Kernel Methods

COMP9417, 22T2

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Primal vs. Dual Algorithms

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Instead of pure parameter based learning (i.e minimising a loss function etc.), dual algorithms introduce **instance-based** learning.

This is where we 'remember' mistakes in our data and adjust the corresponding weights accordingly.

We then use a *similarity function* or **kernel** in our predictions to weight the influence of the training data on the prediction.

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α_i represents the *importance* of a data point (x_i, y_i).

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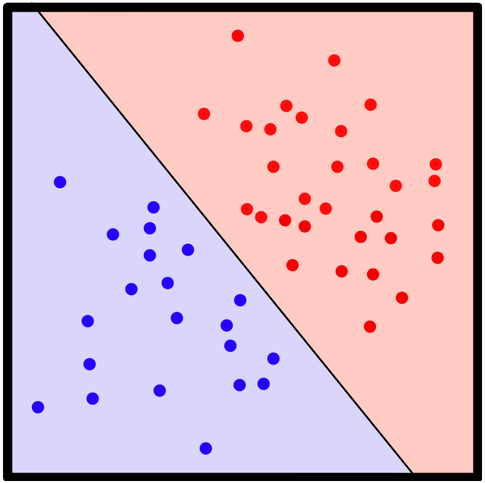

The Dual/Kernel Perceptron

Recall the *primal* perceptron:

```
$converged \leftarrow 0$
**while** not $converged$ **do**
    $converged \leftarrow 1$
    **for** $x_i \in X, y_i \in y$ **do**
        **if** $y_i w \cdot x_i \leq 0$ **then**
            $w \leftarrow w + \eta y_i x_i$
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$$w^{(K)} = \sum_{i=1}^{N} \sum_{j=1}^{K} \mathbf{1}\{y_i w^{(j)} x_i \leq 0\} y_i x_i$$

We can simply our expression and take out the indicator variable:

$$
\begin{aligned}
w^{(K)} &= \sum_{i=1}^{N} \sum_{j=1}^{K} \mathbf{1}\{y_i w^{(j)} x_i \leq 0\} y_i x_i \\
&= \sum_{i=1}^{N} \alpha_i y_i x_i
\end{aligned}
$$

where α_i is the number of times the perceptron makes a mistake on a data point (x_i, y_i).

If we sub in $w^{(K)} = \sum_{i=1}^{N} \alpha_i y_i x_i$. We get the algorithm for the **dual** perceptron.

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Gram Matrix

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$$G = \begin{bmatrix} \langle x_1, x_1 \rangle & \langle x_1, x_2 \rangle & \cdots & \langle x_1, x_n \rangle \\ \langle x_2, x_1 \rangle & \langle x_2, x_2 \rangle & \cdots & \langle x_2, x_n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle x_n, x_1 \rangle & \langle x_n, x_2 \rangle & \cdots & \langle x_n, x_n \rangle \end{bmatrix}$$

$$G_{i,j} = \langle x_i, x_j \rangle$$

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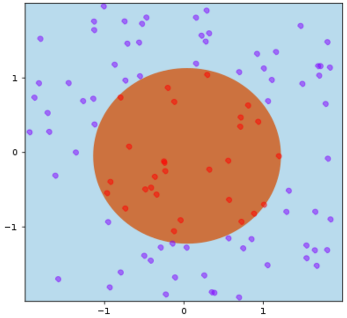
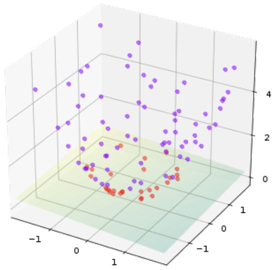
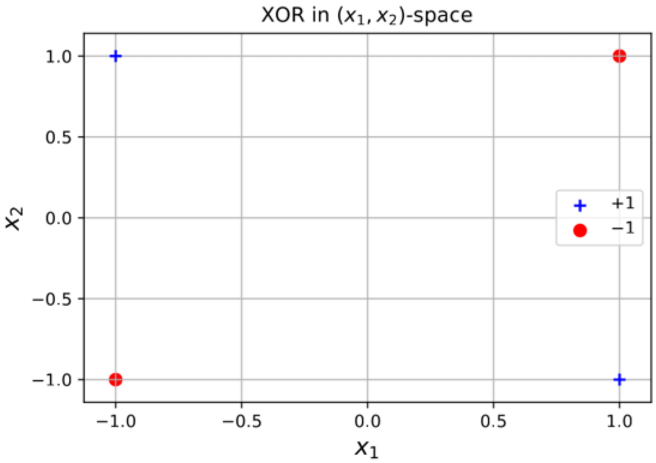




Let's revisit the XOR.



A solution:

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For our input vectors in the form $\mathbf{x} = [x_1, x_2]^T$, use a transformation:

$$\phi(\mathbf{x}) = \begin{bmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{bmatrix}$$

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$$\phi\left(\begin{bmatrix}1\\1\end{bmatrix}\right)=\begin{bmatrix}1\\\sqrt{2}\\\sqrt{2}\\1\\1\\\sqrt{2}\end{bmatrix}\phi\left(\begin{bmatrix}-1\\-1\end{bmatrix}\right)=\begin{bmatrix}1\\-\sqrt{2}\\-\sqrt{2}\\1\\1\\\sqrt{2}\end{bmatrix}\quad\phi\left(\begin{bmatrix}-1\\1\end{bmatrix}\right)=\begin{bmatrix}1\\-\sqrt{2}\\\sqrt{2}\\1\\1\\-\sqrt{2}\end{bmatrix}\quad\phi\left(\begin{bmatrix}1\\-1\end{bmatrix}\right)=\begin{bmatrix}1\\\sqrt{2}\\-\sqrt{2}\\1\\1\\-\sqrt{2}\end{bmatrix}$$

For the negative class:

$$\phi\left(\begin{bmatrix}1\\1\end{bmatrix}\right)_{2,6} = \begin{bmatrix}\sqrt{2}\\\sqrt{2}\end{bmatrix}$$

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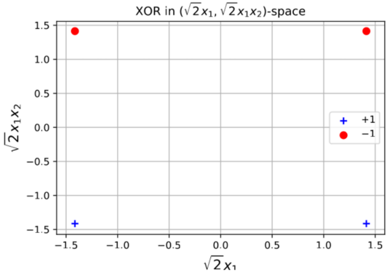

We may have a problem, recall the **dual perceptron**.

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Recall the transformation $\phi : \mathbb{R}^p \rightarrow \mathbb{R}^k$.

Recall the transformation $\phi : \mathbb{R}^p \to \mathbb{R}^k$. For an arbitrarily large k,

$$G = \begin{bmatrix} \langle \phi(x_1), \phi(x_1) \rangle & \langle \phi(x_1), \phi(x_2) \rangle & \cdots & \langle \phi(x_1), x_n \rangle \\ \langle \phi(x_2), \phi(x_1) \rangle & \langle \phi(x_2), \phi(x_2) \rangle & \cdots & \langle \phi(x_2), \phi(x_n) \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \phi(x_n), \phi(x_1) \rangle & \langle \phi(x_n), \phi(x_2) \rangle & \cdots & \langle \phi(x_n), \phi(x_n) \rangle \end{bmatrix}$$

the Gram matrix becomes far too complex to compute.

The Kernel Trick

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An absolute mathemagical idea which allows us to calculate the values of the Gram matrix for cheap.

Recall the transformation to the XOR data:

$$\phi(\mathbf{x}) = \begin{bmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{bmatrix}$$

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$$\phi(\mathbf{x}) \cdot \phi(\mathbf{y}) = 1 + 2x_1 y_1 + 2x_2 y_2 + x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 x_2 y_1 y_2$$

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Why is this useful?

Support Vector Machines