Machine Learning and Intelligent Systems

Kernels (Part 1)

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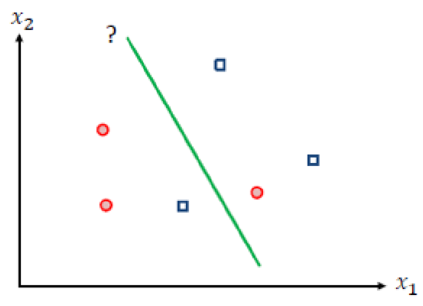
Recap: Limitations of Hard SVM

Hard Margin SVMs: Limitations

- Real data, most likely, will not meet the of linear separable assumption
- Hard margin loss is too limiting when there is class overlapping
- Hard margin SVM wont be able to deal with it



Hard Margin SVMs: Limitations

- Real data, most likely, will not meet the of linear separable assumption
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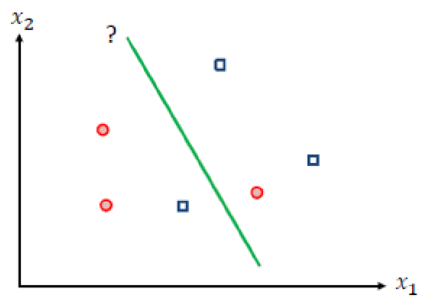
Possible solutions:

1. **Transform the data**
2. Relax the constraints
3. Combination of both

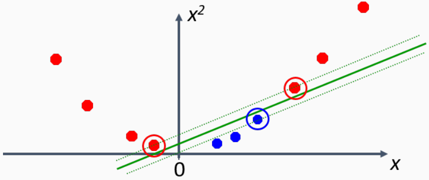


Non-linear Decision Boundary

Idea: move data into a higher dimension space and search for a linear separator

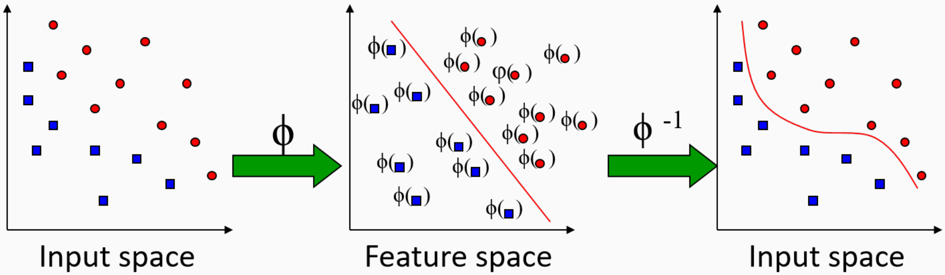
1. 1D problem: Not linearly separable
2. 1D to 2D transformation
3. 2D problem: Linearly separable

$$X \rightarrow (X, X^2)$$



Non-linear Decision Boundary

- **Idea:** Define a transform ϕ from input space to feature space, $\mathbf{x} \to \phi(\mathbf{x})$. It will:
- Solve a linear problem in the feature space
- Result in a non-linear classifier in the input space
- $\phi(\mathbf{x}) \in \mathbb{R}^d$, with typically $d \gg D$



The naïve approach: Hand-crafted features

1. Choose/design a linear model
2. Choose/design a high-dimensional transformation $\phi(\mathbf{x})$
3. After adding many features some of them will make the data linearly separable (fingers crossed)
4. **For each** training example, and **for each** new sample point compute $\phi(\mathbf{x})$
5. Train classifier. Later on, do predictions

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Problem: Impractical to compute $\phi(\mathbf{x})$ for high-dimensional $\phi(\mathbf{x})$-spaces

Example

Consider $\mathbf{x} = [x^1, \ldots, x^D]^T$ and let us define

$$\phi(\mathbf{x}) = \begin{pmatrix} 1 \\ x^1 \\ \vdots \\ x^D \\ x^1 x^2 \\ \vdots \\ x^1 x^D \\ \vdots \\ x^1 x^2 \ldots x^D \end{pmatrix}$$

What is the dimension of the transformed data?

Kernels

The Kernel Trick

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The Kernel Trick

- It is possible to avoid the direct estimation of $\phi(\mathbf{x})$ for every point
- It is even possible to avoid the estimation of $\hat{\mathbf{w}}$
- It is possible to express a linear classifier in term of inner products. This is known as **the kernel trick**
- **Principle:** If we use gradient descent with one of the loss functions we know so far, it is possible to express the gradient as a linear combination of the input samples, $\mathbf{x}$

Sketching the Kernel Trick

- **Claim:** The model parameters can be expressed as a linear combination of all input vectors:

$$\mathbf{w} = \sum_{i=1}^{N} \alpha_i \mathbf{x}_i \tag{1}$$

for a given assignment of α

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- Let us assume our classifier is trained with the squared loss. We have:

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{N} (\mathbf{w}^T \mathbf{x}_i - y_i)^2, \qquad \frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \sum_{i=1}^{N} 2(\mathbf{w}^T \mathbf{x}_i - y_i)\mathbf{x}_i \tag{2}$$

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- Using Eq. 1, the term $\mathbf{w}^T \mathbf{x}_i$ can be estimated as:

$$\mathbf{w}^T \mathbf{x}_j = \sum_{i=1}^{N} \alpha_i \underbrace{\mathbf{x}_i^T \mathbf{x}_j}_{\mathbf{K}_{ij}}$$

Proof: Setup

Let us recall the gradient descent expression:

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \lambda \frac{\partial \mathcal{L}}{\partial \mathbf{w}} \tag{3}$$

Note: We will use λ instead of α for the learning rate in the next slides

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Given the squared loss we chose in Eq. 2, let us do some reorganization of its derivative

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}} = \sum_{i=1}^{N} \underbrace{2(\mathbf{w}^{T}\mathbf{x}_i - y_i)}_{\gamma_i\text{:function of } \mathbf{w}^T\mathbf{x}_i} \mathbf{x}_i$$

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Let's move to the proof

Proof by Induction: Sketch

- We will use gradient descent to estimate the model parameters $\mathbf{w}$
- **Important:** Since the squared loss is convex, no matter how we initialize $\mathbf{w}$ the solution is always the same

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- Answer: $\alpha_i = 0 \quad \forall\, i$ (base case)

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Let us now see what happens in a given round of gradient descent

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By induction we proof for $\mathbf{w}^{(\tau)}$ and it follows for $\mathbf{w}^{(\tau+1)}$

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It is possible to perform gradient descent without ever expressing $\mathbf{w}$ explicitly

Algorithm

The update rule for $\alpha^{(\tau)}$ is

$$\alpha^{(\tau+1)} = \alpha^{(\tau)} - \lambda\gamma_i^{(\tau)} \tag{4}$$

Training Algorithm:

1. Initialize $\alpha_i = 0 \quad \forall\, i, i = 1, \ldots, N$
2. Estimate γ_i
3. Update α using the update rule (eq. 4)
4. Go to step 2

Prediction: For an unseen point $\mathbf{x}^*$,

$$h(\mathbf{x}^*) = \hat{\mathbf{w}}^T\mathbf{x}^* = \sum_{i=1}^{N} \alpha_i \mathbf{x}_i^T \mathbf{x}^*$$

Kernels

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- With the kernel trick we avoid the direct estimation of $\mathbf{w}$. However, we still need to estimate $\phi(\mathbf{x})$
- If d is of very high dimension the estimation of the inner products $\mathbf{K}_{ij}$ can be a very expensive operation. **We have gained nothing!**

Kernels

- **Idea:** Compute the value of **K** without explicitly writing the expensive representation

- Example: Consider $\mathbf{u} = [u_1]$, $\mathbf{v} = [v_1]$, and a transformation $\phi(\mathbf{x}) = [x_1^2, \sqrt{2c}x_1, c]^T$, with c a constant. Estimate:
  - $\phi(\mathbf{u}) =$
  - $\phi(\mathbf{v}) =$
  - $\phi(\mathbf{u})^T\phi(\mathbf{v}) =$
- Alternatively, this can be computed as $(u_1 v_1 + c)^2$

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- We denote $k(\mathbf{u}, \mathbf{v}) = (u_1 v_1 + c)^2 = \phi(\mathbf{u})^T\phi(\mathbf{v})$ a **kernel function**

- With a finite training set of N samples, the inner products can be cheaply pre-computed and stored in a **kernel matrix**:

$$\mathbf{K}_{ij} = \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j)$$

Wrap-up

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- We proposed to transform the input space to address the problem of non-linear separability
- We showed that thanks to the kernel trick it is possible to avoid the direct estimation of $\mathbf{w}$ by using inner products
- We showed that certain type of functions, the kernel functions, avoid the need to estimate inner products
- We introduced the kernel matrix
- **What comes next:**
  - We will present different kernel functions
  - We will present the kernel version of some covered methods

Key Concepts

- Feature transformation
- Kernel trick
- Kernel function
- Kernel matrix
- Proof by induction