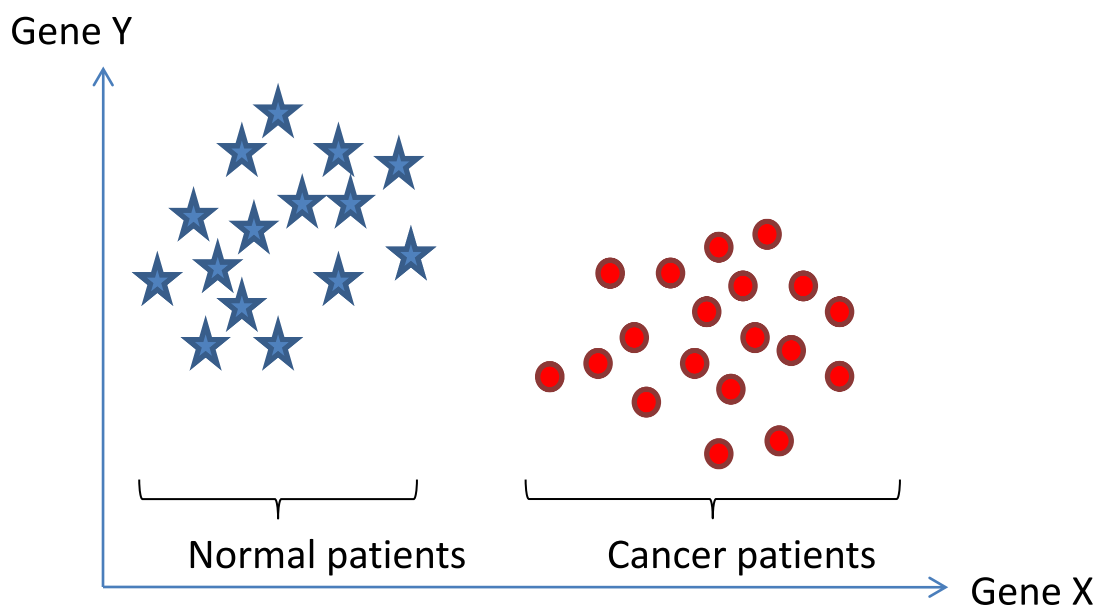
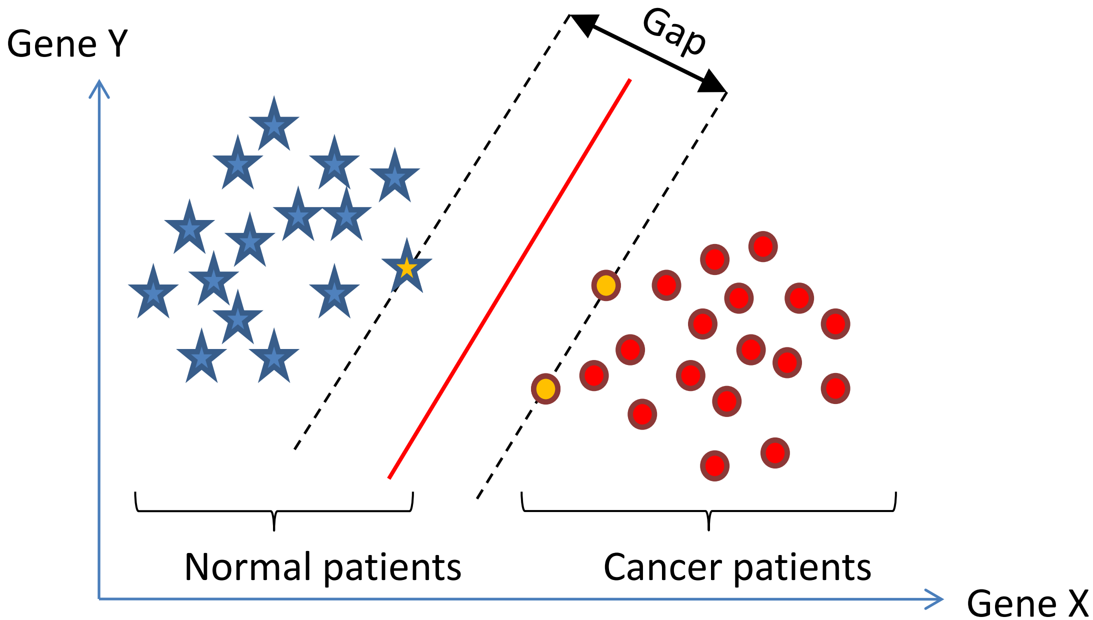
Main ideas of SVMs



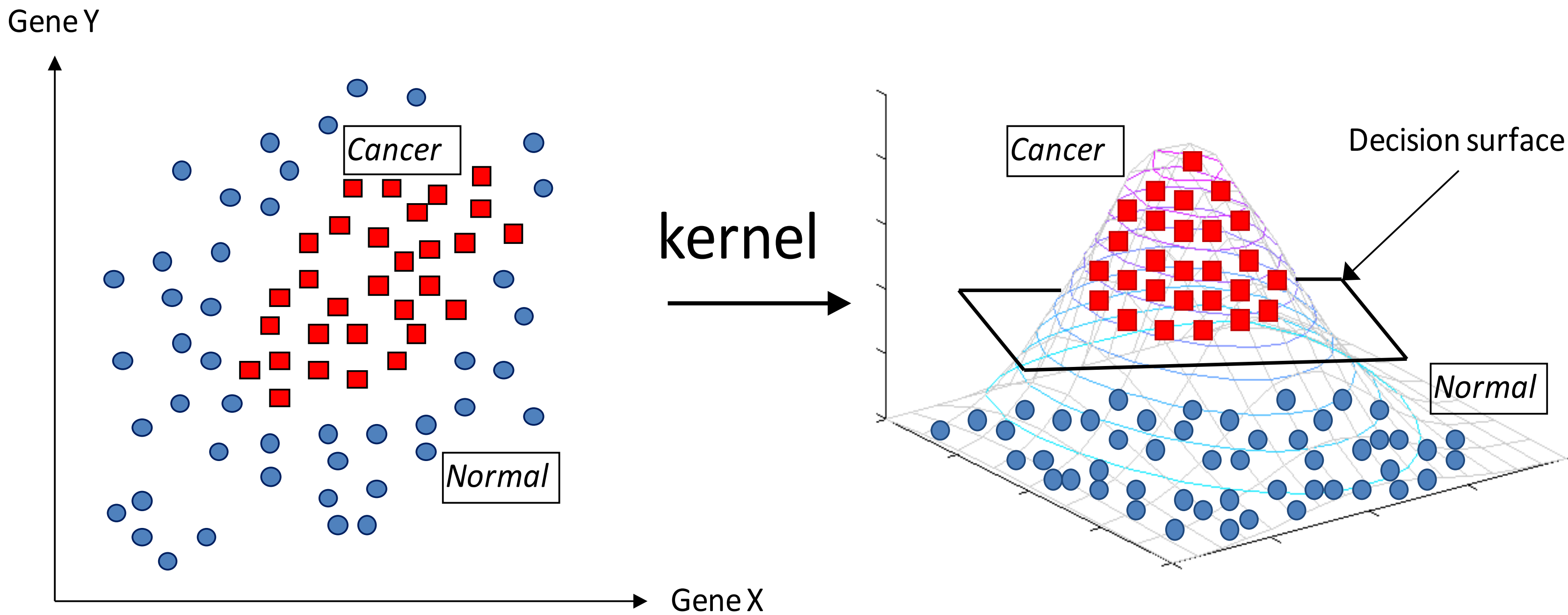
- Consider example dataset described by 2 genes, gene X and gene Y
- Represent patients geometrically (by "vectors")

Main ideas of SVMs



- Find a linear decision surface (“hyperplane”) that can separate patient classes <u>and</u> has the largest distance (i.e., largest “gap” or “margin”) between border-line patients (i.e., “support vectors”);

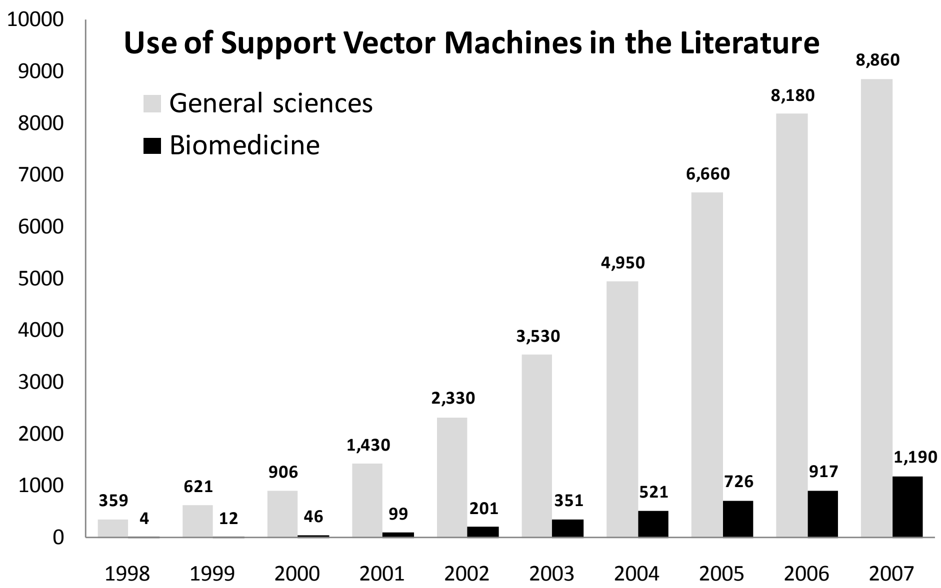
Main ideas of SVMs

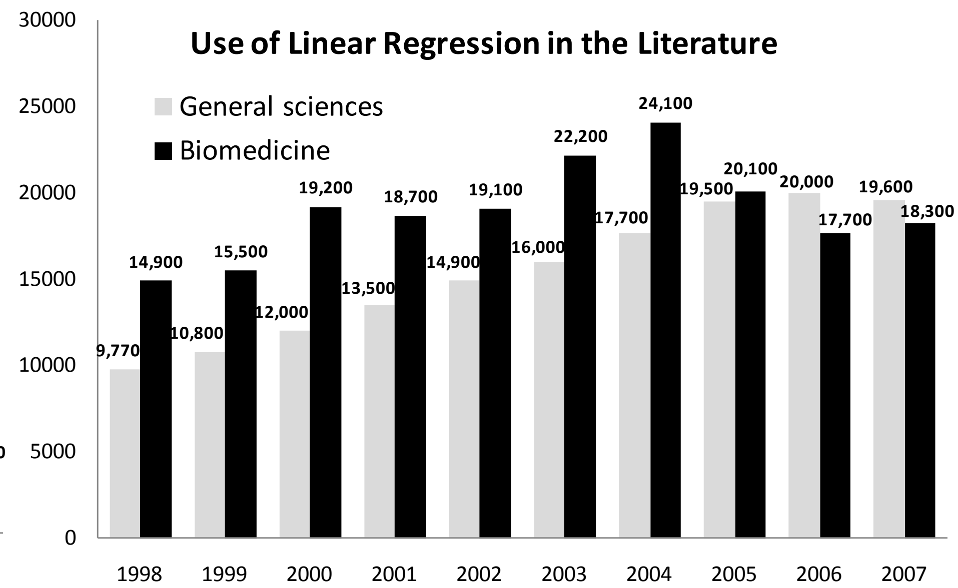


- If such linear decision surface does not exist, the data is mapped into a much higher dimensional space ("feature space") where the separating decision surface is found;
- The feature space is constructed via very clever mathematical projection ("kernel trick").

History of SVMs and usage in the literature

- Support vector machine classifiers have a long history of development starting from the 1960's.
- The most important milestone for development of modern SVMs is the 1992 paper by Boser, Guyon, and Vapnik ("*A training algorithm for optimal margin classifiers*")





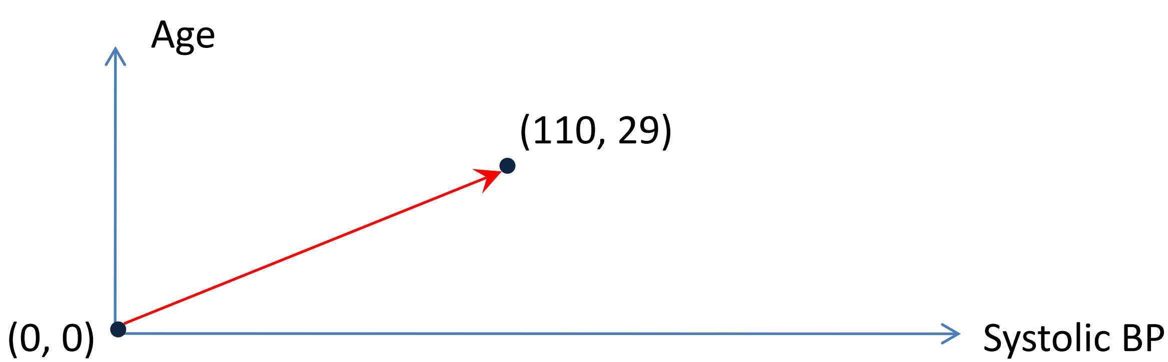
Necessary mathematical concepts

How to represent samples geometrically? Vectors in n-dimensional space ($\mathbb{R}^n$)

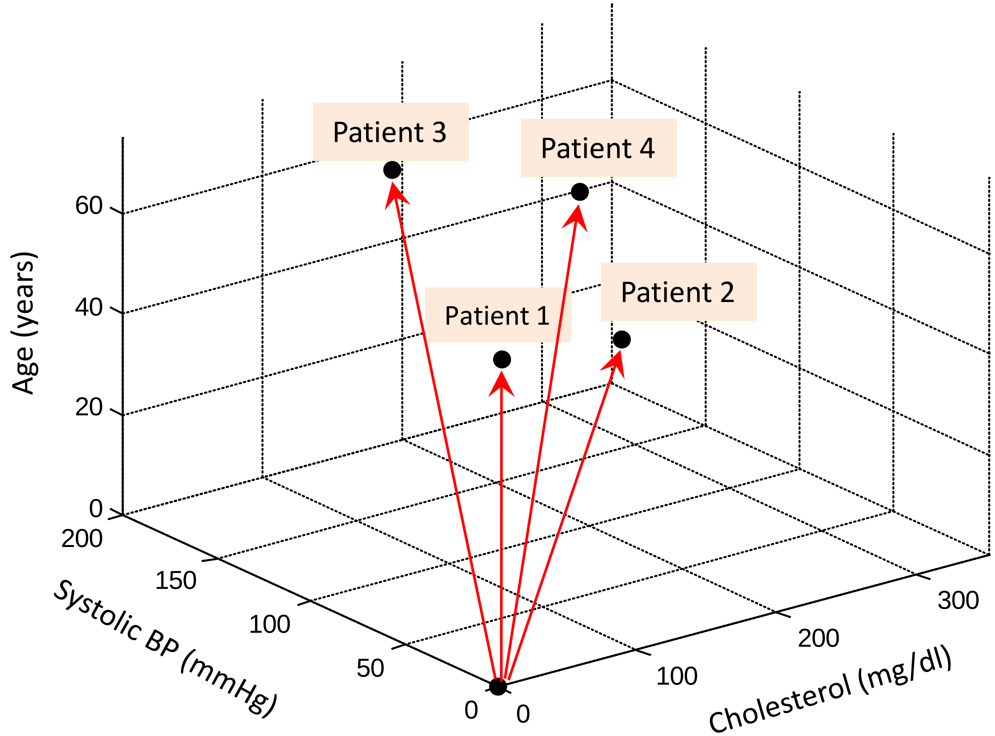
- Assume that a sample/patient is described by *n* characteristics ("features" or "variables")
- **<u>Representation:</u>** Every sample/patient is a vector in $\mathbb{R}^n$ with tail at point with 0 coordinates and arrow-head at point with the feature values.
- **<u>Example:</u>** Consider a patient described by 2 features:

  Systolic BP = 110 and *Age* = 29.

  This patient can be represented as a vector in $\mathbb{R}^2$:

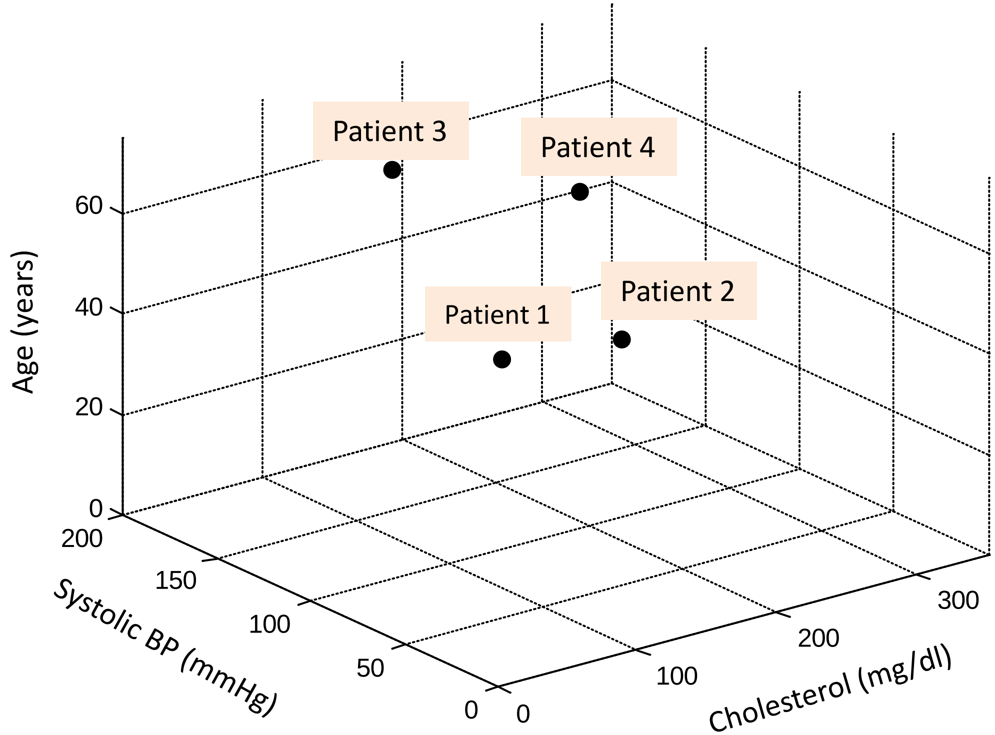


How to represent samples geometrically? Vectors in n-dimensional space ($\mathbb{R}^n$)



Patient id	Cholesterol (mg/dl)	Systolic BP (mmHg)	Age (years)	Tail of the vector	Arrow-head of the vector
1	150	110	35	(0,0,0)	(150, 110, 35)
2	250	120	30	(0,0,0)	(250, 120, 30)
3	140	160	65	(0,0,0)	(140, 160, 65)
4	300	180	45	(0,0,0)	(300, 180, 45)

How to represent samples geometrically? Vectors in n-dimensional space ($\mathbb{R}^n$)

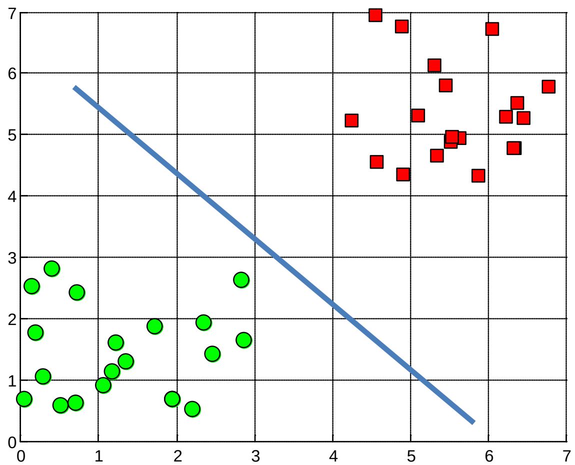


Since we assume that the tail of each vector is at point with 0 coordinates, we will also depict vectors as points (where the arrow-head is pointing).

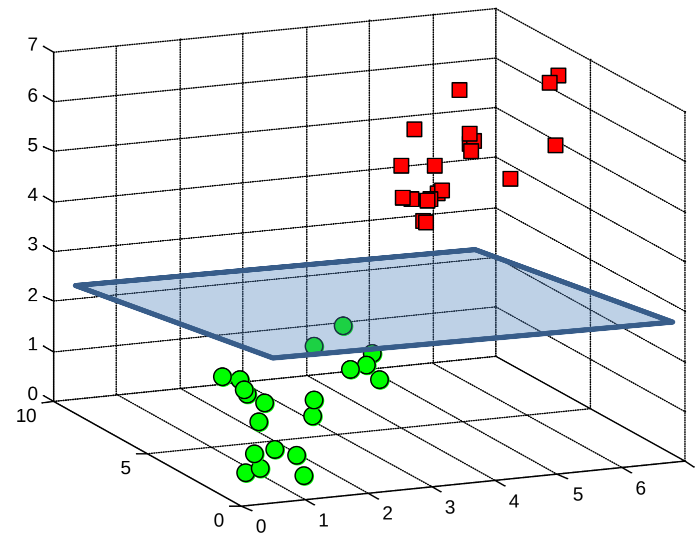
Purpose of vector representation

- Having represented each sample/patient as a vector allows now to geometrically represent the decision surface that separates two groups of samples/patients.

A decision surface in $\mathbb{R}^2$



A decision surface in $\mathbb{R}^3$



- In order to define the decision surface, we need to introduce some basic math elements…

Basic operation on vectors in $\mathbb{R}^n$

1. Multiplication by a scalar

Consider a vector $\vec{a} = (a_1, a_2, \ldots, a_n)$ and a scalar c

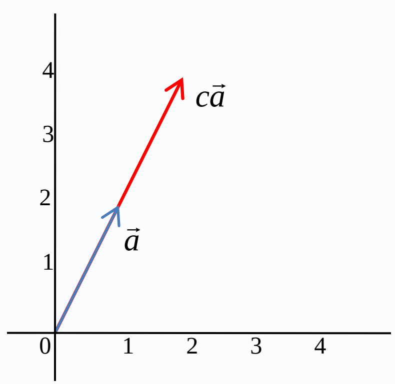
Define: $c\vec{a} = (ca_1, ca_2, \ldots, ca_n)$

When you multiply a vector by a scalar, you "stretch" it in the same or opposite direction depending on whether the scalar is positive or negative.

$\vec{a} = (1,2)$

$c = 2$

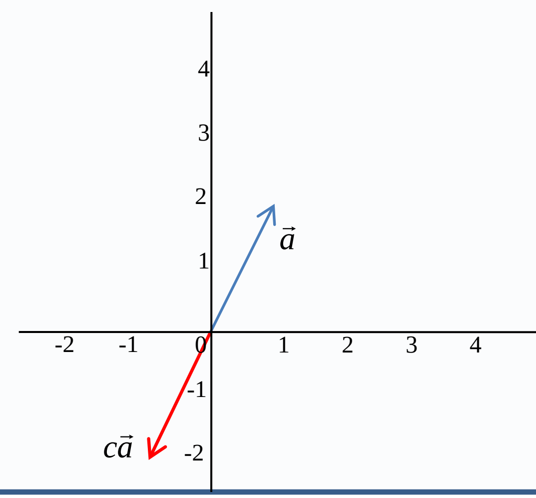
$\vec{c}a = (2,4)$



$\vec{a} = (1,2)$

$c = -1$

$\vec{c}a = (-1,-2)$



Basic operation on vectors in $\mathbb{R}^n$

2. Addition

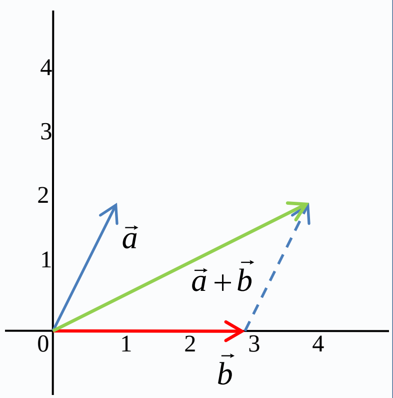
Consider vectors $\vec{a} = (a_1, a_2, \ldots, a_n)$ and $\vec{b} = (b_1, b_2, \ldots, b_n)$

Define: $\vec{a} + \vec{b} = (a_1 + b_1, a_2 + b_2, \ldots, a_n + b_n)$

$\vec{a} = (1,2)$

$\vec{b} = (3,0)$

$\vec{a} + \vec{b} = (4,2)$



Recall addition of forces in classical mechanics.

Basic operation on vectors in $\mathbb{R}^n$

3. Subtraction

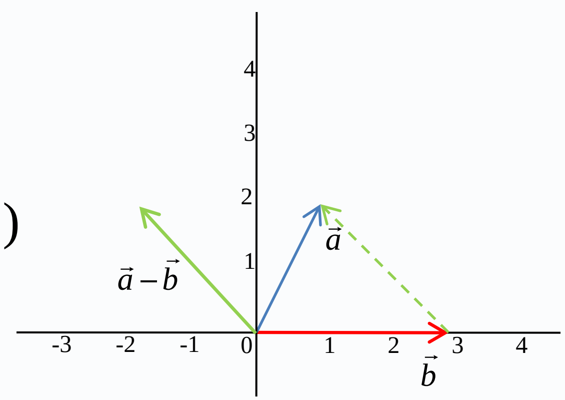
Consider vectors $\vec{a} = (a_1, a_2, \ldots, a_n)$ and $\vec{b} = (b_1, b_2, \ldots, b_n)$

Define: $\vec{a} - \vec{b} = (a_1 - b_1, a_2 - b_2, \ldots, a_n - b_n)$

$\vec{a} = (1,2)$

$\vec{b} = (3,0)$

$\vec{a} - \vec{b} = (-2,2)$



What vector do we need to add to $\vec{b}$ to get $\vec{a}$? I.e., similar to subtraction of real numbers.

Basic operation on vectors in $\mathbb{R}^n$

4. Euclidian length or L2-norm

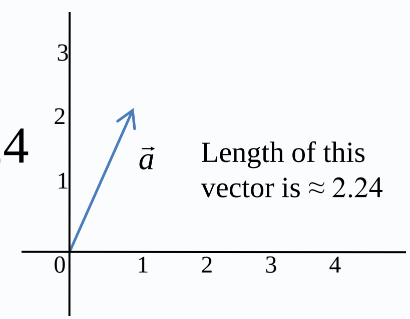
Consider a vector $\vec{a} = (a_1, a_2, \ldots, a_n)$

Define the L2-norm: $\|\vec{a}\|_2 = \sqrt{a_1^2 + a_2^2 + \ldots + a_n^2}$

We often denote the L2-norm without subscript, i.e. $\|\vec{a}\|$

$\vec{a} = (1,2)$

$\|\vec{a}\|_2 = \sqrt{5} \approx 2.24$



L2-norm is a typical way to measure length of a vector; other methods to measure length also exist.

Basic operation on vectors in $\mathbb{R}^n$

5. Dot product

Consider vectors $\vec{a} = (a_1, a_2, \ldots, a_n)$ and $\vec{b} = (b_1, b_2, \ldots, b_n)$

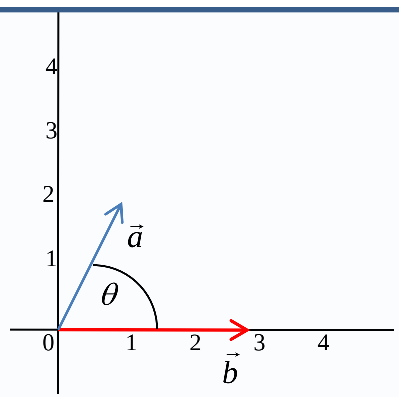
Define dot product: $\vec{a} \cdot \vec{b} = a_1 b_1 + a_2 b_2 + \ldots + a_n b_n = \sum_{i=1}^{n} a_i b_i$

The law of cosines says that $\vec{a} \cdot \vec{b} = \|\vec{a}\|_2 \|\vec{b}\|_2 \cos\theta$ where θ is the angle between $\vec{a}$ and $\vec{b}$. Therefore, when the vectors are perpendicular $\vec{a} \cdot \vec{b} = 0$.

$\vec{a} = (1,2)$

$\vec{b} = (3,0)$

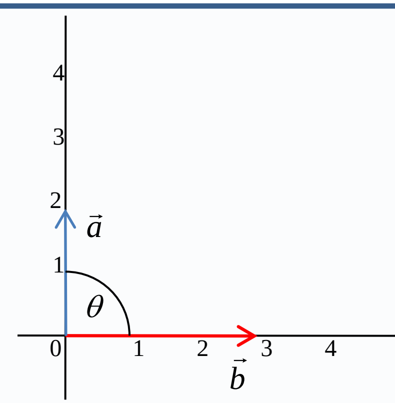
$\vec{a} \cdot \vec{b} = 3$



$\vec{a} = (0,2)$

$\vec{b} = (3,0)$

$\vec{a} \cdot \vec{b} = 0$



Basic operation on vectors in $\mathbb{R}^n$

5. Dot product (continued)

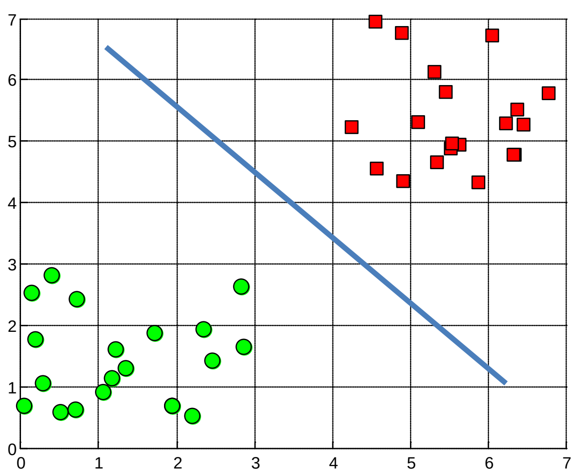
$$\vec{a} \cdot \vec{b} = a_1 b_1 + a_2 b_2 + \ldots + a_n b_n = \sum_{i=1}^{n} a_i b_i$$

- Property: $\vec{a} \cdot \vec{a} = a_1 a_1 + a_2 a_2 + \ldots + a_n a_n = \|\vec{a}\|_2^2$
- In the classical regression equation $y = \vec{w} \cdot \vec{x} + b$ the response variable *y* is just a dot product of the vector representing patient characteristics ($\vec{x}$) and the regression weights vector ($\vec{w}$) which is common across all patients plus an offset *b*.

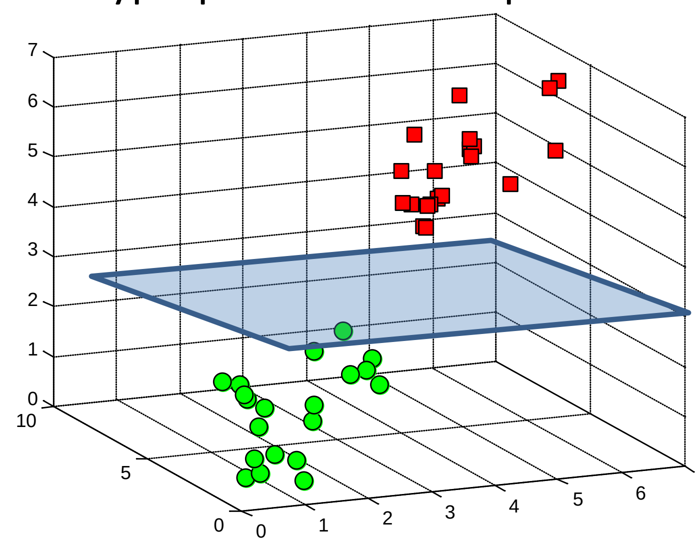
Hyperplanes as decision surfaces

- A hyperplane is a linear decision surface that splits the space into two parts;
- It is obvious that a hyperplane is a binary classifier.

A hyperplane in $\mathbb{R}^2$ is a line



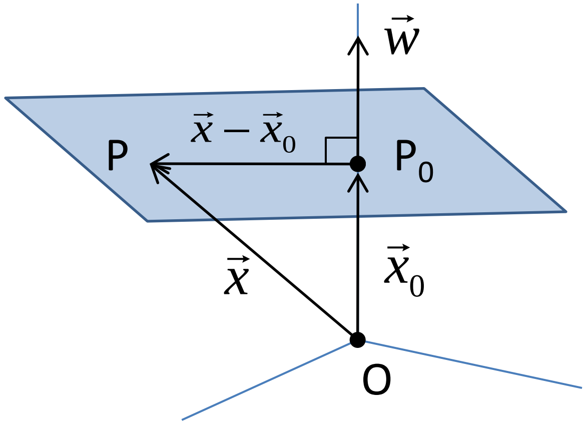
A hyperplane in $\mathbb{R}^3$ is a plane



A hyperplane in $\mathbb{R}^n$ is an n-1 dimensional subspace

Equation of a hyperplane

Consider the case of $\mathbb{R}^3$:



An equation of a hyperplane is defined by a point (P_0) and a perpendicular vector to the plane ($\vec{w}$) at that point.

Define vectors: $\vec{x}_0 = \overrightarrow{OP_0}$ and $\vec{x} = \overrightarrow{OP}$, where *P* is an arbitrary point on a hyperplane.

A condition for *P* to be on the plane is that the vector $\vec{x}-\vec{x}_0$ is perpendicular to $\vec{w}$:

$$\vec{w}\cdot(\vec{x}-\vec{x}_0)=0 \quad \text{or}$$

$$\vec{w}\cdot\vec{x}-\vec{w}\cdot\vec{x}_0=0 \quad \text{define } b=-\vec{w}\cdot\vec{x}_0$$

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

The above equations also hold for $\mathbb{R}^n$ when n>3.

Equation of a hyperplane

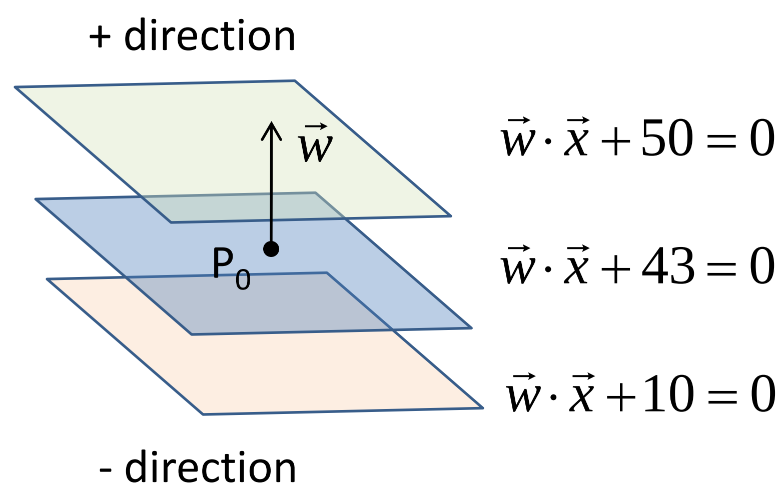
<u>Example</u>

$\vec{w} = (4,-1,6)$

$P_0 = (0,1,-7)$

$b = -\vec{w}\cdot\vec{x}_0 = -(0-1-42) = 43$

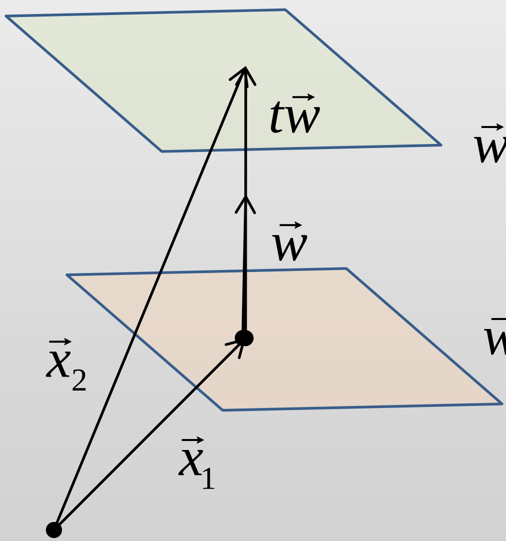
$$\boxed{\begin{aligned}&\Rightarrow \vec{w}\cdot\vec{x} + 43 = 0\\ &\Rightarrow (4,-1,6)\cdot\vec{x} + 43 = 0\\ &\Rightarrow (4,-1,6)\cdot(x_{(1)}, x_{(2)}, x_{(3)}) + 43 = 0\\ &\Rightarrow 4x_{(1)} - x_{(2)} + 6x_{(3)} + 43 = 0\end{aligned}}$$



What happens if the *b* coefficient changes?
The hyperplane moves along the direction of $\vec{w}$.
We obtain "parallel hyperplanes".

Distance between two parallel hyperplanes $\vec{w}\cdot\vec{x} + b_1 = 0$ and $\vec{w}\cdot\vec{x} + b_2 = 0$ is equal to $D = |b_1 - b_2| / \|\vec{w}\|$.

(Derivation of the distance between two parallel hyperplanes)



$$\vec{w}\cdot\vec{x}+b_2=0$$

$$\vec{w}\cdot\vec{x}+b_1=0$$

$$\vec{x}_2=\vec{x}_1+t\vec{w}$$

$$D=\|t\vec{w}\|=|t|\|\vec{w}\|$$

$$\vec{w}\cdot\vec{x}_2+b_2=0$$

$$\vec{w}\cdot(\vec{x}_1+t\vec{w})+b_2=0$$

$$\vec{w}\cdot\vec{x}_1+t\|\vec{w}\|^2+b_2=0$$

$$(\vec{w}\cdot\vec{x}_1+b_1)-b_1+t\|\vec{w}\|^2+b_2=0$$

$$-b_1+t\|\vec{w}\|^2+b_2=0$$

$$t=(b_1-b_2)/\|\vec{w}\|^2$$

$$\boxed{\Rightarrow D=|t|\|\vec{w}\|=|b_1-b_2|/\|\vec{w}\|}$$

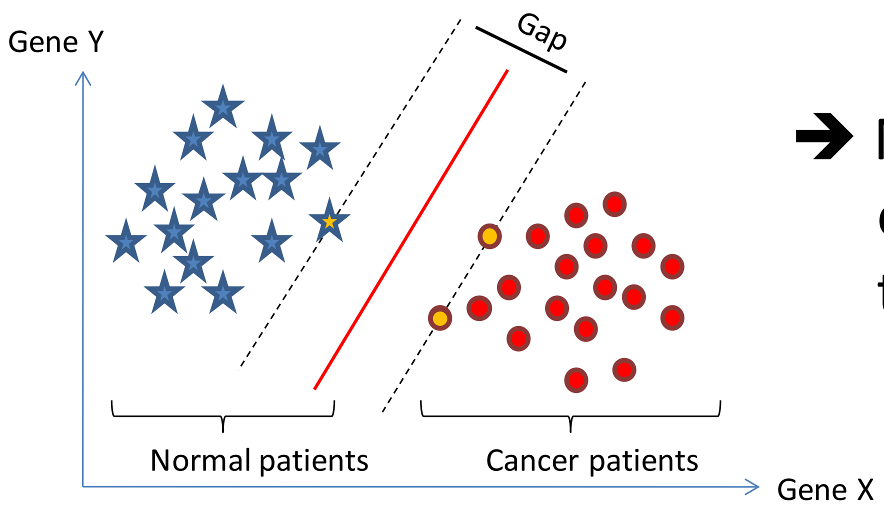
Recap

We know…

- How to represent patients (as "vectors")
- How to define a linear decision surface ("hyperplane")

We need to know…

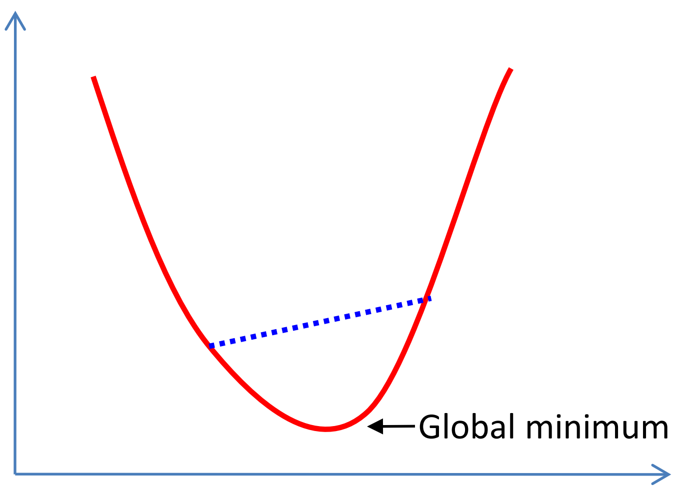
- How to efficiently compute the hyperplane that separates two classes with the largest "gap"?



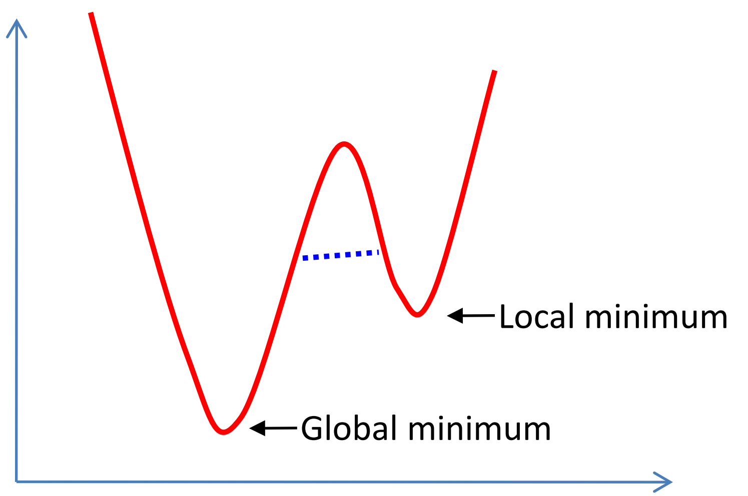
➔ Need to introduce basics of relevant optimization theory

Basics of optimization: Convex functions

- A function is called *convex* if the function lies below the straight line segment connecting two points, for any two points in the interval.
- Property: Any local minimum is a global minimum!



Convex function



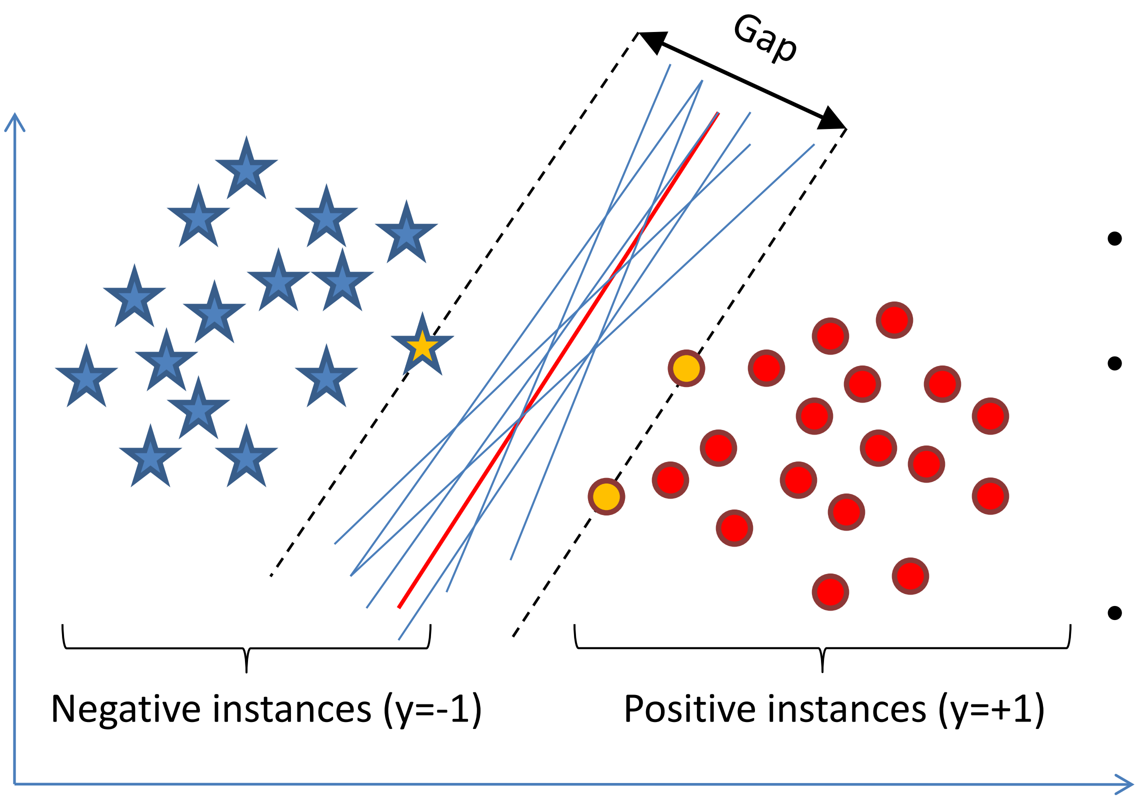
Non-convex function

Support vector machines for binary classification: classical formulation

Case 1: Linearly separable data; "Hard-margin" linear SVM

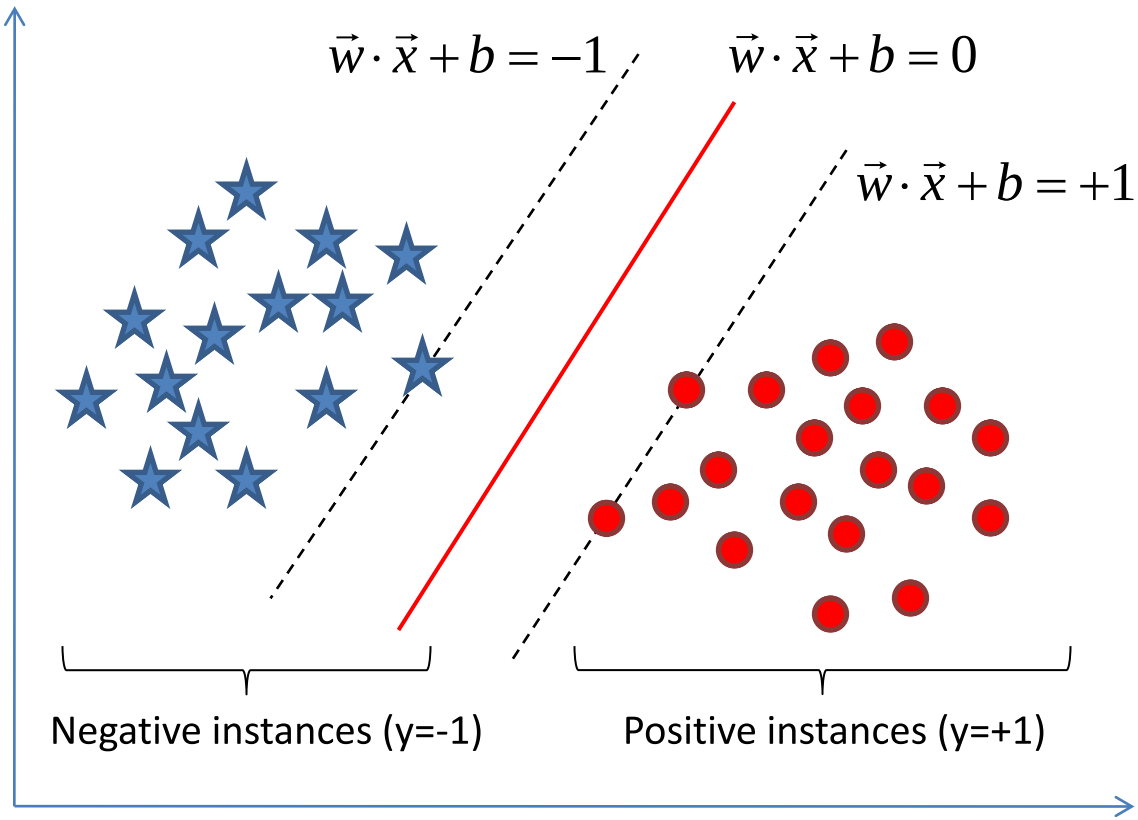
Given training data: $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N \in R^n$

$y_1, y_2, \ldots, y_N \in \{-1, +1\}$



- Want to find a classifier (hyperplane) to separate negative instances from the positive ones.
- An infinite number of such hyperplanes exist.
- SVMs finds the hyperplane that maximizes the gap between data points on the boundaries (so-called "support vectors").
- If the points on the boundaries are not informative (e.g., due to noise), SVMs will not do well.

Statement of linear SVM classifier



The gap is distance between parallel hyperplanes:

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

Or equivalently:

$$\vec{w}\cdot\vec{x}+(b+1)=0$$
$$\vec{w}\cdot\vec{x}+(b-1)=0$$

We know that

$$D=|b_1-b_2|/\|\vec{w}\|$$

Therefore:

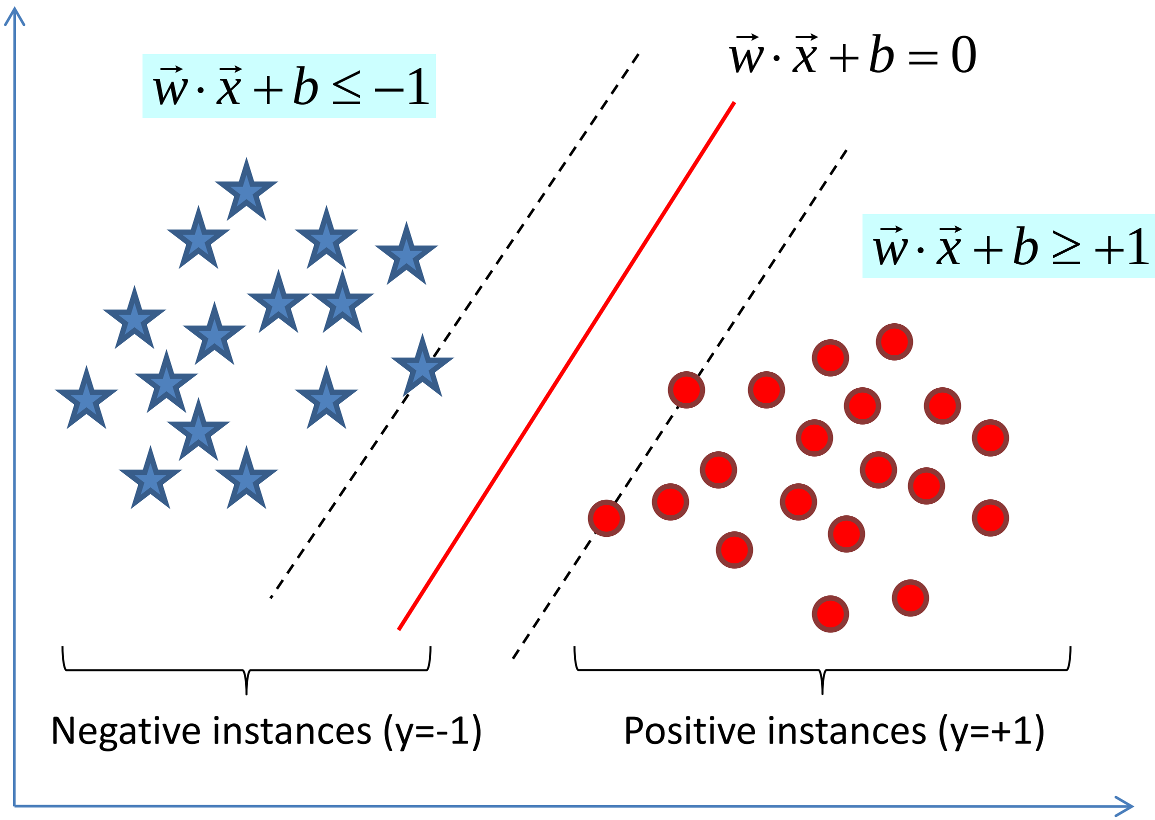
$$\boxed{D=2/\|\vec{w}\|}$$

Since we want to maximize the gap,

we need to minimize $\|\vec{w}\|$

or equivalently $\boxed{\text{minimize } \tfrac{1}{2}\|\vec{w}\|^2}$ ($\frac{1}{2}$ is convenient for taking derivative later on)

Statement of linear SVM classifier



In addition we need to impose constraints that all instances are correctly classified. In our case:

$\vec{w}\cdot\vec{x}_i+b\leq -1$ if $y_i=-1$
$\vec{w}\cdot\vec{x}_i+b\geq +1$ if $y_i=+1$

Equivalently:

$$\boxed{y_i(\vec{w}\cdot\vec{x}_i+b)\geq 1}$$

<u>In summary:</u>

Want to minimize $\frac{1}{2}\left\|\vec{w}\right\|^2$ subject to $y_i(\vec{w}\cdot\vec{x}_i+b)\geq 1$ for $i=1,\ldots,N$

Then given a new instance x, the classifier is $f(\vec{x})=sign(\vec{w}\cdot\vec{x}+b)$

SVM optimization problem: Primal formulation

Minimize $\boxed{\frac{1}{2}\sum_{i=1}^{n} w_i^2}$ subject to $\boxed{y_i(\vec{w}\cdot\vec{x}_i + b) - 1 \geq 0}$ for $i = 1,\ldots,N$

Objective function

Constraints

- This is called "*primal formulation of linear SVMs*".
- It is a convex quadratic programming (QP) optimization problem with *n* variables (w_i, i = 1,…,n), where *n* is the number of features in the dataset.

SVM optimization problem: Dual formulation

- The previous problem can be recast in the so-called "*dual form*" giving rise to "*dual formulation of linear SVMs*".
- It is also a convex quadratic programming problem but with *N* variables (α_i ,i = 1,…,N), where *N* is the number of samples.

Maximize $\boxed{\sum_{i=1}^{N} \alpha_i - \tfrac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \vec{x}_i \cdot \vec{x}_j}$ subject to $\boxed{\alpha_i \geq 0 \text{ and } \sum_{i=1}^{N} \alpha_i y_i = 0}$.

Objective function

Constraints

Then the *w*-vector is defined in terms of α_i: $\vec{w} = \sum_{i=1}^{N} \alpha_i y_i \vec{x}_i$

And the solution becomes: $f(\vec{x}) = sign(\sum_{i=1}^{N} \alpha_i y_i \vec{x}_i \cdot \vec{x} + b)$

SVM optimization problem: Benefits of using dual formulation

1) No need to access original data, need to access only dot products.

Objective function: $\sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \boxed{\vec{x}_i \cdot \vec{x}_j}$

Solution: $f(\vec{x}) = sign(\sum_{i=1}^{N} \alpha_i y_i \boxed{\vec{x}_i \cdot \vec{x}} + b)$

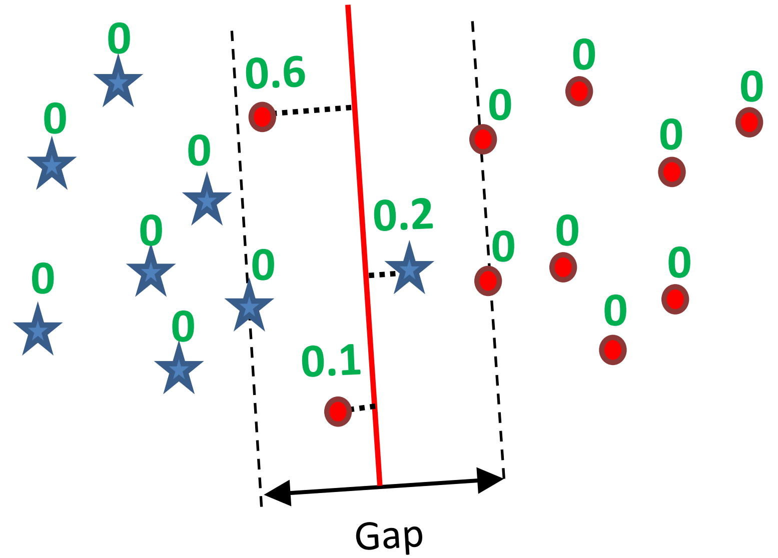
2) Number of free parameters is bounded by the number of support vectors and not by the number of variables (beneficial for high-dimensional problems).

E.g., if a microarray dataset contains 20,000 genes and 100 patients, then need to find only up to 100 parameters!

Case 2: Not linearly separable data; "Soft-margin" linear SVM

What if the data is not linearly separable? E.g., there are outliers or noisy measurements, or the data is slightly non-linear.

Want to handle this case without changing the family of decision functions.



Approach:

Assign a "slack variable" to each instance $\xi_i \geq 0$, which can be thought of distance from the separating hyperplane if an instance is misclassified and 0 otherwise.

Want to minimize $\frac{1}{2}\|\vec{w}\|^2 + C\sum_{i=1}^{N}\xi_i$ subject to $y_i(\vec{w}\cdot\vec{x}_i + b) \geq 1 - \xi_i$ for $i = 1,\ldots,N$

Then given a new instance *x*, the classifier is $f(x) = sign(\vec{w}\cdot\vec{x} + b)$

Two formulations of soft-margin linear SVM

Primal formulation:

Minimize $\boxed{\frac{1}{2}\sum_{i=1}^{n} w_i^2 + C\sum_{i=1}^{N}\xi_i}$ subject to $\boxed{y_i(\vec{w}\cdot\vec{x}_i + b) \geq 1 - \xi_i}$ for $i = 1,\ldots,N$

Objective function

Constraints

Dual formulation:

Minimize $\boxed{\sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{N}\alpha_i\alpha_j y_i y_j \vec{x}_i \cdot \vec{x}_j}$ subject to $\boxed{0 \leq \alpha_i \leq C \text{ and } \sum_{i=1}^{N}\alpha_i y_i = 0}$

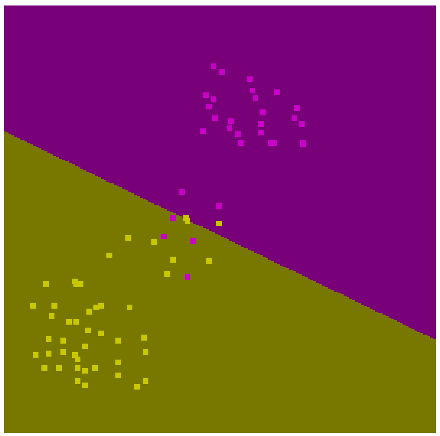
for $i = 1,\ldots,N$.

Objective function

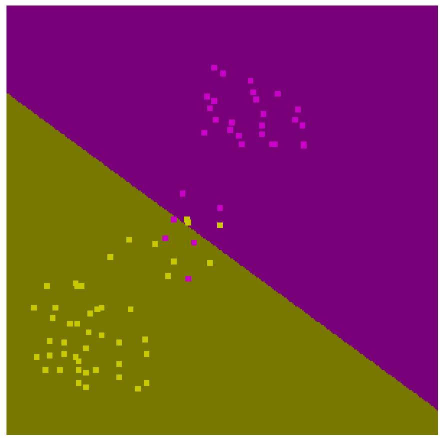
Constraints

Parameter *C* in soft-margin SVM

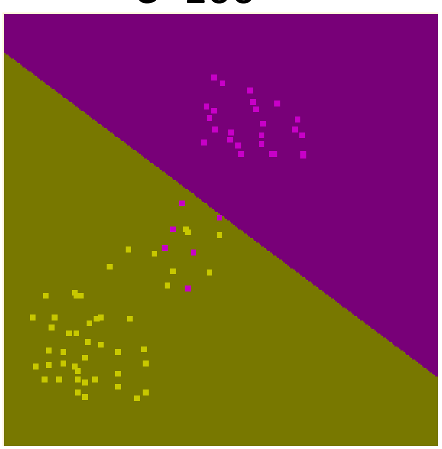
Minimize $\frac{1}{2}\left\|\vec{w}\right\|^2 + \boxed{C}\sum_{i=1}^{N}\xi_i$ subject to $y_i(\vec{w}\cdot\vec{x}_i + b) \geq 1 - \xi_i$ for $i = 1,\ldots,N$



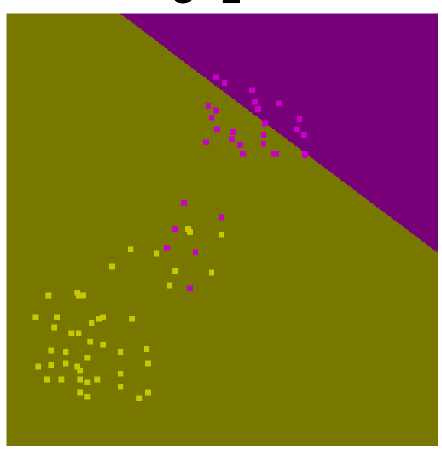
C=100



C=1



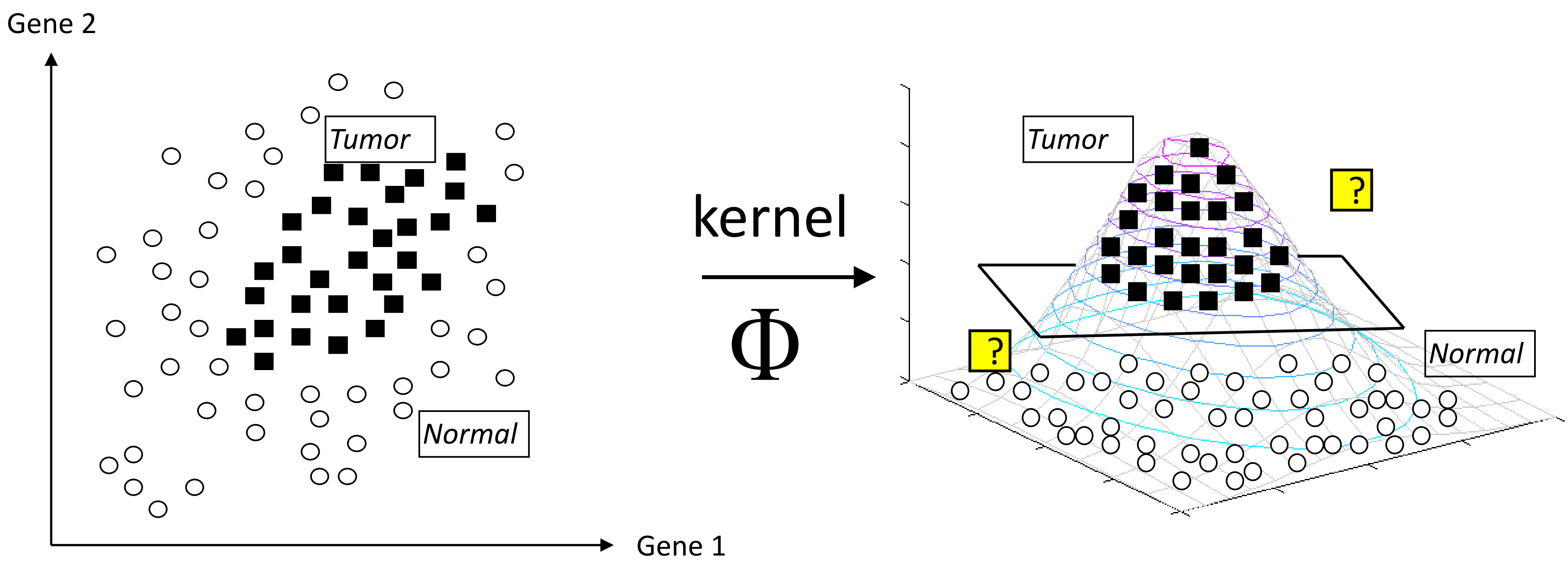
C=0.15



C=0.1

- When *C* is very large, the soft-margin SVM is equivalent to hard-margin SVM;
- When *C* is very small, we admit misclassifications in the training data at the expense of having w-vector with small norm;
- *C* has to be selected for the distribution at hand as it will be discussed later in this tutorial.

Case 3: Not linearly separable data; Kernel trick



Data is not linearly separable in the input space

Data is linearly separable in the feature space obtained by a kernel

$$\Phi : \mathbf{R}^N \rightarrow \mathbf{H}$$

Kernel trick

Original data $\vec{x}$ (in input space)

$$f(x) = sign(\vec{w} \cdot \vec{x} + b)$$

$$\vec{w} = \sum_{i=1}^{N} \alpha_i y_i \vec{x}_i$$

Data in a higher dimensional feature space $\Phi(\vec{x})$

$$f(x) = sign(\vec{w} \cdot \Phi(\vec{x}) + b)$$

$$\vec{w} = \sum_{i=1}^{N} \alpha_i y_i \Phi(\vec{x}_i)$$

$$f(x) = sign(\sum_{i=1}^{N} \alpha_i y_i \Phi(\vec{x}_i) \cdot \Phi(\vec{x}) + b)$$

$$f(x) = sign(\sum_{i=1}^{N} \alpha_i y_i K(\vec{x}_i, \vec{x}) + b)$$

Therefore, we do not need to know Φ explicitly, we just need to define function $K(\cdot, \cdot)$: $\mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}$.

Not every function $\mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}$ can be a valid kernel; it has to satisfy so-called Mercer conditions. Otherwise, the underlying quadratic program may not be solvable.

Popular kernels

A kernel is a dot product in *some* feature space:

$$K(\vec{x}_i, \vec{x}_j) = \Phi(\vec{x}_i) \cdot \Phi(\vec{x}_j)$$

<u>Examples:</u>

$K(\vec{x}_i, \vec{x}_j) = \vec{x}_i \cdot \vec{x}_j$	Linear kernel
$K(\vec{x}_i, \vec{x}_j) = \exp(-\gamma \left\|\vec{x}_i - \vec{x}_j\right\|^2)$	Gaussian kernel
$K(\vec{x}_i, \vec{x}_j) = \exp(-\gamma \left\|\vec{x}_i - \vec{x}_j\right\|)$	Exponential kernel
$K(\vec{x}_i, \vec{x}_j) = (p + \vec{x}_i \cdot \vec{x}_j)^q$	Polynomial kernel
$K(\vec{x}_i, \vec{x}_j) = (p + \vec{x}_i \cdot \vec{x}_j)^q \exp(-\gamma \left\|\vec{x}_i - \vec{x}_j\right\|^2)$	Hybrid kernel
$K(\vec{x}_i, \vec{x}_j) = \tanh(k\vec{x}_i \cdot \vec{x}_j - \delta)$	Sigmoidal