CS 474/574 Machine Learning
2. Linear Classifiers

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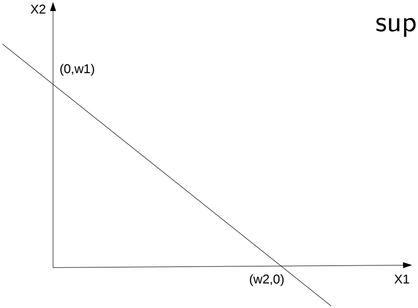
The hyperplane



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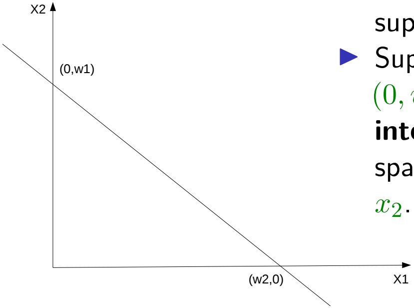

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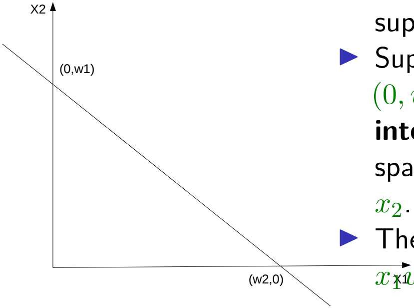

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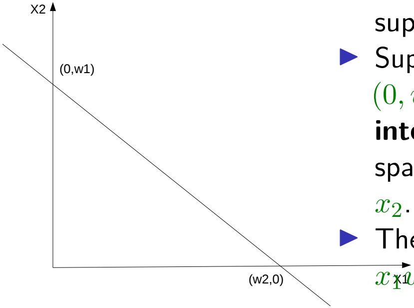

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- In matrix form:

$$(x_1, x_2, 1) \begin{pmatrix} w_1 \\ w_2 \\ -w_1 w_2 \end{pmatrix} = \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ 1 \end{pmatrix}^T}_{\mathbf{x}^T} \underbrace{\begin{pmatrix} w_1 \\ w_2 \\ -w_1 w_2 \end{pmatrix}}_{\mathbf{w}} = 0$$

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- Let

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ 1 \end{pmatrix}$$

  and

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- x_1 and x_2 are two **feature values** comprising the feature vector. 1 is **augmented** for the bias $-w_1 w_2$.
- Then the equation is rewritten into matrix form: $\mathbf{x}^T \cdot \mathbf{w} = 0$. For space sake, $\mathbf{x}^T \mathbf{w} = \mathbf{x}^T \cdot \mathbf{w}$.

The hyperplane (cond.)

- Expand to n-dimension.

$$\mathbf{X} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \\ 1 \end{pmatrix}$$

and

$$\mathbf{W} = \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \\ -w_1 w_2 \end{pmatrix}.$$

Then $\mathbf{X}^T \cdot \mathbf{W} = 0$, denoted as the *hyperplane* in $\mathbb{R}^n$.

Binary Linear Classifier

- A binary linear classier is a function $f(X) = \mathbf{W}\mathbf{X}$, such that

$$\begin{cases} \mathbf{W}^T\mathbf{X} > 0 & \forall X \in C_1 \\ \mathbf{W}^T\mathbf{X} < 0 & \forall X \in C_2 \end{cases} \tag{1}$$

  where C_1 and C_2 are the two classes. Note that the $\mathbf{X}$ has been augmented with 1 as mentioned before.

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- Example. Let $\mathbf{W}^T = (2, 4, -8)$, what's the class for new sample $\mathbf{X} = (1, 1, 1)$ (1 is augmented)?
- $\mathbf{W}^T\mathbf{X} = -2 < 0$. Hence the sample of feature value $(1, 1)$ belongs to class C_1.

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  - First, augment: $\mathbf{x}_1 = (0,0,1)^T$, $\mathbf{x}_2 = (0,1,1)^T$, $\mathbf{x}_3 = (1,0,1)^T$, $\mathbf{x}_4 = (1,1,1)^T$

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  - First, augment: $\mathbf{x}_1 = (0, 0, 1)^T$, $\mathbf{x}_2 = (0, 1, 1)^T$, $\mathbf{x}_3 = (1, 0, 1)^T$, $\mathbf{x}_4 = (1, 1, 1)^T$
  - Then, normalize $\mathbf{x}''_1 = \mathbf{x}_1$, $\mathbf{x}''_2 = \mathbf{x}_2$, $\mathbf{x}''_3 = -\mathbf{x}_3 = (-1, 0, -1)^T$, $\mathbf{x}''_4 = \mathbf{x}_4 = (-1, -1, -1)^T$

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- *normalize* the feature vector: $\mathbf{X}_i y_i$ for $y_i \in \{+1, -1\}$.
- Example:
  - $\mathbf{x}_1' = (0,0)^T$, $\mathbf{x}_2' = (0,1)^T$, $\mathbf{x}_3' = (1,0)^T$, $\mathbf{x}_4' = (1,1)^T$,
  - $y_1 = 1, y_2 = 1, y_3 = -1, y_4 = -1$
  - First, augment: $\mathbf{x}_1 = (0,0,1)^T$, $\mathbf{x}_2 = (0,1,1)^T$, $\mathbf{x}_3 = (1,0,1)^T$, $\mathbf{x}_4 = (1,1,1)^T$
  - Then, normalize $\mathbf{x}_1'' = \mathbf{x}_1$, $\mathbf{x}_2'' = \mathbf{x}_2$, $\mathbf{x}_3'' = -\mathbf{x}_3 = (-1,0,-1)^T$, $\mathbf{x}_4'' = \mathbf{x}_4 = (-1,-1,-1)^T$
- Please note that the term ''normalized" could have different meanings in different context of ML.

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- Let $\mathbf{W}^T = (w_1, w_2)$. In the training process, we can establish 4 inequalities:

$$\begin{cases} 4w_1 + w_2 & > 0 \\ 5w_1 + w_2 & > 0 \\ w_1 + w_2 & < 0 \\ 2w_1 + w_2 & < 0 \end{cases}$$

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- We can find many w_1 and w_2 to satisfy the inequalities. But, how to pick the best?

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- if a function is convex, a local minimum/maxinum is the *global minimum/maximum*.

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- One intuitive criterion can be the sum of error square:

$$J(\mathbf{W}) = \sum_{i=1}^{N} (\mathbf{W}^T \mathbf{x}_i - y_i)^2 = \sum_{i=1}^{N} (\mathbf{x}_i^T \mathbf{W} - y_i)^2$$

where $\mathbf{x}_i$ is the i-th sample (we have N samples here), y_i the corresponding label, $\mathbf{W}^T\mathbf{X}$ is the prediction.

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  where $\mathbf{x}_i$ is the i-th sample (we have N samples here), y_i the corresponding label, $\mathbf{W}^T\mathbf{X}$ is the prediction.
- For each sample $\mathbf{x}_i$, the error of the classifier is $\mathbf{W}^T\mathbf{x} - y_i$. The square is to avoid that errors on difference samples cancele out, e.g., $[+1-(-1)]-[-1-(+1)]=0$.

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- Minimizing $J(\mathbf{W})$ means:
  $\frac{\partial J(\mathbf{W})}{\partial \mathbf{W}} = 2 \sum_{i=1}^{N} \mathbf{x}_i(\mathbf{x}_i^T\mathbf{W} - y_i) = (0, \dots, 0)^T$

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- Hence, $\sum_{i=1}^{N} \mathbf{x}_i\mathbf{x}_i^T\mathbf{W} = \sum_{i=1}^{N} \mathbf{x}_i y_i$

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- Hence, $\sum_{i=1}^{N} \mathbf{x}_i\mathbf{x}_i^T\mathbf{W} = \sum_{i=1}^{N} \mathbf{x}_i y_i$
- The sum of a column vector multiplied with a row vector produces a matrix.

$$\sum_{i=1}^{N} \mathbf{x}_i\mathbf{x}_i^T = \begin{pmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_N \\ | & | & & | \end{pmatrix} \begin{pmatrix} — & \mathbf{x}_1^T & — \\ — & \mathbf{x}_2^T & — \\ & \vdots & \\ — & \mathbf{x}_N^T & — \end{pmatrix} = \mathbb{X}^T\mathbb{X}$$

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- $\mathbb{X}^T \mathbb{X} \mathbf{W} = \mathbb{X}^T \mathbf{y}$
- $(\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbb{X} \mathbf{W} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbf{y}$

Finding the linear classifier via zero-gradient (cond.)

- $$\sum_{i=1}^{N} \mathbf{x}_i y_i = \begin{pmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_N \\ | & | & & | \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = \mathbb{X}^T \mathbf{y}$$
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Gradient descent approach

Since we define the target function as $J(\mathbf{W})$, finding $J(\mathbf{W}) = 0$ or minimizing $J(\mathbf{W})$ is intuitively the same as reducing $J(\mathbf{W})$ along the gradient. The algorithm below is a general approach to minimize any multivariate function: changing the input variable proportionally to the gradient.

Algorithm 1: pseudocode for gradient descent approach

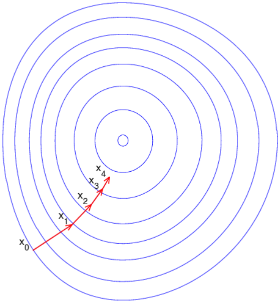
Input: an initial $\mathbf{w}$, stop criterion θ, a learning rate function $\rho(\cdot)$, iteration step $k = 0$

while $\nabla J(\mathbf{w}) > \theta$ **do**

  $\mathbf{w}_{k+1} := \mathbf{w}_k - \rho(k)\nabla J(\mathbf{w})$

  $k := k + 1$

end while



Gradient descent approach (cond.)

In many cases, the $\rho(k)$'s amplitude (why amplitude but not the value?) decreases as k increases, e.g., $\rho(k) = \frac{1}{k}$, in order to shrink the adjustment.Also in some cases, the stop condition is $\rho(k)\nabla J(\mathbf{w}) > \theta$. The limit on k can also be included in stop condition – do not run forever.

Fisher's linear discriminant

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- Quantify this goal ($\mathbf{x}$ is **not augmented** because the bias has equal impact on both classes):

$$\max J(\mathbf{w}) = \frac{(\tilde{m}_1 - \tilde{m}_2)^2}{\tilde{s}_1^2 + \tilde{s}_2^2}$$

where $\tilde{m}_i = \frac{1}{|C_i|} \sum_{\mathbf{x} \in C_i} \mathbf{w}^T\mathbf{x}$ is the post-projection center of class i and $\tilde{\mathbf{s}}_i^2 = \sum_{\mathbf{x} \in C_i} (\mathbf{w}^T\mathbf{x} - \tilde{m}_i)^2$ is the post-projection, inter-class variance for class i.

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- Tails of the distributions of both classes is less likely to overlap. A new sample projected is clearly proximate to one of the two classes.

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- $(\tilde{m}_1 - \tilde{m}_2)^2 = (\mathbf{w}^T(\mathbf{m_1} - \mathbf{m_2}))^2 = \mathbf{w}^T \overbrace{(\mathbf{m_1} - \mathbf{m_2})(\mathbf{m_1} - \mathbf{m_2})^T}^{\mathbf{S}_B} \mathbf{w}$
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- Hence $J(\mathbf{w}) = \frac{\mathbf{w}^T\mathbf{S}_B\mathbf{w}}{\mathbf{w}^T(\mathbf{S}_1 + \mathbf{S}_2)\mathbf{w}} = \frac{\mathbf{w}^T\mathbf{S}_B\mathbf{w}}{\mathbf{w}^T\mathbf{S}_w\mathbf{w}}$. This expression is known as *Rayleigh quotient*. To maximize $J(\mathbf{w})$, the $\mathbf{w}$ must satisfy $\mathbf{S}_B\mathbf{w} = \lambda\mathbf{S}_w\mathbf{w}$.

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