Kernel Methods

COMP9417, 23T1

Section 1

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

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$$\alpha_i \qquad \text{for } i \in [1, n]$$

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

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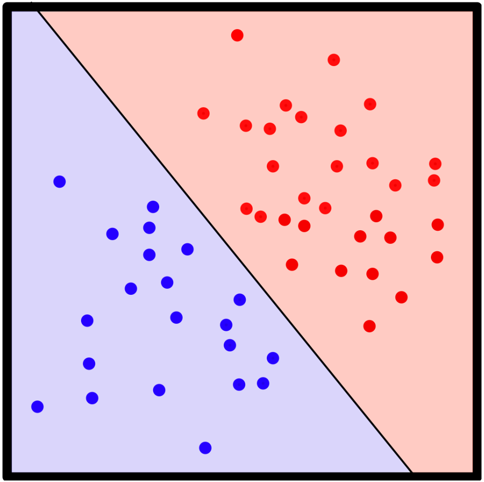

The Dual/Kernel Perceptron

Provide an explanation of how the dual version of the perceptron relates to the original.

Recall the *primal* perceptron:

$converged \leftarrow 0$
while not $converged$ **do**
  $converged \leftarrow 1$
  for $x_i \in X, y_i \in y$ **do**
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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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$$G_{i,j} = \langle x_i, x_j \rangle$$

Section 3

Transformations

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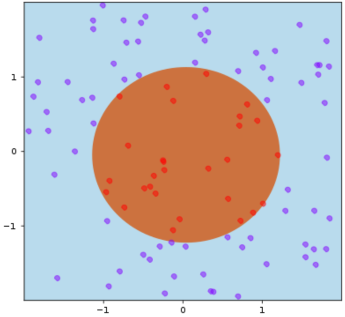
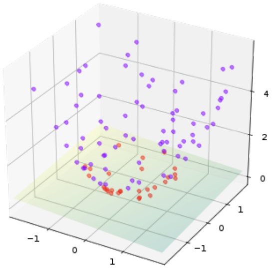
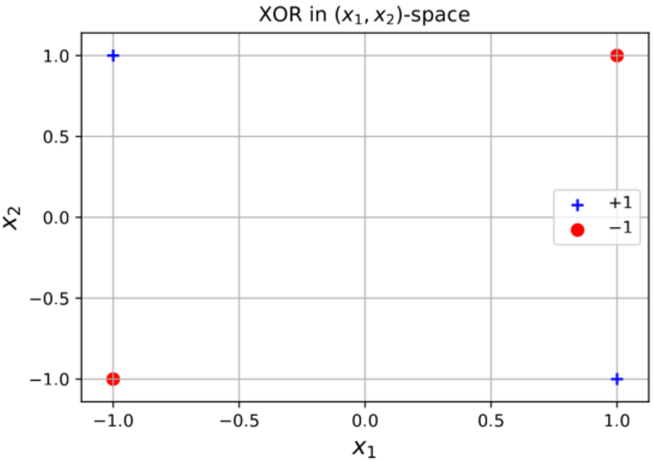




Let's revisit the XOR.



Extend the dual perceptron to learn the XOR function.

A solution:

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

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

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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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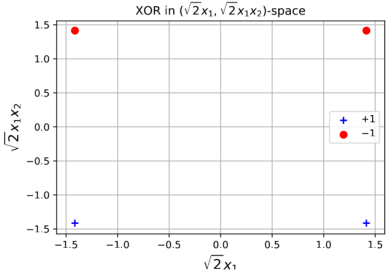

To use the **dual perceptron** on our transformed data, we simply need to redefine it.

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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 costly to compute.

Section 4

The Kernel Trick

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Show how computational issues in the previous section can be mitigated by using the Kernel trick.

Recall the transformation to the XOR data:

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Show how computational issues in the previous section can be mitigated by using the Kernel trick.

Recall the transformation to the XOR data:

$$\phi(\mathbf{x}) \cdot \phi(\mathbf{y}) = \begin{bmatrix} 1 \\ \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ x_1^2 \\ x_2^2 \\ \sqrt{2}x_1x_2 \end{bmatrix} \begin{bmatrix} 1 \\ \sqrt{2}y_1 \\ \sqrt{2}y_2 \\ y_1^2 \\ y_2^2 \\ \sqrt{2}y_1y_2 \end{bmatrix}$$

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

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So our Gram matrix is:

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Why is this useful?

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Why is this useful? We've essentially gotten a 6-dimensional transformation with the cost of a 2-dimensional dot-product.

The kernel perceptron is now defined as:

$converged \leftarrow 0$
while not $converged$ **do**
  $converged \leftarrow 1$
  for $x_i \in X, y_i \in y$ **do**
    if $y_i \sum_{j=1}^{N} \alpha_j y_j k(x_j, x_i) \leq 0$ **then**
      $\alpha_i \leftarrow \alpha_i + 1$
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Section 5

Support Vector Machines

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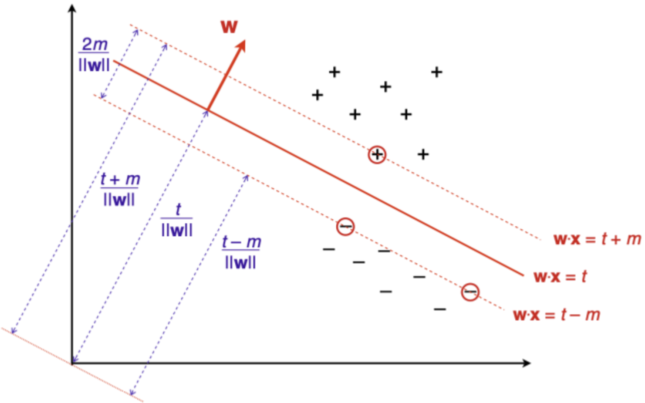

The basic SVM is a linear classifier defined by:

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

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

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$$\Lambda(x, y, \lambda) = xy + \lambda(x + y - 4)$$

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

If we have a 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 ($m = 1$):

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

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From the general form, we can take the vector 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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$$\Lambda(w,t,\alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{n}\alpha_i y_i(w \cdot x_i) + t\sum_{i=1}^{n}\alpha_i y_i + \sum_{i=1}^{n}\alpha_i$$

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We can see that at $\frac{\partial \Lambda}{\partial w} = 0$

$$w = \sum_{i=1}^{n} \alpha_i y_i x_i$$

Repeating a similar process for t,

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

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Repeating a similar process for t,

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

$$\frac{\partial \Lambda}{\partial t} = \sum_{i=1}^{n} \alpha_i y_i$$

We can see that at $\frac{\partial \Lambda}{\partial t} = 0$

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

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

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

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

Our final problem now has relaxed constraints:

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

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

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

Section 6

Question 7

Question 7

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

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

$$\mathbf{y} = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}$$

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

1. 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 $\mathbf{X}'(\mathbf{X}')^T$.

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

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

2. Set up the expression to be minimised

Recall the dual problem for the SVM:

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

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

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

2. Set up the expression to be minimised

Recall the dual problem for the SVM:

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

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

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

Recall the gram matrix:

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

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

Recall the gram matrix:

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

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

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

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 $\alpha_3 = \alpha_1 + \alpha_2$, out final maximisation problem becomes:

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

$$\begin{aligned} \sum_{i=1}^{3} \alpha_i y_i &= 0 \\ \alpha_1 + \alpha_2 - \alpha_3 &= 0 \\ \alpha_3 &= \alpha_1 + \alpha_2 \end{aligned}$$

Therefore if we substitute in $\alpha_3 = \alpha_1 + \alpha_2$, out 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 ($\sum_i \alpha_i y_i = 0$),

$$\begin{aligned}\sum_{i=1}^{3} \alpha_i y_i &= 0 \\ \alpha_1 + \alpha_2 - \alpha_3 &= 0 \\ \alpha_3 &= \alpha_1 + \alpha_2\end{aligned}$$

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

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

3. Take partial derivatives

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

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 α_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 α_1,

$$-5\alpha_1 - 2\alpha_2 + 2 = 0$$
$$\alpha_1 = -\frac{(2\alpha_2 - 2)}{5}$$

For α_2,

$$-2\alpha_1 - 4\alpha_2 + 2 = 0$$
$$\frac{2}{5}(2\alpha_2 - 2) - 4\alpha_2 + 2 = 0$$
$$2\alpha_2 - 2 - 10\alpha_2 + 5 = 0$$
$$\alpha_2 = \frac{3}{8} \qquad \alpha_1 = \frac{1}{4} \qquad \alpha_3 = \frac{5}{8}$$

5. Solve for w

What did we define w as for the dual problem?

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$$w = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x_i}$$

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What did we define w as for the dual problem?

$$w = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x_i}$$

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?

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? A projection to infinite dimensions!