Week 4 Note

Support Vector Machine: Soft Margin

Making preditions based on the dual representation

- Primal:

$$h(x) = \vec{w}^T\phi(\vec{x}) + b \begin{cases} h(\vec{x}) > 0 \rightarrow \text{class} + 1 \\ h(\vec{x}) < 0 \rightarrow \text{class - 1} \end{cases}$$

- Dual:

$$h(\vec{x}) = \sum_{n=1}^{N} a^{(n)}y^{(y)}k(\vec{x}, \vec{x}^{(n)}) + b \begin{cases} h(\vec{x}) > 0 \rightarrow \text{class} + 1 \\ h(\vec{x}) < 0 \rightarrow \text{class - 1} \end{cases}$$

  where Substituting $\vec{w} = \sum_{n=1}^{N} a^{(n)}y^{(y)}\phi(\vec{x}^{(n)})$

- For every training example
  - It will be correctly classified(if the SVM problem is feasible)
  - Either: $a^{(n)} = 0$, so the value of $y^{(n)}k(\vec{x}, \vec{x}^{(n)})$ won't matter
  - Or: $a^{(n)} > 0$ and $1 - y^{(n)}(\vec{w}^T\phi(\vec{x}^{(n)}) + b) = 0$, this is a support vector

$$g(\vec{w}, b) = \max_{\vec{a}} \sum_{n=1}^{N} a^{(n)}(1 - y^{(n)}(\vec{w}^T\phi(\vec{x}^{(n)}) + b))$$

- We only need to store the suport vectors for making predictions

$$h(\vec{x}) = \sum_{n \in S} a^{(n)}y^{(y)}k(\vec{x}, \vec{x}^{(n)}) + b$$

  where S is the set of indexes of the support vectors

> - Primal Representation
>
> $$\arg\min_{\vec{w}, b}\{\frac{1}{2}||\vec{w}||^2\}$$
>
> Subject to: $y^{(n)}(\vec{w}^T\phi(\vec{x}^{(n)}) + b) \geq 1 \, \forall(\vec{x}^{(n)}, y^{(n)} \in J)$
>
> - Dual Representation
>
> $$\arg\max_{a} \tilde{L}(\vec{a}) \sum_{n=1}^{N} a^{(n)} - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a^{(n)}a^{(m)}y^{(n)}y^{(m)}k(\vec{x}^{(n)}, \vec{x}^{(m)})$$

> where: $k(\vec{x}^{(n)}, \vec{x}^{(m)}) = \phi(\vec{x}^{(n)})^T \phi(\vec{x}^{(m)})$
>
> Subject to: $a^{(n)} \leq 0$, $\forall n \in \{1, ..., N\}$ $\sum_{n=1}^{N} a^{(n)} y^{(n)} = 0$

- Clalculating b
  - Note that $y^{(n)} h(\vec{x}^{(n)}) = 1$ for all support vectors

$$b = y^{(n)} - \sum_{m \in S} a^{(m)} y^{(m)} k(\vec{x}^{(n)}, \vec{x}^{(m)})$$

- AAveraging for All Support Vectors
  - We have N_S support vectors
  - We can compute b for each of them and average the results to get a numerically more stable solution:

$$b = \frac{1}{N_S} \sum_{n \in S} (y^{(n)} - \sum_{m \in S} a^{(m)} y^{(m)} k(\vec{x}^{(n)}, \vec{x}^{(m)}))$$

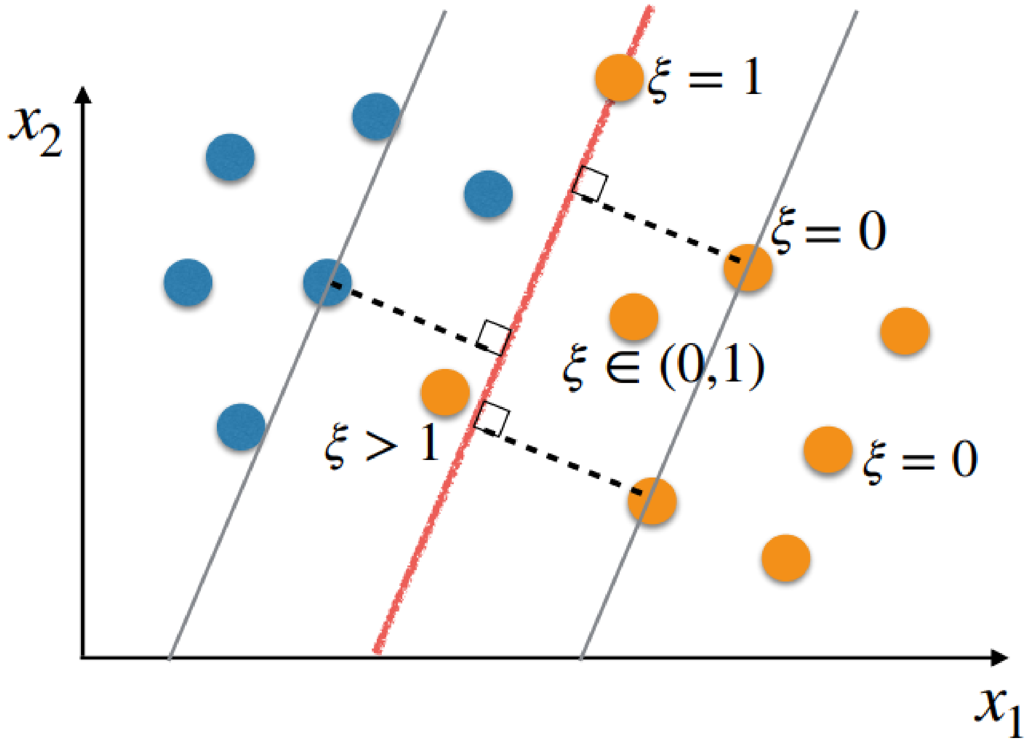
where S is the set of indexes of the support vectors and N_S is the number of support vectors

> Adopting the dual representation enables us to adopt powerful kernels, e.g., the Gaussian kernel, which takes us to an infinite dimensional embedding
>
> Predictions when using the dual representation are based on the support vectors

Soft margin SVM

- Slack Variables ξ
  - On slack variable $\xi^{(n)} \geq 0$ is associated to each training example $(\vec{x}^{(n)}, y^{(n)})$
  - These variables tell us by how much an example can be within the margin or on the wrong side of the decision boundary

$$y^{(n)} h(\vec{x}^{(n)}) \geq 1 - \xi^{(n)}$$



> - The effect of ξ
>   - $y^{(n)}h(\vec{x}^{(n)}) \geq 1 - \xi^{(n)}$
>   - $\xi^{(n)} = 0 \rightarrow y^{(n)}h(\vec{x}^{(n)}) \geq 1$
>   - $\xi^{(n)} \in (0,1) \rightarrow y^{(n)}h(\vec{x}^{(n)}) \in (0,1)$
>   - $\xi^{(n)} = 1 \rightarrow y^{(n)}h(\vec{x}^{(n)}) \geq 0$
>   - $\xi^{(n)} > 1 \rightarrow y^{(n)}h(\vec{x}^{(n)}) < 0$

- Margin
    - Our margin was previously defined by

$$dist(h, \vec{x}^{(k)}) = \frac{y^{(k)}h(\vec{x}^{(k)})}{||\vec{w}||} = \frac{1}{||\vec{w}||}$$

where $(\vec{x}^{(k)}, y^{(k)})$ was the closest example to the decision boundary

Primal

- New Optimisation Problem

$$\arg\min_{\vec{w},b,\xi}\{\frac{1}{2}||\vec{w}||^2 + C\sum_{n=1}^{N}\xi^{(n)}\}$$

Subject to: $y^{(n)}h(\vec{x}^{(n)}) \geq 1 - \xi^{(n)}, \forall n \in \{1, 2, ..., N\}, \xi^{(n)} \geq 0$

> C is a hyperparameter that controls the trade-off between the slack variable penalty and the margin

> When we allow slacks > 0, the margin is called a "`soft margin`", as opposed to a "`hard margin`".

Dual

- Using Slack

$$\arg\max_{a} \tilde{L}(\vec{a}) \sum_{n=1}^{N} a^{(n)} - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a^{(n)} a^{(m)} y^{(n)} y^{(m)} k(\vec{x}^{(n)}, \vec{x}^{(m)})$$

Subject to: $a^{(n)} \leq 0 \leq C, \forall n \in \{1, ..., N\} \sum_{n=1}^{N} a^{(n)} y^{(n)} = 0$

- Calculation of b

$$b = \frac{1}{N_M} \sum_{n \in M} (y^{(n)} - \sum_{m \in S} a^{(m)} y^{(m)} k(\vec{x}^{(n)}, \vec{x}^{(m)}))$$

where M is the set of indexes of the support vectors that are on the margin and N_M is the number of such support vectors

Support Vector Machines: Sequential Minimal Optimisation(SMO)

- Solving the Optimisation Problem
  - Sequential minimal optimisation is one of the most popular techniques.
    - It breaks the quadratic programming problem into subquadratic programming problems that can be solved analytically one at a time. -> a subset of a.
    - Uses heuristics to decide which of these smaller problems to solve at each step -> which subset of a to solve
- Sequential Minimal Optimisation(SMO)

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Initialise a
Repeat for a maximum number of iterations:
  Select a pair of Lagrange multipliers a(i) and a(j) to update next
  Optimise L(a) with respect to a(i) and a(j), while holding all other Lag
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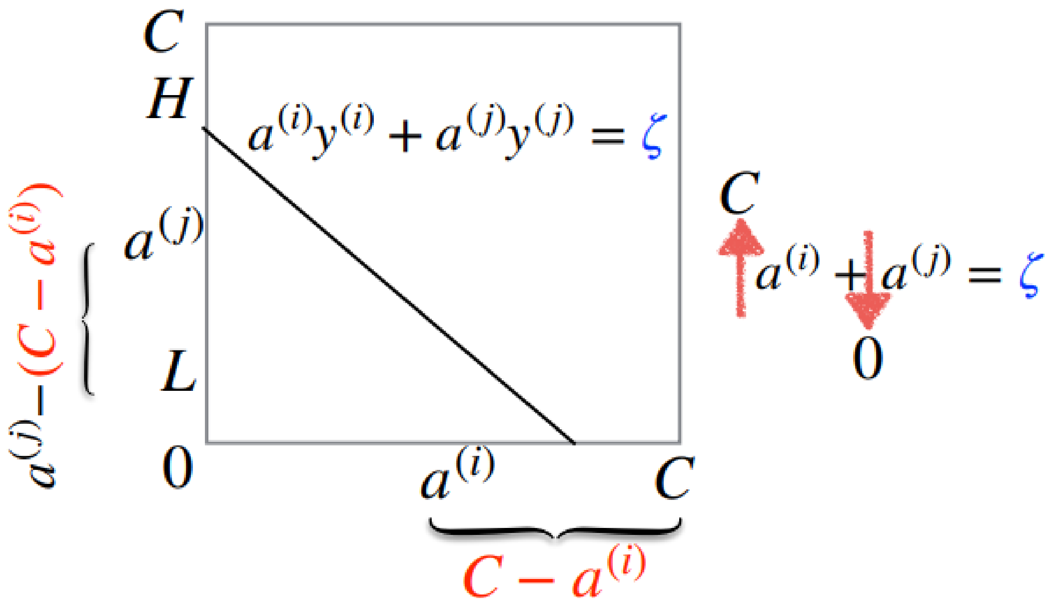
  - Initialise a

$$0 \geq a^{(n)} \geq C, \forall n \in \{1, ..., N\}$$
$$\sum_{n=1}^{N} a^{(n)} y^{(n)} = 0$$

The simplest way is to choose $a^{(n)} = 0, \forall n \in \{1, ..., N\}$

- Optimise $\tilde{L}(\vec{a})$ with respect to $a^{(i)}$ and $a^{(j)}$, while Dealing With Constrains

$$\sum_{n=1}^{N} a^{(n)} y^{(n)} = 0$$
$$a^{(i)} y^{(i)} + a^{(j)} y^{(j)} = - \sum_{n \neq i,j} a^{(n)} y^{(n)}$$
$$a^{(i)} y^{(i)} + a^{(j)} y^{(j)} = \xi$$



  - Lower and Higeher Possible Values For $\vec{a}$
    - If $y^{(i)} = y^{(j)}$

$$L = \max(0, a^{(i)} + a^{(j)} - C)$$
$$H = \min(C, a^{(i)} + a^{(j)})$$

    - If $y^{(i)} \neq y^{(j)}$

$$L = \max(0, a^{(j)} - a^{(i)})$$
$$H = \min(C, C + a^{(j)} - a^{(i)})$$

- Optimising for $a^{(j)}$

$$a^{(j,new)} = a^{(j)} + \frac{y^{(j)}(E^{(i)} - E^{(j)})}{k(\vec{x}^{(i)}, \vec{x}^{(i)}) + k(\vec{x}^{(j)}, \vec{x}^{(j)}) - 2k(\vec{x}^{(i)}, \vec{x}^{(j)})}$$

where the following is the error on training example i:

$$E^{(i)} = h(\vec{x}^{(i)}) - y^{(i)}$$

- Clipping the Value of $a^{(j)}$
  - This update rule may lead to violations in the box constraints(not only for $a^{(j)}$ but also for $a^{(i)}$, since $a^{(i)}$ is set based on $a^{(j)}$).

$$a^{(j,new,clipped)} = \begin{cases} H \quad if\ a^{(j,new)} \geq H \\ a^{(j,new)} \quad if\ L < a^{(j,new)} < H \\ L \quad if\ a^{(j,new)} \leq L \end{cases}$$

> This will ensure that the box constraints are satisfied for $a^{(j)}$.

- Obtaining $a^{(i)}$

$$a^{(i,new)} = \frac{\xi - a^{(j,new,clipped)y^{(j)}}}{y^{(i)}}$$

> This will ensure that $\sum_{n=1}^{N} a^{(n)}y^{(n)} = 0$ is satisfied(and the box constraint for $a^{(i)}$ too)

- Karush-Kuhn-Tucker (KKT) Conditions
    - KKT conditions are conditions that have been proved to be necessary and sufficient for a solution of a quadratic programming problem to be optimal.
    - For soft margin SVM, they boil down to the following,$\forall n \in \{1, .., N\}$:
        - $0 < a^{(n)} < C \iff y^{(n)}h(\vec{x}^{(n)}) = 1$
        - $a^{(n)} = C \iff y^{(n)}h(\vec{x}^{(n)}) \leq 1$
        - $a^{(n)} = 0 \iff y^{(n)}h(\vec{x}^{(n)}) \geq 1$

Selecting Pair $a^{(i)}$ and $a^{(j)}$ To Optimise Next

- Selection is done heuristically.
- We first select a value for $a^{(i)}$ and then for $a^{(j)}$.
- The Lagrange multiplier $a^{(i)}$ is selected by alternating between the following two strategies:
    - Selected randomly among those corresponding to training examples that violate the KKT conditions with a certain margin of error .
    - Selected randomly among those corresponding to training examples that violate the KKT conditions given the margin and $0 < a^{(i)} < C$(support vectors on the margin)
- The Lagrange multiplier $a^{(j)}$ is selected by trying the following strategies in the following order, until a positive improvement in the objective is observed:
    - Pick the $a^{(j)}$ associated to the example that will obtain the largest change in the $a^{(j)}$ value (which would hopefully result in a large increase in the objective). Largest step size approximated based on $|E^{(i)} - E^{(j)}|$

$$a^{(j,new)} = a^{(j)} + \frac{y^{(j)}(E^{(i)} - E^{(j)})}{k(\vec{x}^{(i)}, \vec{x}^{(i)}) + k(\vec{x}^{(j)}, \vec{x}^{(j)}) - 2k(\vec{x}^{(i)}, \vec{x}^{(j)})}$$

    - Pick each $0 < a^{(i)} < C$ in turn.
    - Look through the entire training set.
    - Replace $a^{(i)}$ and try again