

## Kernel Methods

COMP9417, 23T1

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## Section 1

### Kernel Methods

## Section 2

### 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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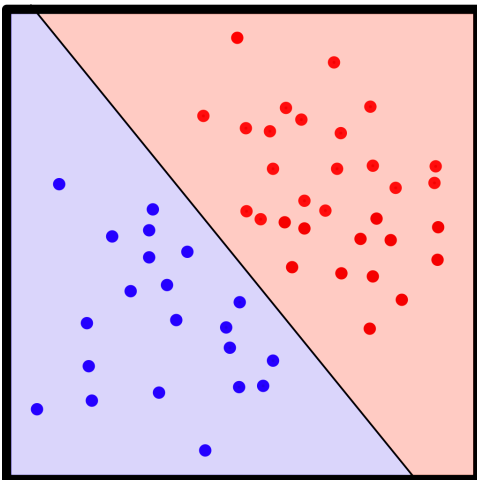
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$\alpha_i$  represents the *importance* of a data point  $(x_i, y_i)$ .

## What do we mean by importance?

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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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If we define the number of iterations the perceptron makes as  $K \in \mathbb{N}^+$  and assume  $\eta = 1$ . We can derive an expression for the final weight vector  $w^{(K)}$ :

$$w^{(K)} = \sum_{i=1}^N \sum_{j=1}^K \mathbf{1}_{\{y_i w^{(j)} \cdot x_i \leq 0\}} y_i x_i$$

We can simplify 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  $\alpha_i$  is the number of times the perceptron makes a mistake on a data point  $(x_i, y_i)$ .



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## Gram Matrix

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## Section 3

# Transformations

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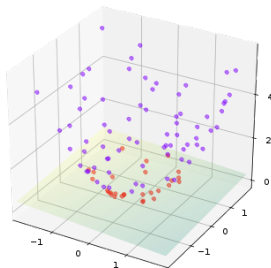
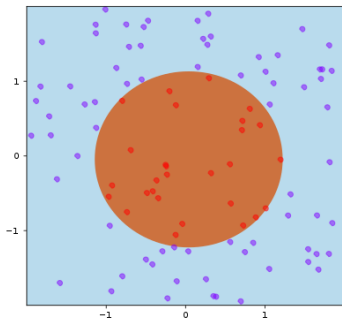
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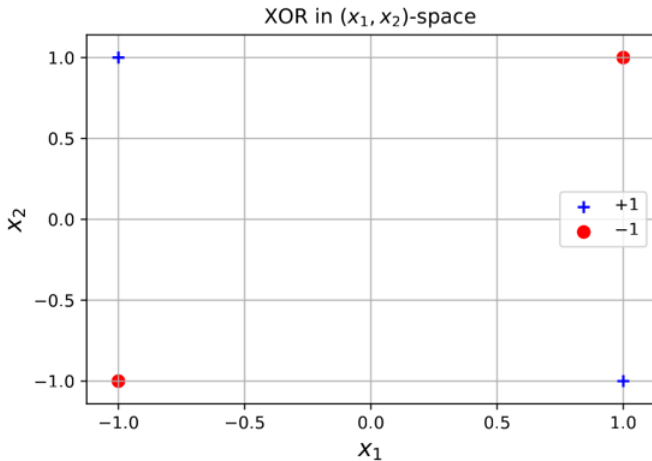
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Let's revisit the XOR.



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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For the negative class:

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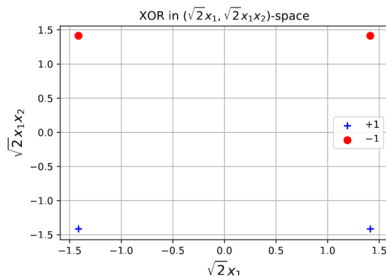
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Recall the transformation  $\phi : \mathbb{R}^p \rightarrow \mathbb{R}^k$ .

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

the Gram matrix becomes far too complex to compute.

## Section 4

### The Kernel Trick

# The Kernel Trick

An absolute mathematical 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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So our Gram matrix is:

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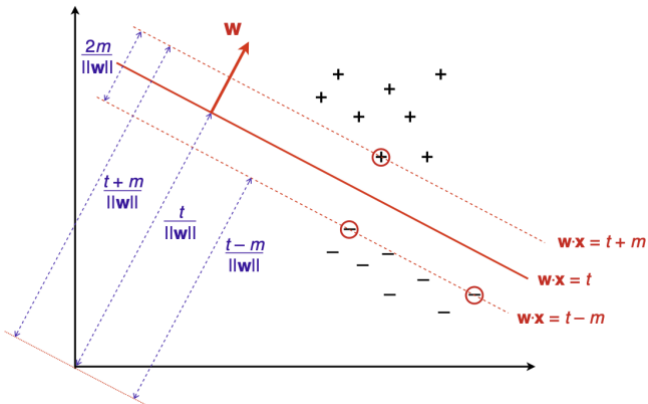
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**Why is this useful?**

## Section 5

# Support Vector Machines

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The basic SVM is a linear classifier defined by:

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

where  $t$  is the line's intercept, and we 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

Say we have a problem as follows:

$$\max_{x,y} xy$$

$$\text{subject to } x + y = 4$$

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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The general *dual* problem is:

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

# The Dual Problem for SVM

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

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

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From the general form, we can take the vector  $\alpha$  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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We've derived that for an optimal solution,  $\sum_{i=1}^n \alpha_i y_i = 0$  and  $w = \sum_{i=1}^n \alpha_i y_i x_i$

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

# The Dual Problem for SVM

We've derived that for an optimal solution,  $\sum_{i=1}^n \alpha_i y_i = 0$  and  $w = \sum_{i=1}^n \alpha_i y_i x_i$

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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:

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

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

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

## Section 6

### Question 7



## Question 7

Given data  $\mathbf{X}$  and targets  $\mathbf{y}$ , with transformed data  $\mathbf{X}'$ .

$$\mathbf{X} = \begin{bmatrix} 1 & 3 \\ 2 & 1 \\ 0 & 1 \end{bmatrix} \quad \mathbf{X}' = \begin{bmatrix} 1 & 3 \\ 2 & 1 \\ 0 & -1 \end{bmatrix}$$
$$\mathbf{y} = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}$$

solve the SVM problem by hand.

The steps given are:

- 1 Set up the Gram matrix for labelled data
- 2 Set up the expression to be minimised
- 3 Take partial derivatives
- 4 Set to zero and solve for each multiplier
- 5 Solve for  $w$
- 6 Solve for  $t$
- 7 Solve for  $m$

- ④ Set up the Gram matrix for labelled data

The Gram matrix is just the product  $\mathbf{X}'(\mathbf{X}')^T$ .

$$\mathbf{X}'(\mathbf{X}')^T = \begin{bmatrix} 1 & 3 \\ 2 & 1 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 0 \\ 3 & 1 & -1 \end{bmatrix}$$

# 1 Set up the Gram matrix for labelled data

The Gram matrix is just the product  $\mathbf{X}'(\mathbf{X}')^T$ .

$$\begin{aligned}\mathbf{X}'(\mathbf{X}')^T &= \begin{bmatrix} 1 & 3 \\ 2 & 1 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 0 \\ 3 & 1 & -1 \end{bmatrix} \\ &= \begin{bmatrix} 10 & 5 & -1 \\ 5 & 5 & -1 \\ -3 & -1 & 1 \end{bmatrix}\end{aligned}$$

② Set up the expression to be minimised

Recall the dual problem for the SVM:

$$\arg \min_{\alpha_1, \dots, \alpha_n} -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j (x_i \cdot x_j) + \sum_{i=1}^n \alpha_i$$

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

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

② Set up the expression to be minimised

Recall the dual problem for the SVM:

$$\arg \min_{\alpha_1, \alpha_2, \alpha_3} -\frac{1}{2} \sum_{i=1}^3 \sum_{j=1}^3 \alpha_i \alpha_j y_i y_j \mathbf{G}[i, j] + \sum_{i=1}^3 \alpha_i$$

$$\text{subject to } \sum_{i=1}^3 \alpha_i y_i = 0$$

$$\alpha_i \geq 0 \text{ for } i = 1, \dots, 3$$

Recall the gram matrix:

$$\mathbf{G} = \begin{bmatrix} 10 & 5 & -1 \\ 5 & 5 & -1 \\ -3 & -1 & 1 \end{bmatrix}$$

$$\arg \min_{\alpha_1, \alpha_2, \alpha_3} -\frac{1}{2} \sum_{i=1}^3 \sum_{j=1}^3 \alpha_i \alpha_j y_i y_j \mathbf{G}[i, j] + \sum_{i=1}^3 \alpha_i$$

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$$\arg \min_{\alpha_1, \alpha_2, \alpha_3} -\frac{1}{2} \left( 10\alpha_1^2 + 10\alpha_1\alpha_2 - 6\alpha_1\alpha_3 + 5\alpha_2^2 - 2\alpha_2\alpha_3 + \alpha_3^2 \right) + \alpha_1 + \alpha_2 + \alpha_3$$



If we look at the constraints ( $\sum_i \alpha_i y_i = 0$ ),

$$\sum_{i=1}^3 \alpha_i y_i = 0$$

Therefore if we substitute in  $\alpha_3 = \alpha_1 + \alpha_2$ , our final maximisation problem becomes:

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$$\alpha_1 + \alpha_2 - \alpha_3 = 0$$

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Therefore if we substitute in  $\alpha_3 = \alpha_1 + \alpha_2$ , our final maximisation problem becomes:

$$\arg \min_{\alpha_1, \alpha_2} -\frac{1}{2} \left( 10\alpha_1^2 + 10\alpha_1\alpha_2 - 6\alpha_1(\alpha_1 + \alpha_2) + 5\alpha_2^2 - 2\alpha_2(\alpha_1 + \alpha_2) + (\alpha_1 + \alpha_2)^2 \right) + \alpha_1 + \alpha_2 + (\alpha_1 + \alpha_2)$$

If we look at the constraints ( $\sum_i \alpha_i y_i = 0$ ),

$$\sum_{i=1}^3 \alpha_i y_i = 0$$

$$\alpha_1 + \alpha_2 - \alpha_3 = 0$$

$$\alpha_3 = \alpha_1 + \alpha_2$$

Therefore if we substitute in  $\alpha_3 = \alpha_1 + \alpha_2$ , our final maximisation problem becomes:

$$\arg \min_{\alpha_1, \alpha_2} -\frac{1}{2} (5\alpha_1^2 + 4\alpha_1\alpha_2 + 3\alpha_2^2) + 2\alpha_1 + 2\alpha_2$$

### 3 Take partial derivatives

$$\arg \min_{\alpha_1, \alpha_2} -\frac{1}{2} \left( 5\alpha_1^2 + 4\alpha_1\alpha_2 + 3\alpha_2^2 \right) + 2\alpha_1 + 2\alpha_2$$

### 3 Take partial derivatives

$$\arg \min_{\alpha_1, \alpha_2} -\frac{1}{2} \left( 5\alpha_1^2 + 4\alpha_1\alpha_2 + 3\alpha_2^2 \right) + 2\alpha_1 + 2\alpha_2$$

$$\frac{\partial}{\partial \alpha_1} = -5\alpha_1 - 2\alpha_2 + 2$$

$$\frac{\partial}{\partial \alpha_2} = -2\alpha_1 - 4\alpha_2 + 2$$

4 Set to zero and solve for each multiplier

For  $\alpha_1$ ,

$$-5\alpha_1 - 2\alpha_2 + 2 = 0$$

$$\alpha_1 = -\frac{(2\alpha_2 - 2)}{5}$$

#### 4 Set to zero and solve for each multiplier

For  $\alpha_1$ ,

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$$\alpha_1 = -\frac{(2\alpha_2 - 2)}{5}$$

For  $\alpha_2$ ,

$$-2\alpha_1 - 4\alpha_2 + 2 = 0$$

$$\frac{2}{5}(2\alpha_2 - 2) - 4\alpha_2 + 2 = 0$$

$$2\alpha_2 - 2 - 10\alpha_2 + 5 = 0$$

$$\alpha_2 = \frac{3}{8} \quad \alpha_1 = \frac{1}{4} \quad \alpha_3 = \frac{5}{8}$$

## 5 Solve for $w$

What did we define  $w$  as for the dual problem?



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So, in this case:

$$\begin{aligned} w &= \frac{1}{4}x_1 + \frac{3}{8}x_2 + \frac{5}{8}x_3 \\ &= \frac{1}{4} \begin{bmatrix} 1 \\ 3 \end{bmatrix} + \frac{3}{8} \begin{bmatrix} 2 \\ 1 \end{bmatrix} + \frac{5}{8} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 \\ \frac{1}{2} \end{bmatrix} \end{aligned}$$

## 6 Solve for $t$

The constraint  $y_i(\langle w, x_i \rangle - t) = 1$  for all support vectors. We can use the 3rd data point:

$$\begin{aligned}y_3(\langle w, x_3 \rangle - t) &= 1 \\ -\left(\frac{1}{2} - t\right) &= 1 \\ t &= \frac{3}{2}\end{aligned}$$

## 7 Solve for $m$

$$m = \frac{1}{\|w\|} = \frac{2}{\sqrt{5}}$$

## Section 7

### Extension: The RBF Kernel

## Extension: The RBF Kernel

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:

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

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

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

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



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

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!