Kernel Methods

COMP9417, 22T2

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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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$$\mathbf{w} \in \mathbb{R}^p$$

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

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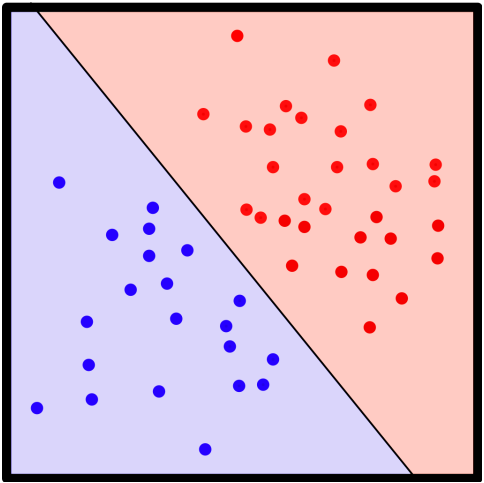

The Dual/Kernel Perceptron

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

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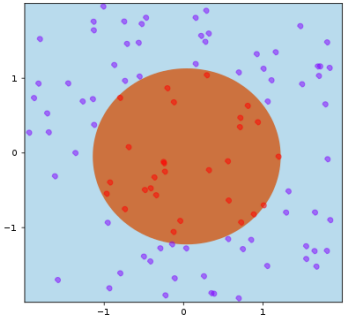
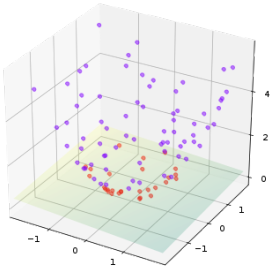
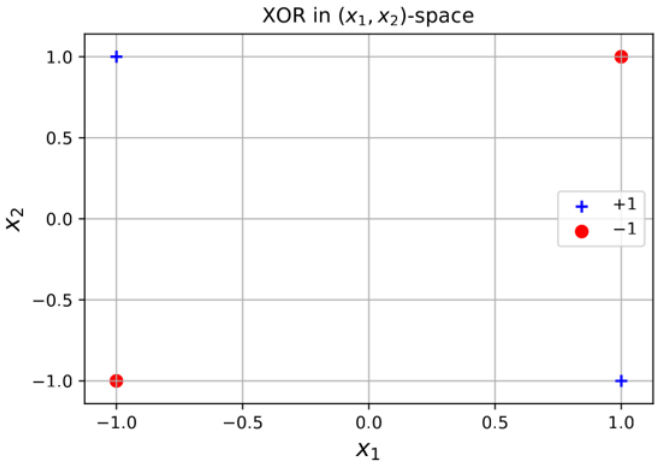




Let's revisit the XOR.



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

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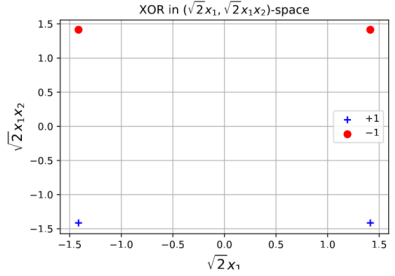

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$$G = \begin{bmatrix} \langle \phi(x_1), \phi(x_1) \rangle & \langle \phi(x_1), \phi(x_2) \rangle & \cdots & \langle \phi(x_1), x_n \rangle \\ \langle \phi(x_2), \phi(x_1) \rangle & \langle \phi(x_2), \phi(x_2) \rangle & \cdots & \langle \phi(x_2),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

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:

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$$\phi(\mathbf{x}) \cdot \phi(\mathbf{y}) = 1 + 2x_1y_1 + 2x_2y_2 + x_1^2y_1^2 + x_2^2y_2^2 + 2x_1x_2y_1y_2$$

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Why is this useful?

Support Vector Machines

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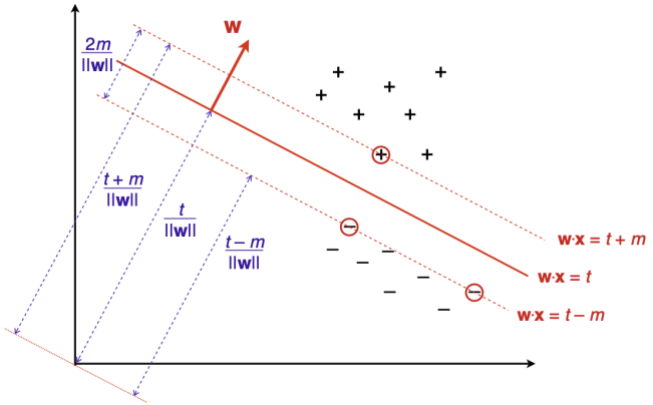

The basic SVM is a linear classifier defined by:

$$\arg\min_{w,t} \frac{1}{2}\|w\|^2 \qquad \text{subject to } y_i(\langle x_i, w\rangle - t) \geq m$$

where t is the line's intercept, and we a consider a margin m. Typically, we'll see $m = 1$ for a standardised dataset.

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This formulation means that we find the **maximal margin** classifier for the dataset.

Aside: Lagrangian Dual Problem

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$$\max_{x,y} xy \qquad \text{subject to } x + y = 4$$

we can also consider the constraint as $x + y - 4 = 0$.

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To solve this, we can calculate $\frac{\partial L}{\partial x}$, $\frac{\partial L}{\partial y}$ and $\frac{\partial L}{\partial \lambda}$ and solve the remaining system of equations.

The General Form of a Dual Problem

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$$\Lambda(\mathbf{x}, \lambda) = f(\mathbf{x}) + \sum_{i=1}^{n} \lambda_i g_i(x_i)$$

The Dual Problem for SVM

If we take the general SVM problem ($m = 1$):

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From the general form, we can take the vector α to form the dual problem:

$$\Lambda(w, t, \alpha) = \frac{1}{2}\|w\|^2 + \left(-\sum_{i=1}^{n} \alpha_i y_i(\langle x_i, w\rangle - t) - 1)\right)$$

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$$\Lambda(w, \alpha) = \frac{1}{2} w^T w - w^T w + \sum_{i=1}^{n} \alpha_i$$

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$$\Lambda(\alpha) = -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j (x_i \cdot x_j) + \sum_{i=1}^{n} \alpha_i$$

Our final problem now has relaxed constraints:

$$\Lambda(\alpha) = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j (x_i \cdot x_j) + \sum_{i=1}^{n}\alpha_i$$

$$\text{subject to } \sum_{i=1}^{n}\alpha_i y_i = 0$$

$$\alpha_i \geq 0 \text{ for } i = 1, \ldots, n$$

Soft Margin SVM

Our current model is a **maximum** or hard margin classifier. To allow for errors *within* the supporting hyperplanes, we can redefine the primal problem as:

$$\arg\min_{w,t,\xi} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i \qquad \text{subject to } y_i(\langle x_i, w\rangle - t) \geq 1 - \xi_i \text{ where } \xi_i \geq 0$$

we typically take ξ_i as the *hinge loss* of a point.

A Slight Extension: Hinge Loss

We define hinge loss for a data point at (x_i, y_i) as:

$$\xi_i = \max(0, 1 - y_i(w^T x_i - b))$$

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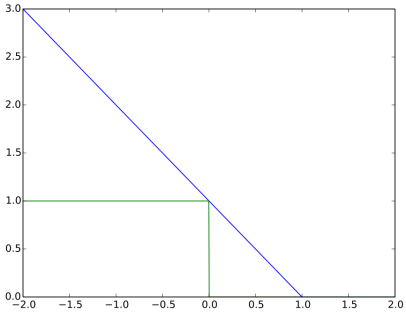

So, the function we minimise is essentially:

$$\arg\min_{w,t,\xi} \frac{1}{2}\|w\|^2 + C \max(0, 1 - y_i(w^T x_i - b))$$

$$\text{subject to } y_i(\langle x_i, w\rangle - t) \geq 1 - \max(0, 1 - y_i(w^T x_i - b))$$

Extension: The RBF Kernel

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A popular Kernel is the Radial Basis Function kernel, defined below:

$$K(x, y) = \exp\left(-\frac{\|x - y\|^2}{2\sigma^2}\right)$$

for scalar values:

$$K(x, y) = \exp\left(-\frac{(x - y)^2}{2\sigma^2}\right)$$

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$$
\begin{aligned}
K(x, y) &= \exp\left(\frac{(x-y)^2}{2\sigma^2}\right) \\
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&= \exp\left(\frac{-x^2}{2\sigma^2}\right) \exp\left(\frac{-y^2}{2\sigma^2}\right) \exp\left(\frac{xy}{\sigma^2}\right)
\end{aligned}
$$

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K(x,y) &= \exp\left(\frac{(x-y)^2}{2\sigma^2}\right) \\
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&= \exp\left(\frac{-x^2}{2\sigma^2}\right)\exp\left(\frac{-y^2}{2\sigma^2}\right)\exp\left(\frac{xy}{\sigma^2}\right) \\
&= \exp\left(\frac{-x^2}{2\sigma^2}\right)\exp\left(\frac{-y^2}{2\sigma^2}\right)\sum_{i=1}^{\infty}\frac{(xy)^k}{\sigma^{2k}k!}
\end{aligned}
$$

By definition

$$\langle \phi(x), \phi(y) \rangle = \exp\left(\frac{-x^2}{2\sigma^2}\right) \exp\left(\frac{-y^2}{2\sigma^2}\right) \sum_{i=1}^{\infty} \frac{(xy)^k}{\sigma^{2k} k!}$$

So, our basis transformation is:

$$\phi(x) = \exp\left(\frac{-x^2}{2\sigma^2}\right) \sum_{i=1}^{\infty} \frac{x^k}{\sigma^k \sqrt{k!}}$$

What does this represent?

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What does this represent? A projection to infinite dimensions!