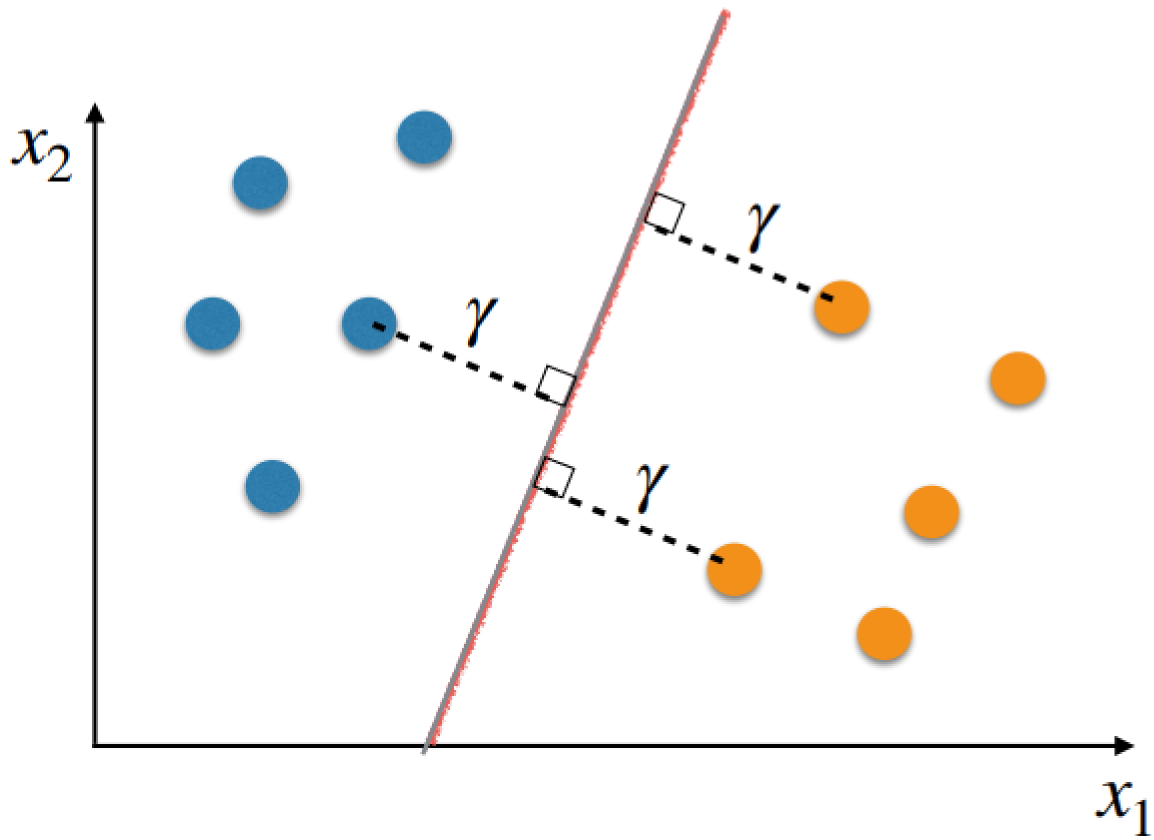
# Week 3 Note

## Support Vector Machines(SVMs)




- The perpendicular distance $\gamma$ between the decision boundary and the closest training examole is called the `margin`
- The decision boundary can be chosen so as to maximise the margin
- Training examples that are exactly on the margin are called `support vectors`
- `Given` a set of training examples

  $$J = \{(\vec{x}^{(1)}, y^{(1)}), (\vec{x}^{(2)}, y^{(2)}), ..., (\vec{x}^{(N)}, y^{(N)})\}$$

  where $(\vec{x}^{(i)}, y^{(i)}) \in X \times Y$ are drawn from a fixed albeit unkown joint probability distribution $P(\vec{x}, y) = P(y|\vec{x})P(\vec{x})$
- `Goal`: to learn a function $g$ able to `generalise` to unseen(test) examples of the same probability distribution $P(\vec{x}, y)$
  - $g$: $X \rightarrow Y$, mapping input space to output space
  - $g$ as a probability distribution approximating $P(y|\vec{x})$

## Hypothesis Set

$$h(\vec{x}) = \begin{cases} +1 & if\ \vec{w}^T\vec{x} + b > 0 \\ -1 & if\ \vec{w}^T\vec{x} + b <> 0 \end{cases}, \forall \vec{w} \in \mathbb{R}^d, \forall b \in \mathbb{R}$$

- Perpendicular Distance From a Point $\vec{x}^{(n)}$ to a Hyperplane $h(\vec{x}) = 0$

$$dist(h, \vec{x}^{(n)}) = \frac{|h(\vec{x}^{(n)})|}{||\vec{w}||} = \frac{y^{(n)}h(\vec{x}^{(n)})}{||\vec{w}||}$$

where $||w|| = \sqrt{\vec{w}^T\vec{w}}$ is the Euclidean norm(the length of the vector $\vec{w}$)

- Find $\vec{w}$ and $b$ that maximise the margin
- `Constraint`: all training examples must be correctly classified

> $$\min_n dist(h, \vec{x}^{(n)})$$
> $$\downarrow$$
> $$\arg\max_{\vec{w},b}\{\min_n dist(h, \vec{x}^{(n)})\}$$
>
> `Constraint`:
>
> $$Subject\ to\ y^{(n)}h(\vec{x}^{(n)}) > 0, \forall(\vec{x}^{(n)}, y^{(n)}) \in J$$

> $$\arg\max_{\vec{w},b}\{\min_n(\frac{y^{(n)}h(\vec{x}^{(n)})}{||\vec{w}||})\}$$
> $$\downarrow$$
> $$\arg\max_{\vec{w},b}\{\frac{1}{||\vec{w}||}\min_n(y^{(n)}h(\vec{x}^{(n)}))\}$$
>
> `Constraint`:
>
> $$Subject\ to\ y^{(n)}h(\vec{x}^{(n)}) > 0, \forall(\vec{x}^{(n)}, y^{(n)}) \in J$$
> $$Subject\ to\ \min_n y^{(n)}h(\vec{x}^{(n)}) = 1, \forall(\vec{x}^{(n)}, y^{(n)}) \in J$$
>
> > - Why are these two constraints equivalent?
> >     - Rescaling $\vec{w}$ and $b$ does not change the position of the hyperplane, nor the distances of the training examples to it
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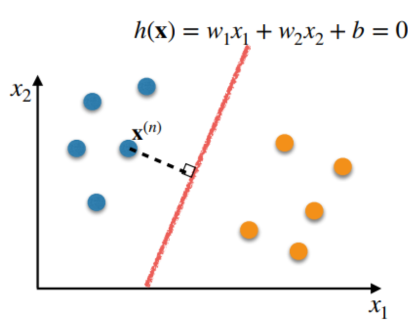
> > 
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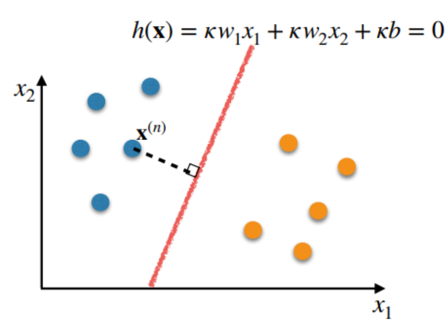
> > 
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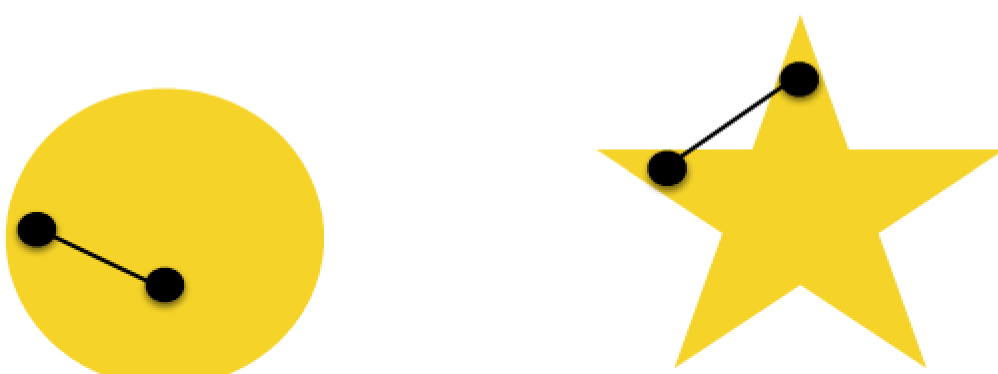
> > - If there is a hyperplane that can separate the training examples, its $\vec{w}$ and $b$ can be divided by $\min_n y^{(n)} h(\vec{x}^{(n)})$ so that $y^{(n)} h(\vec{x}^{(n)}) = 1$ for the closet example
>
> $$\arg\max_{\vec{w},b}\{\frac{1}{||\vec{w}||}\}$$
> $$\downarrow$$
> $$\arg\min_{\vec{w},b}\{||\vec{w}||\}$$
>
> `Constraint`:
>
> $$Subject\ to\ \min_n y^{(n)} h(\vec{x}^{(n)}) = 1, \forall(\vec{x}^{(n)}, y^{(n)}) \in J\ stricter$$
> $$Subject\ to\ y^{(n)} h(\vec{x}^{(n)}) \geq 1, \forall(\vec{x}^{(n)}, y^{(n)}) \in J\ looser$$
>
> > The optimal solution will satisfy the equality in $y^{(n)} h(\vec{x^{(n)}}) \geq 1$ for at least one training example

> $$\arg\min_{\vec{w},b}\{\frac{1}{2}||\vec{w}||^2\}$$
>
> `Constraint`:
>
> $$Subject\ to\ y^{(n)}(\vec{w}^T \phi(\vec{x}^{(n)} + b) \geq 1, \forall(\vec{x}^{(n)}, y^{(n)}) \in J$$

## Convexity

- Convex Sets
  - A set $C$ is convex if the line segment between any two points in $C$ lies in $C$
  - For any two points $\vec{x}^{(1)}, \vec{x}^{(2)} \in C$ and any $\lambda \in (0, 1)$, we have:

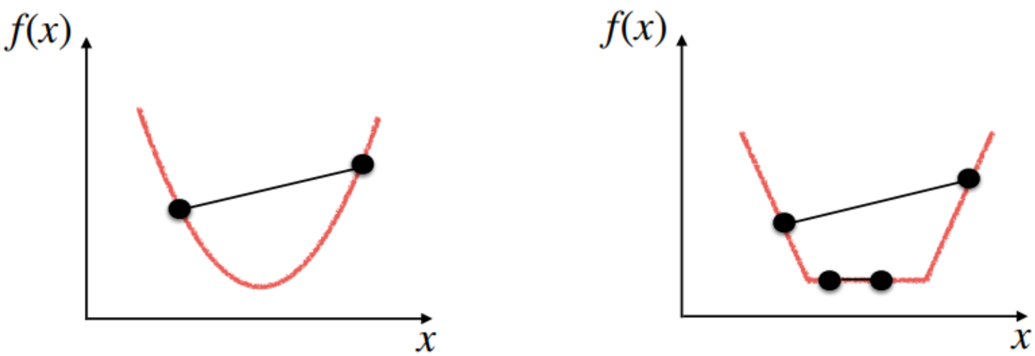
$$\lambda\vec{x}^{(1)} + (1-\lambda)\vec{x}^{(2)} \in C$$



- Convex Functions
    - A convex function $f(\vec{x})$ is a function with a convex domain $C$ that satisfies the following condition for any $\vec{x}^{(1)}, \vec{x}^{(2)} \in C$ and $\lambda \in (0,1)$

$$f\left(\lambda\vec{x}^{(1)} + (1-\lambda)\vec{x}^{(2)}\right) \leq \lambda f\left(\vec{x}^{(1)}\right) + (1-\lambda) f\left(\vec{x}^{(2)}\right)$$

    - Strictly convex: satisfies the condition with <

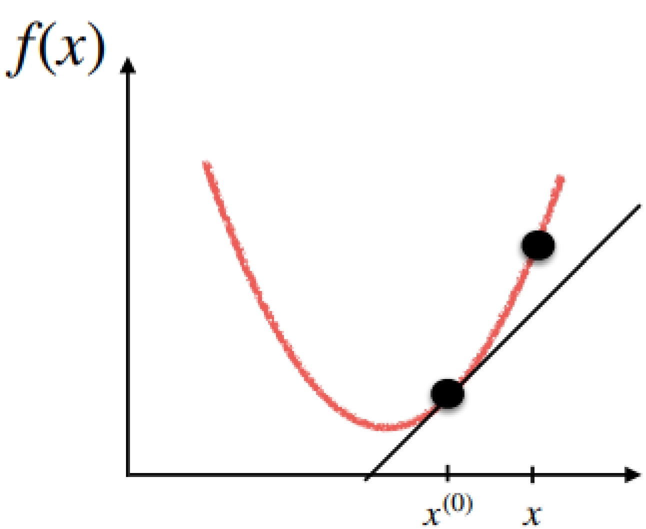



- Importance of Convexity in Machine Learning/Optimisation
    - Any minimum in a convex function is a global minimum
    - A strictly convex function has at most one stationary (critical) point. If such a point exists, it is a global minimum
- Concave: A function $f(\vec{x})$ is concave if $-f(\vec{x})$ is convex

- First-Derivative Characterisation of Convexity
    - A differentiable function $f(\vec{x})$ is convex iff its domain $C$ is convex and it satisfies the following condition for any pair $\vec{x}^{(0)}, \vec{x} \in C$

$$f(\vec{x}) \geq \underbrace{f(\vec{x}^{(0)}) + \nabla f(\vec{x}^{(0)}) \cdot (\vec{x} - \vec{x}^{(0)})}_{\text{Equation of the tangent line}}$$

    - Strictly convex: satisfies the condition with > for any $\vec{x}^{(1)} \neq \vec{x}^{(2)}$



- Second-Derivative Characterisation of Convexity
  - A twice differentiable function $f(\vec{x})$ is convex iff:
    - Its domain $C$ is a convex set and
    - Its Hessian $H_f(\vec{x})$ is positive semidefinite for all $\vec{x} \in C$
  - If a twice differentiable function $f(\vec{x})$
    - has a convex set $C$ as its domain and
    - its Hessian $H_f(\vec{x})$ is positive definite for all $\vec{x} \in C$
  - It is a strictly convex function.(sufficient but not necessary condition)

- First-Order(Partial) Derivatives
  - `(First-order) derivatives` tell us the rate of change of $f(x)$ as we increase x

$$\frac{d}{dx}f(x) = \frac{df}{dx} = f'(x) = f^{(1)}(x)$$

  - `(First-order) partial derivatives` tell us the rate of change of $f(\vec{x})$ as we increase a specific variable $x_i$

$$\frac{\partial f}{\partial x_i}$$

  - `(Partial) derivatives` tell us whether $f(\vec{x})$ is increasing /decreasing (along a specific axis) and how rapidly

- Second-Order(Partial) Derivatives
  - `Second-order derivative`: This is the derivative of the derivative of $f(x)$, denoted as $\frac{d^2 f(x)}{dx^2}$. In simpler terms, it gives the rate of change of the slope $f'(x)$.

$$\frac{d^2}{dx^2}f(x) = \frac{d}{dx}\left(\frac{df}{dx}\right) = \frac{d^2 f}{dx^2} = f''(x) = f^{(2)}$$

  - `Second-order partial derivative``: This is the partial derivative of the partial derivative of $f(x)$. It shows the rate of change of the slope along a specific axis, relative to that same axis or another one.

$$\frac{\partial^2 f}{\partial x_i^2} = \frac{\partial}{\partial x_i}\left(\frac{\partial f}{\partial x_i}\right)$$
$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_i}\left(\frac{\partial f}{\partial x_j}\right)$$

- Hessian - Matrix of Second-Order Partial Derivatives
  - Consider $f(\vec{x})$, where $\vec{x} = (x_0.x_1, ..., x_d)^T$

$$H(f(\vec{x})) = H_f(\vec{x}) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_0^2} & \frac{\partial^2 f}{\partial x_0 \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_0 \partial x_n} \\ \frac{\partial^2 f}{\partial x_1 \partial x_0} & \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_d^2} \end{bmatrix}$$

- Univariate Case
  - The function is convex iff $f''(x) \geq 0$ for all $x$
  - If $f''(0) > 0$ for all $x$, a function is strictly convex(sufficient but not necessary condition)
  - If $f'(x) = 0$ and $f''(x) > 0$, then $x$ is a (local) minimum(sufficient but not necessary condition)
  - The function is concave iff $f''(x) \leq 0$ for all $x$
  - If $f''(0) < 0$ for all $x$, a function is strictly concave(sufficient but not necessary condition)
  - If $f'(x) = 0$ and $f''(x) < 0$, then $x$ is a (local) maximum(sufficient but not necessary condition)
- Multivariate Case
  - The function is convex iff $H_f(\vec{x}) \geq 0$ (positive semidefinite) for all $\vec{x}$
  - If $H_f(\vec{x}) > 0$(positive definite) for all $\vec{x}$, a function is strictly convex(sufficient but not necessary condition)
  - if $\triangledown f(\vec{x}) = 0$ and $H_f(\vec{x}) > 0$, then $x$ is a (local) minimum(sufficient but not necessary condition)
- Positive Semidefinite Matrix
  - A $d \times d$ symmetric matrix $A$ is positive semidefinite iff for any non-zero vector $\vec{z} \in \mathbb{R}^d$ , the following is true:

    $$\vec{z}^T A \vec{z} \geq 0$$

    e.g.

    $$\vec{z}^T A \vec{z} = \begin{pmatrix} z_1 & z_2 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} z_1 & z_2 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = z_1^2 + z_2^2$$

    Satisfying the above with > defines a "positive definite" matrix

- Second-Derivative Characterisation of Convexity
  - A twice differentiable function $f(\vec{x})$ is convex iff:
    - its domain $C$ is a convex set and
    - its Hessian $H_f(\vec{x})$ is positive semidefinite for all $\vec{x} \in C$
  - For any $\vec{z}, \vec{x}$, we have $\vec{z} H_f(\vec{x}) \vec{z} \geq 0$
- Eigenvalues and Eigenvectors

> - The eigenvalues of $H$ capture the direction of the principal curvatures of the function $f(\vec{x})$, where the curvature is most pronounced
> - The eigenvalues of $H$ capture the curvature itself
> - If all eigenvalues are $\geq 0$, the curvature is always positive, "upwards"
> - The eigenvalues are $\geq 0$ iff $H_f(\vec{x}) \geq 0$

## The Dual Representation for SVM

### Dual representation of SVM

- Primal Representation

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

Subject to: $y^{(n)}(\vec{w}^T\phi(\vec{x}^{(n)})+b) \geq 1 \; \forall(\vec{x}^{(n)}, y^{(n)} \in J)$

- Dual Representation

$$\arg\max_{a} \tilde{L}(\vec{a}) \sum_{n=1}^{N} a^{(n)} - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a^{(n)}a^{(m)}y^{(n)}y^{(m)}k(\vec{x}^{(n)}, \vec{x}^{(m)})$$

where: $k(\vec{x}^{(n)}, \vec{x}^{(m)}) = \phi(\vec{x}^{(n)})^T\phi(\vec{x}^{(m)})$
Subject to: $a^{(n)} \leq 0$, $\forall n \in \{1, ..., N\} \sum_{n=1}^{N} a^{(n)}y^{(n)} = 0$

### Kernel trick

- There is a way to compute $k(\vec{x}^{(n)}, \vec{x}^{(m)}) = \phi(\vec{x}^{(n)})^T\phi(\vec{x}^{(m)})$ without having to ever compute $\phi(x)$. This is called the `Kernel Trick`
- This calculation can be generalised to basis expansions composed of all terms of order up to $p$

$$k(\vec{x}, \vec{z}) = \phi(\vec{x})^T\phi(\vec{z}) = (1 + \vec{x}^T\vec{z})^p$$

- Mercer's Condition
  - Consider any finite set of points $\vec{x}^{(1)}, ..., \vec{x}^{(M)}$(not necessarily the training set)
  - Gram matrix: An $M \times M$ similarity matrix $K$, whose elements are given by $K_{i,j} = k(\vec{x}^{(i)}, \vec{x}^{(j)})$
  - Mercer's condition states that $K$ must be symmetric and positive semidefinite.
    - Symmetric: $k(\vec{x}^{(i)}, \vec{x}^{(j)}) = k(\vec{x}^{(j)}, \vec{x}^{(i)})$
    - Positive semidefinite: $\vec{z}K\vec{z} \geq 0 \; \forall \vec{z} \in \mathbb{R}^M$

> If these conditions are satisfied, the inner product defined by the kernel in the feature space respects the properties of inner products.

- Given valid kernels $k_1(x,z)$ and $k_2(x,z)$, the following will also be valid kernels:
    - $k(x,z) = ck_1(x,z)$
        - where $c \geq 0$ is a constant.
    - $k(x,z) = f(x)k_1(x,z)f(z)$
        - where $f(\cdot)$ is any function.
    - $k(x,z) = q(k_1(x,z))$
        - where $q(\cdot)$ is a polynomial with non-negative coefficients.
    - $k(x,z) = e^{k_1(x,z)}$
    - $k(x,z) = k_1(x,z) + k_2(x,z)$
    - $k(x,z) = k_1(x,z)k_2(x,z)$
- Gaussian kernel, a.k.a. Radial Basis Function (RBF) kernel

$$k(\vec{x}, \vec{x}^{(n)}) = e^{-\frac{||x - x^{(n)}||^2}{2\sigma^2}}$$

The embedding $\phi$ is infinite dimensional