = 0$

From complementary slackness condition

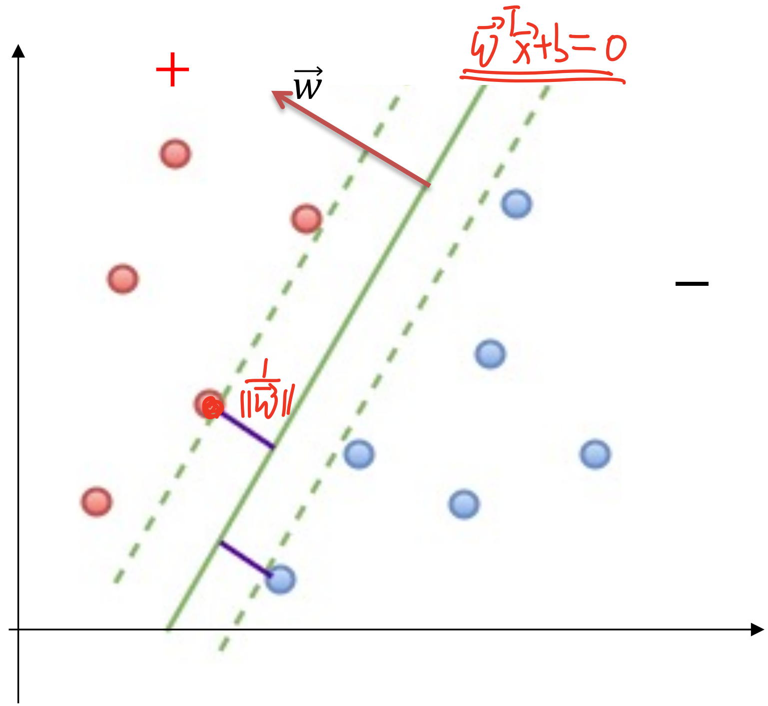
- If $\alpha_i > 0$, then $y^{(i)}(\vec{w}^T\vec{x}^{(i)} + b) = 1$

  So, $\vec{x}^{(i)}$ is a support vector.

- If $y^{(i)}(\vec{w}^T\vec{x}^{(i)} + b) > 1$, then, $\alpha_i = 0$

  So, if $\vec{x}^{(i)}$ is away from boundary, then we don't use those points.

Only support vectors matter!



Plug the condition formulas back to the Lagrangian,

$$L(\vec{w}, b, \vec{\alpha}) := \frac{1}{2}\vec{w}^T\vec{w} + \sum_{i=1}^{n} \alpha_i \left(1 - y^{(i)}\left(\vec{w}^T\vec{x}^{(i)} + b\right)\right)$$

$$= \frac{1}{2}\vec{w}^T\vec{w} + \sum_{i=1}^{n} \alpha_i - \vec{w}^T\vec{w}$$

only inner product!

$$= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} y^{(i)}y^{(j)}\alpha_i\alpha_j \boxed{\langle \vec{x}^{(i)}, \vec{x}^{(j)} \rangle} =: F(\vec{\alpha})$$

Find $\vec{\alpha}$

The new question is to optimize the dual Lagrangian $F(\vec{\alpha})$ with constraints:

$$\max_{\vec{\alpha}} F(\vec{\alpha}) \text{ subject to } \sum_{i=1}^{n} \alpha_i y^{(i)} = 0 \text{ and } \alpha_i \geq 0$$

There is a [Sequential minimal optimization (SMO) algorithm](#) for solving this quadratic programing problem. (1998 by John Platt)

After finding optimal α_i, we can plug back to find optimal $\vec{w}$.

From the distance formula, the intersection term can be calculated by **one support vector** $(\vec{x}^{(s)}, y^{(s)} = 1)$

$$\boxed{b = 1 - \vec{w}^T \vec{x}^{(s)}} = 1 - \sum_{i=1}^{n} \alpha_i y^{(i)} \langle \vec{x}^{(i)}, \vec{x}^{(s)} \rangle$$

$$\vec{w} = \sum_{i=1}^{n} \alpha_i y^{(i)} \vec{x}^{(i)}$$

Or we want to use **all support vectors** $\{(\vec{x}^{(s)}, y^{(s)}) \mid s \in S\}$ and take average for numerically stable solution:

$$b = \frac{1}{|S|} \sum_{s \in S} \left(y^{(s)} - \vec{w}^T \vec{x}^{(s)}\right) = \frac{1}{|S|} \sum_{s \in S} \left(y^{(s)} - \sum_{i=1}^{n} \alpha_i \, y^{(i)} \langle \vec{x}^{(i)}, \vec{x}^{(s)} \rangle\right)$$

Or we want to start with **original data** in computation formula:

$$b = -\frac{\min_{i;y^{(i)}=1} \vec{w}^T \vec{x}^{(i)} + \max_{i;y^{(i)}=-1} \vec{w}^T \vec{x}^{(i)}}{2}$$

we know α_i $\cancel{\vec{w}^T}$, b.

$$\vec{\mathrm{w}} = \sum_{i=1}^{n} \alpha_i y^{(i)} \vec{x}^{(i)}$$

➢ Prediction:

After we have the optimal model (parameters) $\vec{w}^T, b$, we can make predictions for a test data point $\vec{x}$:

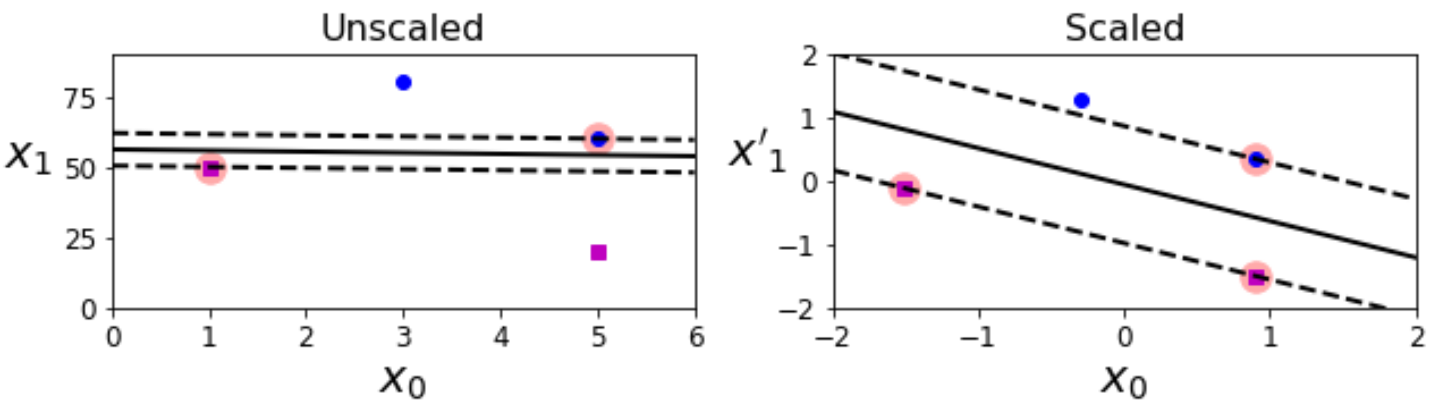
$$f(\vec{x}) = \vec{w}^T \vec{x} + b = \sum_{i=1}^{n} \alpha_i \, y^{(i)} \langle \vec{x}^{(i)}, \vec{x} \rangle + b$$

- Only involves **inner product** of the input data $\{(\vec{x}^{(i)}, y^{(i)}), i = 1, \ldots n\}$!
- $\alpha_i = 0$ except for support vectors. So the formula can also be written as

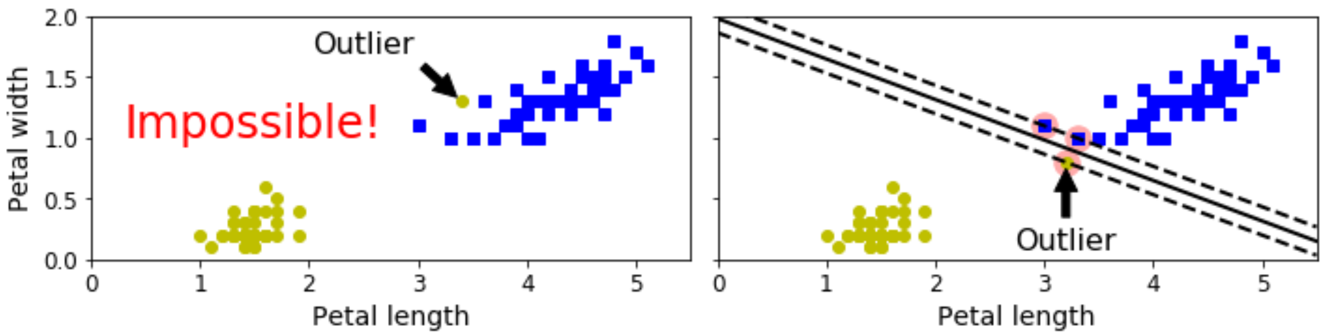
$$f(\vec{x}) = \sum_{i \in S} \alpha_i \, y^{(i)} \langle \vec{x}^{(i)}, \vec{x} \rangle + b$$

where S is the set of indices of support vectors.

Sensitivity to feature scales



Outlier:

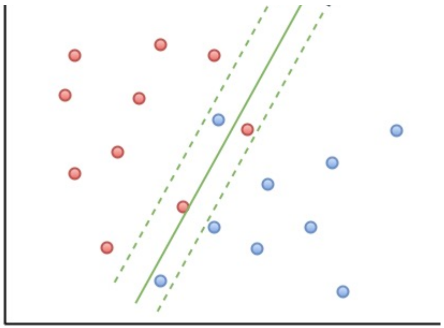


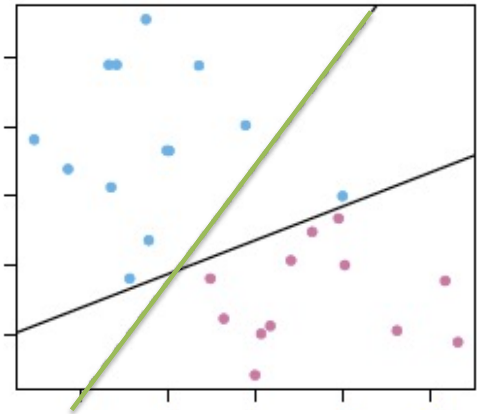
➢ Non-separable cases:

- In general, the two classes are usually **not separable** by any hyperplane.
- Even if they are, the max margin may not be desirable because of its high variance, and thus possible over-fit.
- The generalization of the maximal margin classier to the non-separable case is known as the **support vector classifier.**
- Use a **soft-margin** in place of the max margin.
- **Soft-margin classier** (support vector classier) allow some violation of the margin: some can be on the wrong side of the margin (in the river) or even wrong side of the hyperplane.

➢ **Non-separable cases**: (Soft-margin SVM classifier)

If the datasets are **not *linearly separable***, *or we want SVM less sensitive to **outliers**.*





Soft-margin SVM optimization: find $\vec{w}$ and b

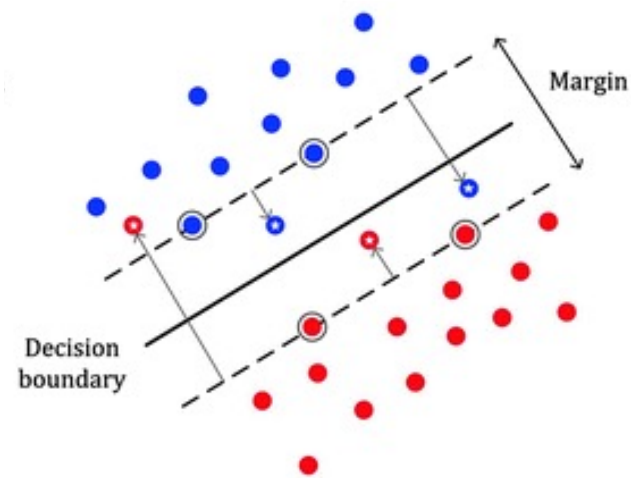
$$\min_{\vec{w},b} \ \frac{1}{2}\vec{w}^T\vec{w} + C\sum_{i=1}^{n} \xi_i$$

such that $1 - \xi_i - y^{(i)}\left(\vec{w}^T\vec{x}^{(i)} + b\right) \leq 0$ for $1 \leq i \leq n$

Here, for each training point, we introduce $\xi_i \geq 0$, which is called a slack variable.

$$\xi_i := \begin{cases} 0 & \text{for data points on or inside the correct margin boundary} \\ |y^{(i)} - f(x^{(i)})| & \text{for other points, where } f\left(\vec{x}^{(i)}\right) = \vec{w} \cdot \vec{x}^{(i)} + b \end{cases}$$

- $0 < \xi_i < 1$ for data points inside the margin, but on the correct side of the decision boundary.
- $\xi_i = 1$ for data points on the decision boundary.
- $\xi_i > 1$ for data points will be misclassified.



The classification constraints $y^{(i)}\left(\vec{w} \cdot \vec{x}^{(i)} + b\right) \geq 1$ will be replaced by

$$y^{(i)}\left(\vec{w} \cdot \vec{x}^{(i)} + b\right) \geq 1 - \xi_i$$

Now we maximize the margin while **softly** penalizing points that lie on the wrong side of the margin boundary (**Soft-margin SVM optimization**)

$$\min_{\vec{w},b} \ \frac{1}{2}\vec{w}^T\vec{w} + C\sum_{i=1}^{n}\xi_i$$

such that $1 - \xi_i - y^{(i)}\left(\vec{w}^T\vec{x}^{(i)} + b\right) \leq 0$ for $1 \leq i \leq n$

Similarly as hard-margin SVM, we use Lagrangian and KKT to simplify the optimization question to be

$$\max_{\vec{\alpha}} F(\vec{\alpha}) \coloneqq \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y^{(i)} y^{(j)} \alpha_i \alpha_j \left\langle \vec{x}^{(i)}, \vec{x}^{(j)} \right\rangle$$

subject to

$$\sum_{i=1}^{n} \alpha_i y^{(i)} = 0$$

$$\text{and } 0 \leq \alpha_i \leq C \qquad \text{for } 1 \leq i \leq n$$

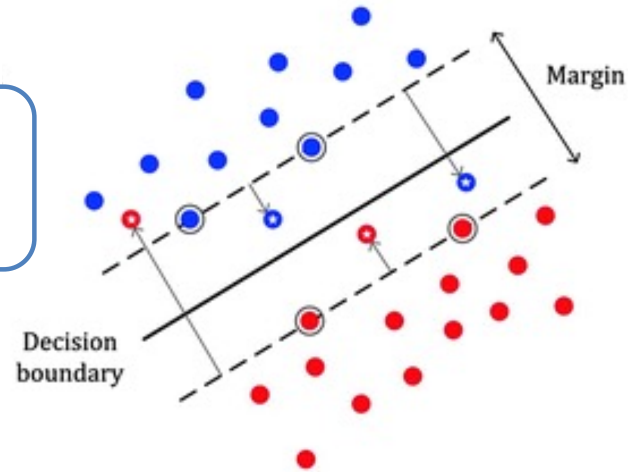
- The hyperparameter $C > 0$ controls the trade-off between the slack variable penalty and the margin.
- If $C \to \infty$, it recover the hard-margin SVM.

The **intersection term** can be calculated by **one support vector** $(\vec{x}^{(s)}, \mathrm{y}^{(s)} = 1)$ with $0 \leq \alpha_i \leq C$ and $\xi_i = 0$

$$b = 1 - \sum_{i=1}^{n} \alpha_i y^{(i)} \langle \vec{x}^{(i)}, \vec{x}^{(s)} \rangle$$

Or we want to use set of **support vectors** $\left\{\left(\vec{x}^{(s)}, \mathrm{y}^{(s)}\right) \mid s \in M\right\}$ with $0 \leq \alpha_i \leq C$ and $\xi_i = 0$, and take average for numerically stable solution:

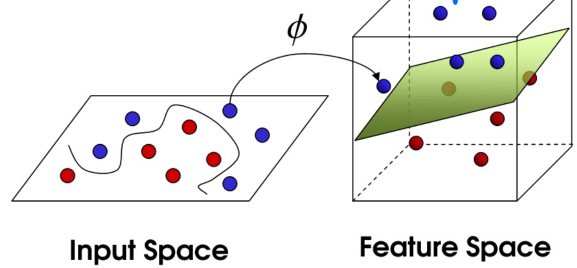
$$b = \frac{1}{|M|} \sum_{s \in M} \left(y^{(s)} - \sum_{i=1}^{n} \alpha_i \, y^{(i)} \langle \vec{x}^{(i)}, \vec{x}^{(s)} \rangle \right)$$



➢ The kernel method

x_1	x_2	x_1^2	x_1x_2	x_2^2	...	y

For any linear method (e.g., linear regression, logistics regression, LDA), we can easily generalize it to non-linear method by introducing new variables (features).



$\theta_0+\theta_1 z_1+\theta_2 z_2+\theta_3 z_3+\cdots=0$

For example,

$$z_1 = x_1, z_2 = x_2,$$
$$z_3 = x_1^2, z_4 = x_2^2, z_5 = x_1x_2,$$
$$z_6 = x_1^3, z_7 = x_2^3, z_8 = x_1^2x_2, z_9 = x_1x_2^2, \ldots$$

Formally, we can consider this procedure as defining a **feature map:**

$$\phi: \mathbb{R}^d \to \mathbb{R}^D$$
$$\vec{x} \to \phi(\vec{x})$$

$$\sum_{i=1}^{m} \binom{i+d-1}{i}$$

The **difficulty** is that dimension D is very large or even infinite.

For example, using polynomial of degree m, there are $D \sim O(d^m)$ parameters.

For a relatively easy question, if $d = 100$ and $m = 4$, there are about $d^4 \approx 4$ million parameters!

Question: How to solve the difficulty?

Answer: The kernel method (trick).

SVM

Suppose there is a machine learning model, in the optimization of the cost and the prediction formula, only **inner products** of the data points are involved: $\langle \vec{x}^{(i)}, \vec{x}^{(j)} \rangle$, or $\langle \vec{x}^{(i)}, \vec{x} \rangle$ for prediction for $\vec{x}$.

After we applied the feature map, $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \to \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \\ x_1 x_1 \\ x_2 x_2 \\ \vdots \end{bmatrix}$

$$\phi\colon \mathbb{R}^d \to \mathbb{R}^D$$

$\langle \phi(\vec{x}^{(i)}), \phi(\vec{x}) \rangle$

$\langle \phi(\vec{x}^{(i)}), \phi(x^{(j)}) \rangle$

all calculations will be replaced by $\phi(\vec{x}) \in \mathbb{R}^D$. (Very large dimension)

We assume that all calculations **only involve inner products**

$$\langle \phi(\vec{x}^{(i)}), \phi(\vec{x}^{(j)}) \rangle \text{ or } \langle \phi(\vec{x}^{(i)}), \phi(\vec{x}\,) \rangle$$

Define it as the **Kernel function**: $K\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

$$K\left(\vec{x}^{(i)}, \vec{x}^{(j)}\right) := \langle \phi(\vec{x}^{(i)}), \phi(\vec{x}^{(j)}) \rangle$$

Example: (quadratic)

For $\vec{x}$ and $\vec{z} \in \mathbb{R}^3$, consider the quadratic feature map:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\phi(\vec{x}) := \begin{bmatrix} x_1x_1 \\ x_1x_2 \\ x_1x_3 \\ x_2x_1 \\ x_2x_2 \\ x_2x_3 \\ x_3x_1 \\ x_3x_2 \\ x_3x_3 \end{bmatrix} \in \mathbb{R}^{3^2}$$

$$\phi(\vec{z}) = \begin{bmatrix} z_1z_1 \\ z_1z_2 \\ z_1z_3 \\ \vdots \end{bmatrix}$$

The **kernel function:**

$$K(\vec{x}, \vec{z}) := \langle \phi(\vec{x}), \phi(\vec{z}) \rangle = \sum_{i=1}^{d} \sum_{j=1}^{d} x_i x_j z_i z_j$$

d^2 - Calculations

$$= \left(\sum_{i=1}^{d} x_i z_i \right) \left(\sum_{j=1}^{d} x_j z_j \right) = \left(\sum_{i=1}^{d} x_i z_i \right)^2 = (\vec{x}^T \vec{z})^2$$

$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ $\vec{z} = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix}$

Recall that in hard-margin SVM,

$$\mathbb{R}^d \xrightarrow{\phi} \mathbb{R}^D$$

$$\max_{\vec{\alpha}} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} y^{(i)} y^{(j)} \alpha_i \alpha_j \underbrace{\langle \phi(\vec{x}^{(i)}), \phi(\vec{x}^{(j)}) \rangle}_{= K(\vec{x}^{(i)}, \vec{x}^{(j)})}$$

subject to $\sum_{i=1}^{n} \alpha_i y^{(i)} = 0$ and $\alpha_i \geq 0$ for $1 \leq i \leq n$

$$b = 1 - \sum_{i=1}^{n} \alpha_i y^{(i)} \underbrace{\langle \phi(\vec{x}^{(i)}), \phi(\vec{x}^{(s)}) \rangle}_{= K(\quad , \quad)}$$

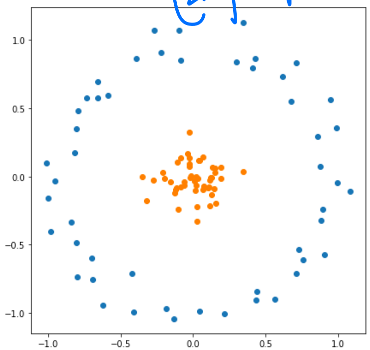
Prediction:

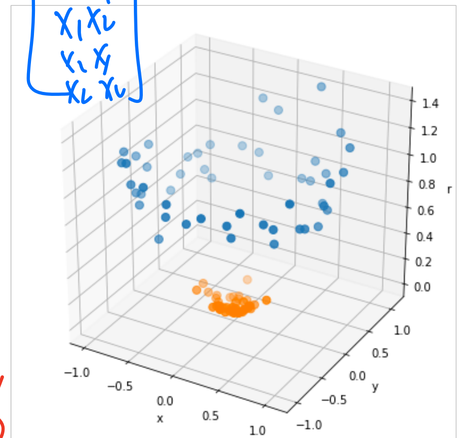
$$f(\vec{x}) = \sum_{i=1}^{n} \alpha_i \, y^{(i)} \underbrace{\langle \phi(\vec{x}^{(i)}), \phi(\vec{x}) \rangle}_{K(\, , \,)} + b$$

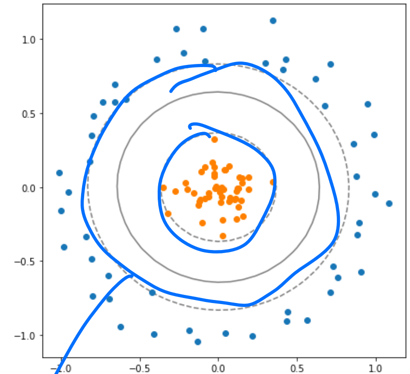
e.g.

$$K(\vec{x}, \vec{z}) := (\vec{x}^T \vec{z})^2$$

$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbb{R}^2 \xrightarrow{\phi} \mathbb{R}^4 \ni \begin{bmatrix} x_1 x_1 \\ x_1 x_2 \\ x_2 x_1 \\ x_2 x_2 \end{bmatrix}$







Σ $\qquad$ $\pm b = \pm 1$

Data in $\mathbb{R}^2$ $\xrightarrow{\phi}$ Feature space $\mathbb{R}^3$

$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \longrightarrow \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{bmatrix}$

x_1	x_2	y

z_1: x_1	z_2: x_2	z_3: $x_1 x_2$	y

Boundary:

$$\sum_{i=1}^{n} \alpha_i\, y^{(i)} K(\vec{x}^{(i)}, \vec{x}) + b = 0$$

$$= (\vec{x}^{(i)T} \vec{x})^2$$

$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

Kernel Functions

1. Quadratic Kernel

$\langle \phi(\vec{x}), \phi(\vec{z}) \rangle = \cdots$

For $\vec{x}$ and $\vec{z} \in \mathbb{R}^d$, define kernel function:

$$K(\vec{x}, \vec{z}) := (\vec{x}^T \vec{z} + c)^2$$

What is the feature map ϕ: $\mathbb{R}^d \to \mathbb{R}^D$?

D =

$$\phi(\vec{x}) := \begin{bmatrix} x_1 x_1 \\ \vdots \\ x_1 x_d \\ \vdots \\ x_d x_d \\ \sqrt{2c}\, x_1 \\ \vdots \\ \sqrt{2c}\, x_d \\ c \end{bmatrix} \in \mathbb{R}^{d^2+d+1}$$

Do we need the feature map ϕ?

2. Polynomial Kernel

Thm

$\phi : \mathbb{R}^d \to \mathbb{R}^D$

exist!

For $\vec{x}$ and $\vec{z} \in \mathbb{R}^d$, define degree n polynomial kernel function:

$$K(\vec{x}, \vec{z}) := (\vec{x}^T \vec{z} + c)^n$$

3. Sigmoid Kernel

For $\vec{x}$ and $\vec{z} \in \mathbb{R}^d$, define Sigmoid kernel function:

$\phi : \mathbb{R}^d \to \mathbb{R}^D$

$$K(\vec{x}, \vec{z}) \coloneqq \tanh(\eta \vec{x}^T \vec{z} + c)$$

where $\tanh(t) = \frac{e^t - e^{-t}}{e^t + e^{-t}}$

4. Gaussian Kernel

$\mathbb{R}^d \longrightarrow \mathbb{R}^D$

For $\vec{x}$ and $\vec{z} \in \mathbb{R}^d$, define Gaussian kernel function:

$$K(\vec{x},\vec{z}) \coloneqq \exp\left(-\frac{\|\vec{x}-\vec{z}\|^2}{2\sigma^2}\right)$$

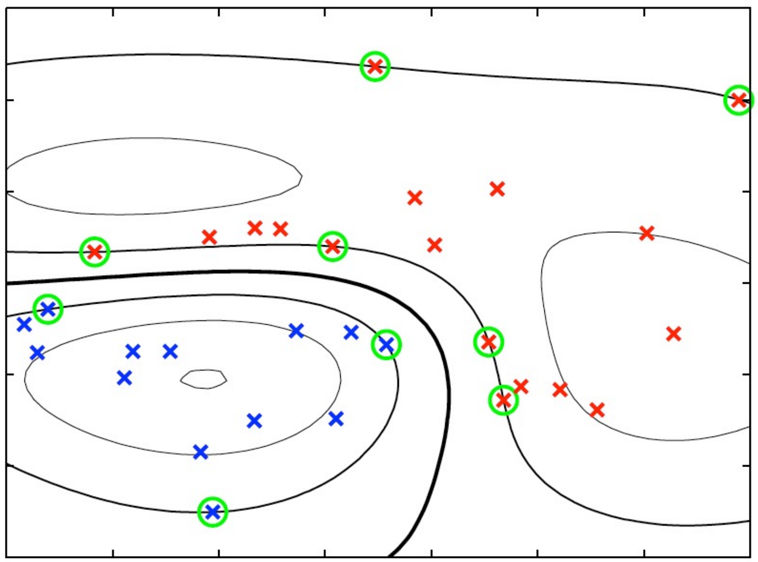
Remark:

- If σ is very small, then overfitting. If σ is very large, then underfitting
- What is the feature map $\boxed{\phi: \mathbb{R}^d \to \mathbb{R}^D}$? exist!

$d=1$

$$\phi(x) = \begin{bmatrix} 1 \\ \frac{x}{\sigma\sqrt{1!}} \\ \frac{x^2}{\sigma^2\sqrt{2!}} \\ \frac{x^3}{\sigma^3\sqrt{3!}} \\ \vdots \end{bmatrix} \exp\left(-\frac{x^2}{2\sigma^2}\right) \in \mathbb{R}^\infty$$

Example: SVM with kernel trick



Example of two classes in two dimensions showing contours of constant $f(\vec{x})$ obtained from a support vector machine having a **Gaussian kernel** function. Also shown are the decision boundary, the margin boundaries, and the support vectors.

scikit-learn

- SVM:

  https://scikit-learn.org/stable/modules/svm.html#svm

- Kernel Functions:

  https://scikit-learn.org/stable/modules/svm.html#kernel-functions

- linear: $\langle x, x' \rangle$.
- polynomial: $(\gamma \langle x, x' \rangle + r)^d$, where d is specified by parameter `degree`, r by `coef0`.
- rbf: $\exp(-\gamma \|x - x'\|^2)$, where γ is specified by parameter `gamma`, must be greater than 0.
- sigmoid $\tanh(\gamma \langle x, x' \rangle + r)$, where r is specified by `coef0`.

How to show a map is a feature maps?

$$K(\vec{x}, \vec{z}) = \langle \phi(\vec{x}), \phi(\vec{z}) \rangle$$

for some ϕ

Theorem: (Mercer 1909)

Let K: $\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ be a binary map.

The map K is a **kernel** function *if and only if* $\Longleftrightarrow$ for any finite sequence $\{\vec{x}^{(1)}, \dots, \vec{x}^{(m)}\}$, the matrix

$$M = \begin{bmatrix} & \vdots & \\ \cdots & K\left(\vec{x}^{(i)}, \vec{x}^{(j)}\right) & \cdots \\ & \vdots & \end{bmatrix}$$

is **symmetric** and **positive semi-definite.**

Proof: "$\Longrightarrow$"

If K is a kernel function, then there exists a map $\phi: \mathbb{R}^d \to \mathbb{R}^D$ such that

$$K\left(\vec{x}^{(i)}, \vec{x}^{(j)}\right) = \left\langle \phi(\vec{x}^{(i)}), \phi(\vec{x}^{(j)}) \right\rangle$$

First, $K\left(\vec{x}^{(i)}, \vec{x}^{(j)}\right) = K\left(\vec{x}^{(j)}, \vec{x}^{(i)}\right)$ by the property of inner product.

Second, the quadratic form

$$\vec{z}^T M \vec{z} = \sum_{i,j}^{d} z_i \left\langle \phi(\vec{x}^{(i)}), \phi(\vec{x}^{(j)}) \right\rangle z_j = \sum_{i,j}^{d} \left\langle z_i \phi(\vec{x}^{(i)}), \phi(\vec{x}^{(j)}) z_j \right\rangle$$

$$= \left\langle \sum_{i=1}^{d} z_i \phi(\vec{x}^{(i)}), \sum_{j=1}^{d} z_j \phi(\vec{x}^{(j)}) \right\rangle = \left\| \sum_{i=1}^{d} z_i \phi(\vec{x}^{(i)}) \right\|^2 \geq 0$$

M defined by inner product this way is called the **Gram matrix**.

“ $\Longleftarrow$ ”

Suppose K is a binary map such that $M = \left[K\left(\vec{x}^{(i)}, \vec{x}^{(j)}\right)\right]$ satisfies the properties.

Consider $\phi_{(\vec{x})}(-) \coloneqq K(-, \vec{x})$, which is map from $\mathbb{R}^n\ to\ \mathbb{R}$.

Let $\mathcal{F} \coloneqq \mathrm{Span}\left\{\phi_{(\vec{x})} \mid \vec{x} \in \mathbb{R}^n\right\}$ be a subspace of the function space $C(\mathbb{R}^n, \mathbb{R})$

Claim 1. $\phi_{(\vec{x})}$ defines a map from $\mathbb{R}^n$ to $\mathcal{F}$.

Claim 2. $\mathcal{F}$ is an **inner product space** with

$$\left\langle \phi_{(\vec{x})}, \phi_{(\vec{z})} \right\rangle_{\mathcal{F}} \coloneqq K(\vec{x}, \vec{z})$$

How to construct feature maps?

e.g. $K_1(\vec{x}, \vec{z}) = (c + \vec{x}^T\vec{z})^n \pm (c + \vec{x}^T\vec{z})^2$

Theorem:

If K_1 *and* K_2 are kernel functions, then the following are also kernel functions.

- $K(\vec{x}, \vec{z}) := aK_1(\vec{x}, \vec{z}) + bK_2(\vec{x}, \vec{z})$, where $a, b \geq 0$
- $K(\vec{x}, \vec{z}) := K_1(\vec{x}, \vec{z})K_2(\vec{x}, \vec{z})$
- $K(\vec{x}, \vec{z}) := K_1\big(f(\vec{x}), f(\vec{z})\big)$, where f is a function from $\mathbb{R}^d \rightarrow \mathbb{R}^M$
- $K(\vec{x}, \vec{z}) := P\big(K_1(\vec{x}, \vec{z})\big)$, where $P(t)$ is a polynomial with non-negative coeffects.
- $K(\vec{x}, \vec{z}) := \exp\big(K_1(\vec{x}, \vec{z})\big)$
- $K(\vec{x}, \vec{z}) := \vec{x}^T S \vec{z}$, where S is a symmetric positive semidefinite matrix.
- $K(\vec{x}, \vec{z}) := f(\vec{x})K_1(\vec{x}, \vec{z})f(\vec{z})$, where $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is any function.

➢ Support Vector Machine - Regression (SVR)

Support Vector Machine can also be used as a **regression** method, maintaining all the main features that characterize the algorithm (maximal margin).

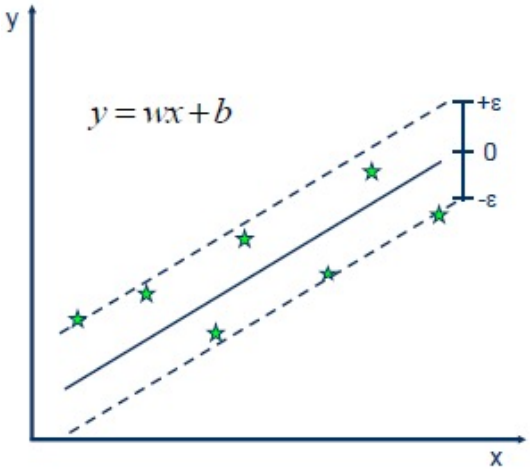
First of all, because output is a real number it becomes very difficult to predict the information at hand, which has infinite possibilities.

In the case of regression, a margin of tolerance (epsilon) is set in approximation to the SVM which would have already requested from the problem.

But besides this fact, there is also a more complicated reason, the algorithm is more complicated therefore to be taken in consideration.

However, the **main idea** is always the same: to minimize error, individualizing the hyperplane which maximizes the margin, keeping in mind that part of the error is tolerated.

Support Vector Machine - Regression (SVR)

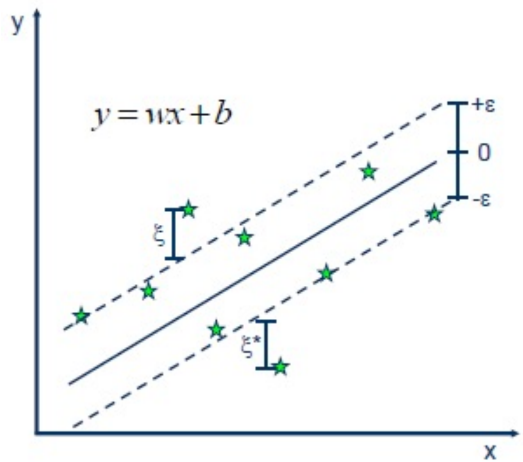


- Solution:

$$\min \frac{1}{2}\|w\|^2$$

- Constraints:

$$y_i - wx_i - b \le \varepsilon$$
$$wx_i + b - y_i \le \varepsilon$$



- Minimize:

$$\frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N}\left(\xi_i + \xi_i^*\right)$$

- Constraints:

$$y_i - wx_i - b \le \varepsilon + \xi_i$$
$$wx_i + b - y_i \le \varepsilon + \xi_i^*$$
$$\xi_i, \xi_i^* \ge 0$$

Linear SVR

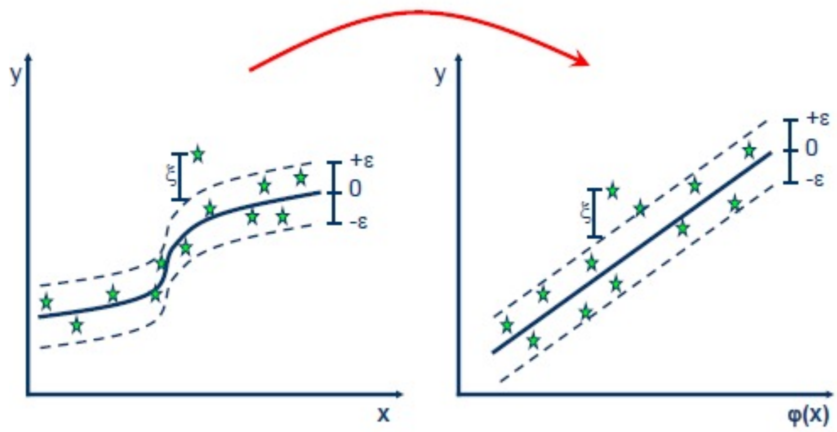
$$y = \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) \cdot \langle x_i, x \rangle + b$$

Non-linear SVR

The kernel functions transform the data into a higher dimensional feature space to make it possible to perform the linear separation.

$$y = \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) \cdot \langle \varphi(x_i), \varphi(x) \rangle + b$$

$$y = \sum_{i=1}^{N} (\alpha_i - \alpha_i^*) \cdot K(x_i, x) + b$$



Apply Kernel Methods to Linear Regressions:

$$X = \begin{bmatrix} \vec{x}^{(1)T} \\ \vec{x}^{(2)T} \\ \vdots \\ \vec{x}^{(n)T} \end{bmatrix} \qquad X^T = \begin{bmatrix} \vec{x}^{(1)} & \cdots & \vec{x}^{(n)} \end{bmatrix}$$

Data: $D = \{(\vec{x}^{(i)}, y^{(i)}) \mid i = 1, \ldots n\}$

Model: $h(\vec{x}) = \vec{\theta}^T \vec{x}$ Not iner prod.

If the **mean** of the data matrix X is **zero**, **Ridge regression** cost function:

$X X^T$

$$J^{Ridge}(\vec{\theta}\,) := (X\vec{\theta} - \vec{y})^T (X\vec{\theta} - \vec{y}) + \lambda \vec{\theta}^T \vec{\theta}$$

The optimal solution is

$$\vec{\theta} = (X^T X + \lambda I)^{-1} X^T \vec{y}$$

Define $\boxed{\vec{\theta} = X^T \vec{\beta}}$ for some new parameter vector $\vec{\beta} \in \mathbb{R}^n$, called dual parameters

$d \times 1$ $\quad d \times n$ $\quad n \times 1$

$$\vec{\theta} = X^T \vec{\beta} = \begin{bmatrix} \vec{x}^{(1)} & \ldots & \vec{x}^{(n)} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_n \end{bmatrix} = \sum_{i=1}^{n} \beta_i \, \vec{x}^{(i)}$$

The **dual model for linear regression** is

$$h(\vec{x}) = \vec{\theta}^T \vec{x} = \langle \vec{x}, \vec{\theta} \rangle = \sum_{i=1}^{n} \beta_i \langle \vec{x}, \vec{x}^{(i)} \rangle$$

The **cost function**

$$J^{Ridge}(\vec{\beta}) := \left(XX^T\vec{\beta} - \vec{y}\right)^T \left(XX^T\vec{\beta} - \vec{y}\right) + \lambda \vec{\beta}^T XX^T \vec{\beta}$$

Solutions of $\vec{\beta}$ for optimizing the cost function:

$$\vec{\beta} = (XX^T + \lambda I)^{-1}\, \vec{y}$$

· kernel ridge

Here, $XX^T = \begin{bmatrix} & \vdots & \\ \cdots & \langle \vec{x}^{(i)}, \vec{x}^{(j)} \rangle & \cdots \\ & \vdots & \end{bmatrix}$

Now you can apply the **kernel tricks** to the dual linear model.

· kernel PCA

References:

- Chapter 7 in Pattern Recognition and Machine Learning by Chris Bishop.
- Chapter 9 An introduction to Statistical Learning by James, Witten, Hastie, Tibshirani
- Chapter 12 The elements of Statistical Learning, by Hastie, Tibshirani, Friedman
- https://see.stanford.edu/materials/aimlcs229/cs229-notes3.pdf