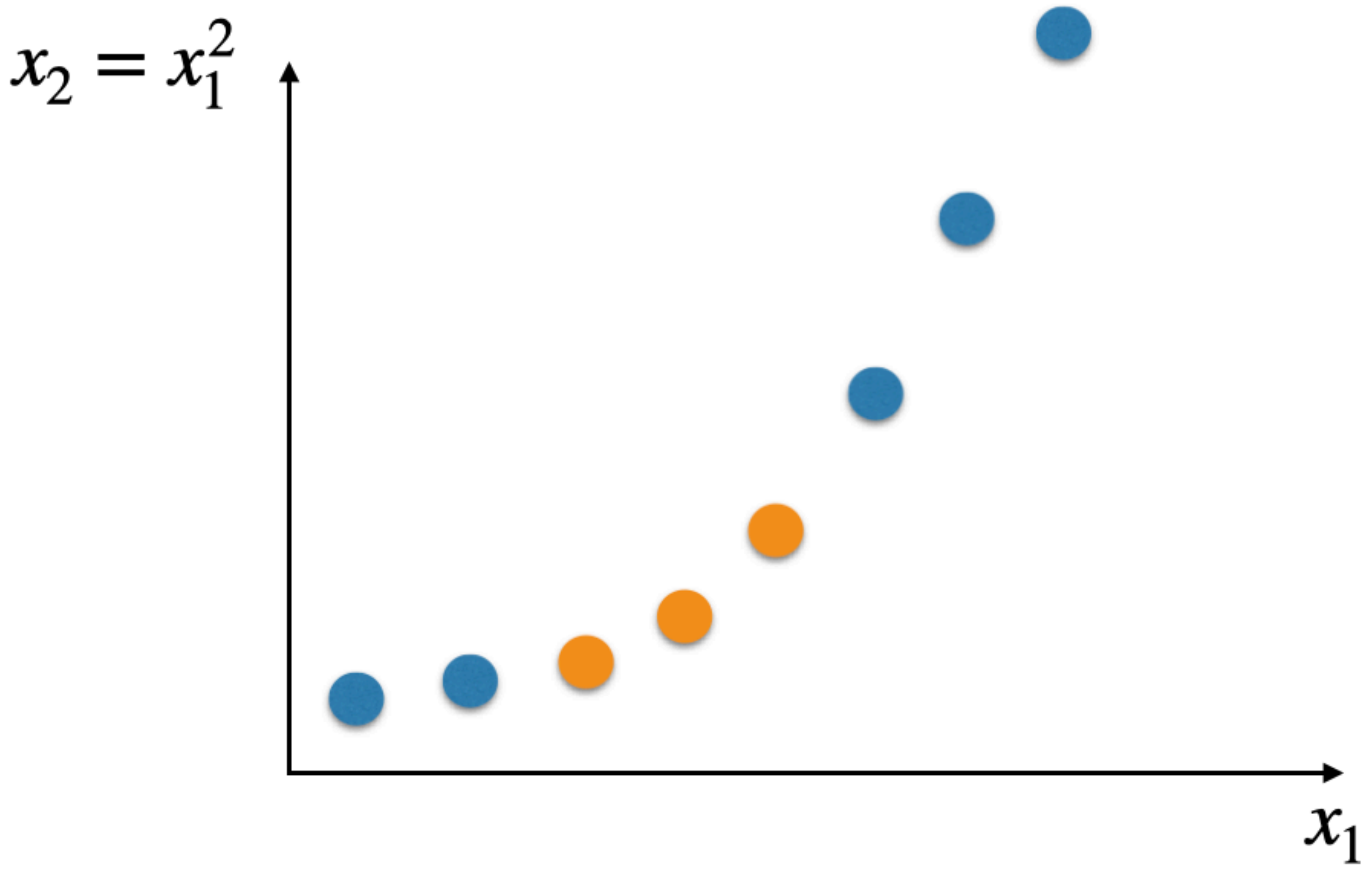
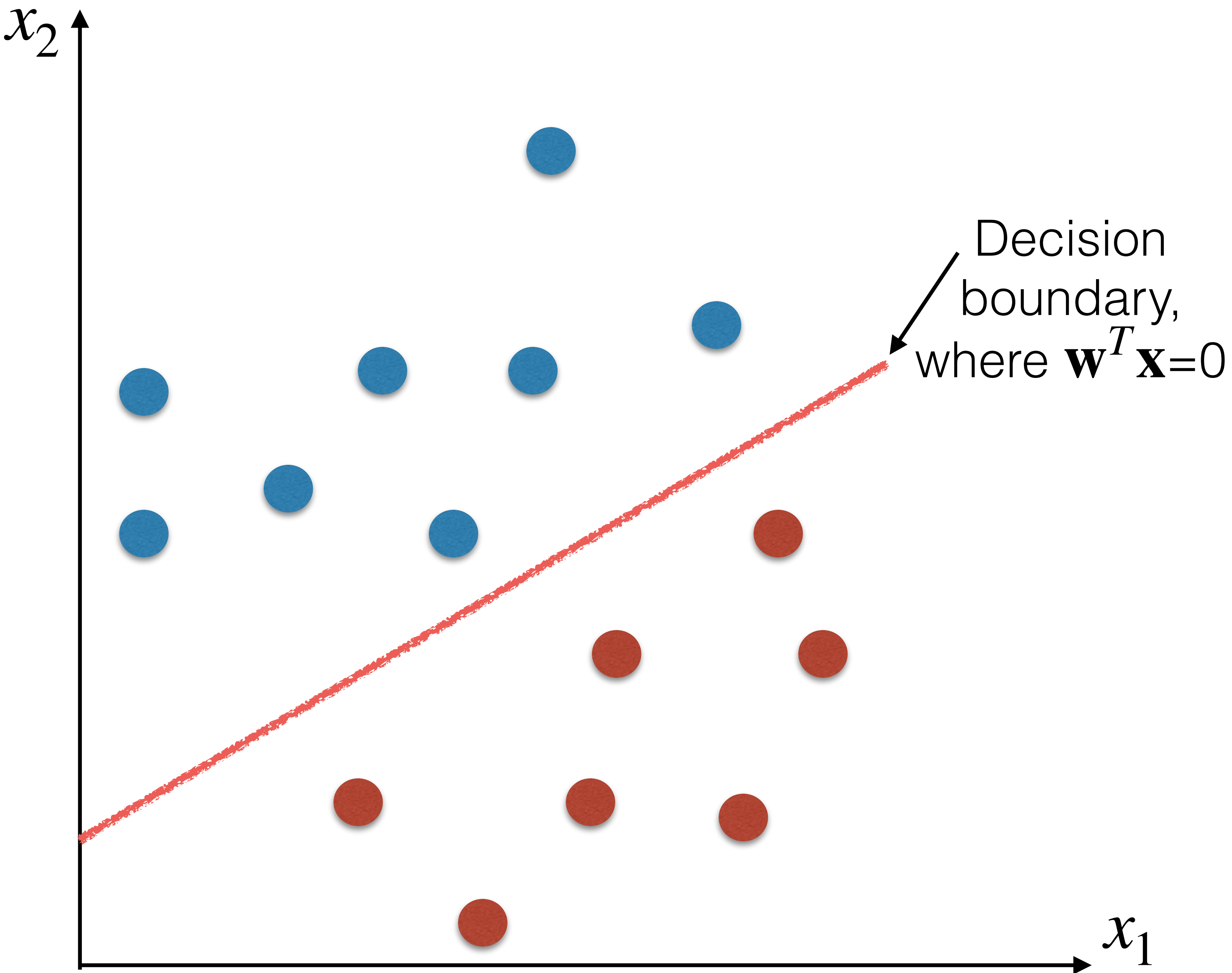


Nonlinear Transformations

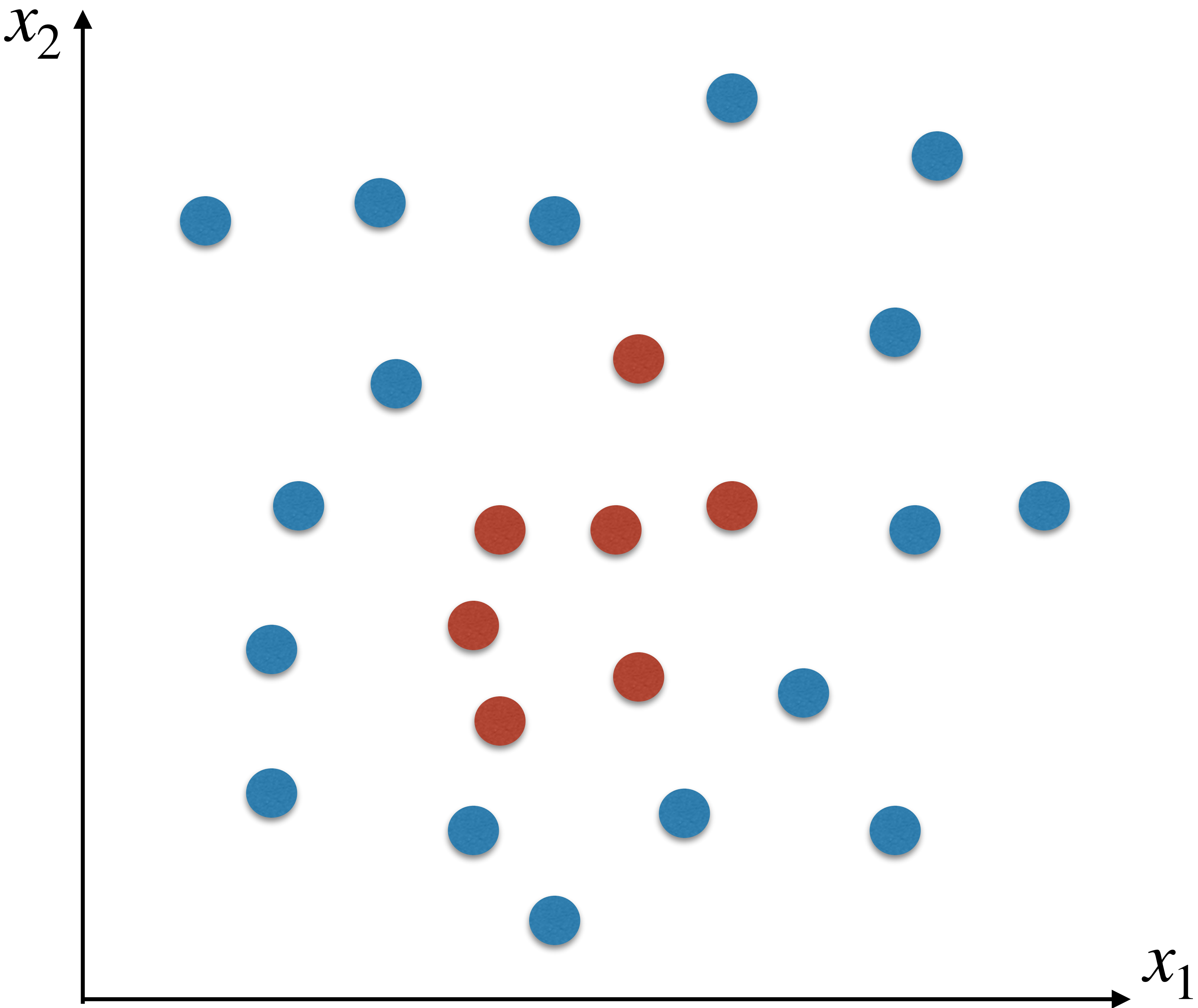
Leandro L. Minku

Linearly Separable Problems

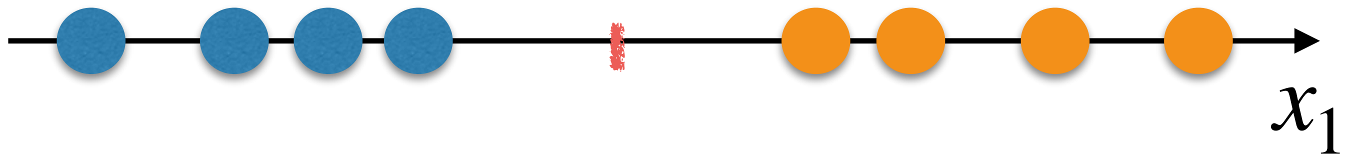
$\text{logit}(p_1) = \mathbf{w}^T\mathbf{x}$



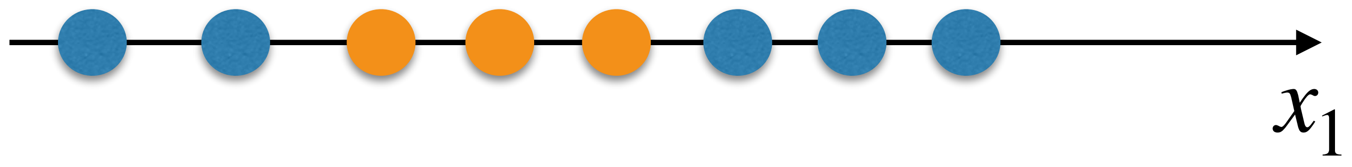
Nonlinearly Separable Problems



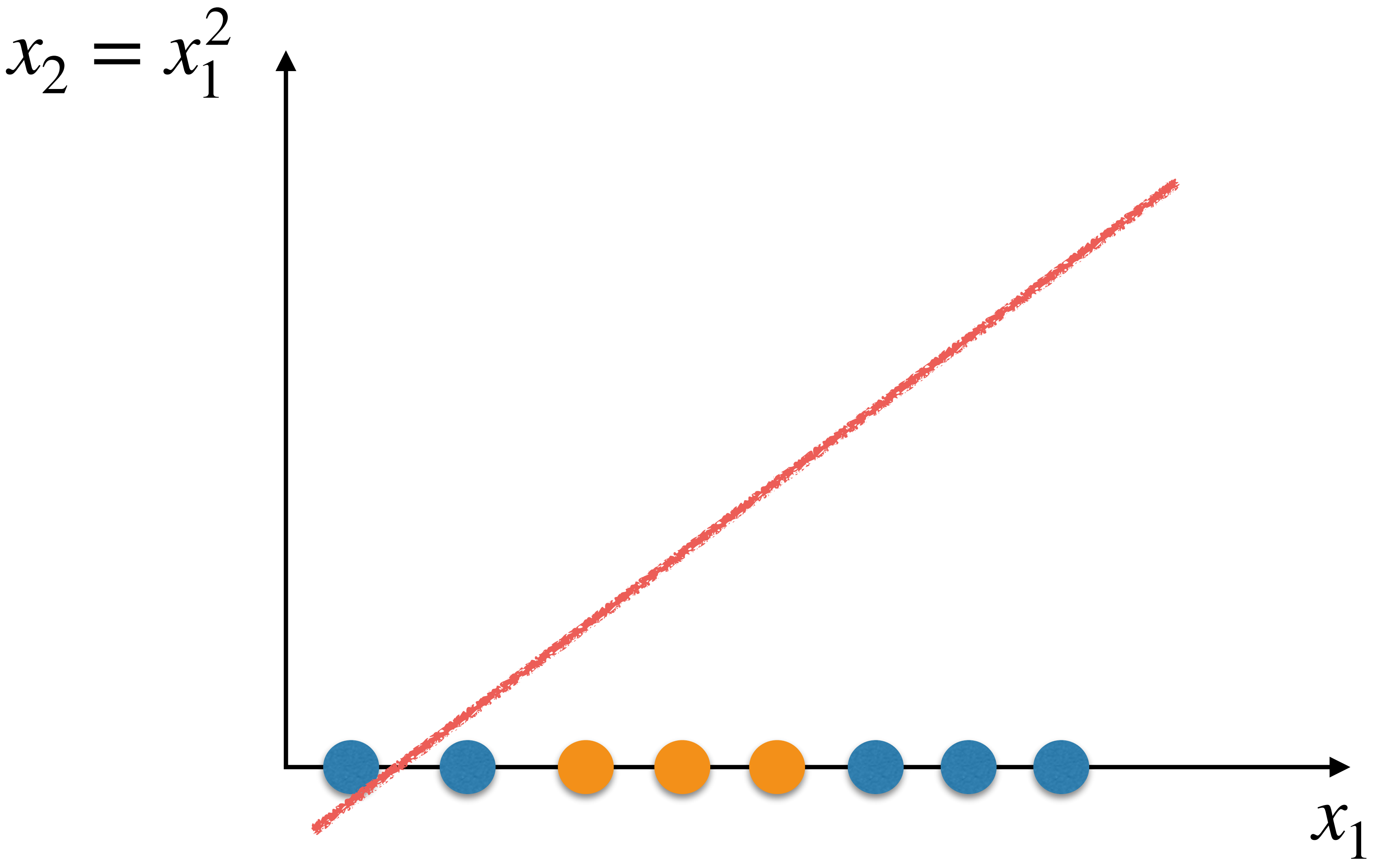
Linearly Separable Problems



Non-Linearly Separable Problems

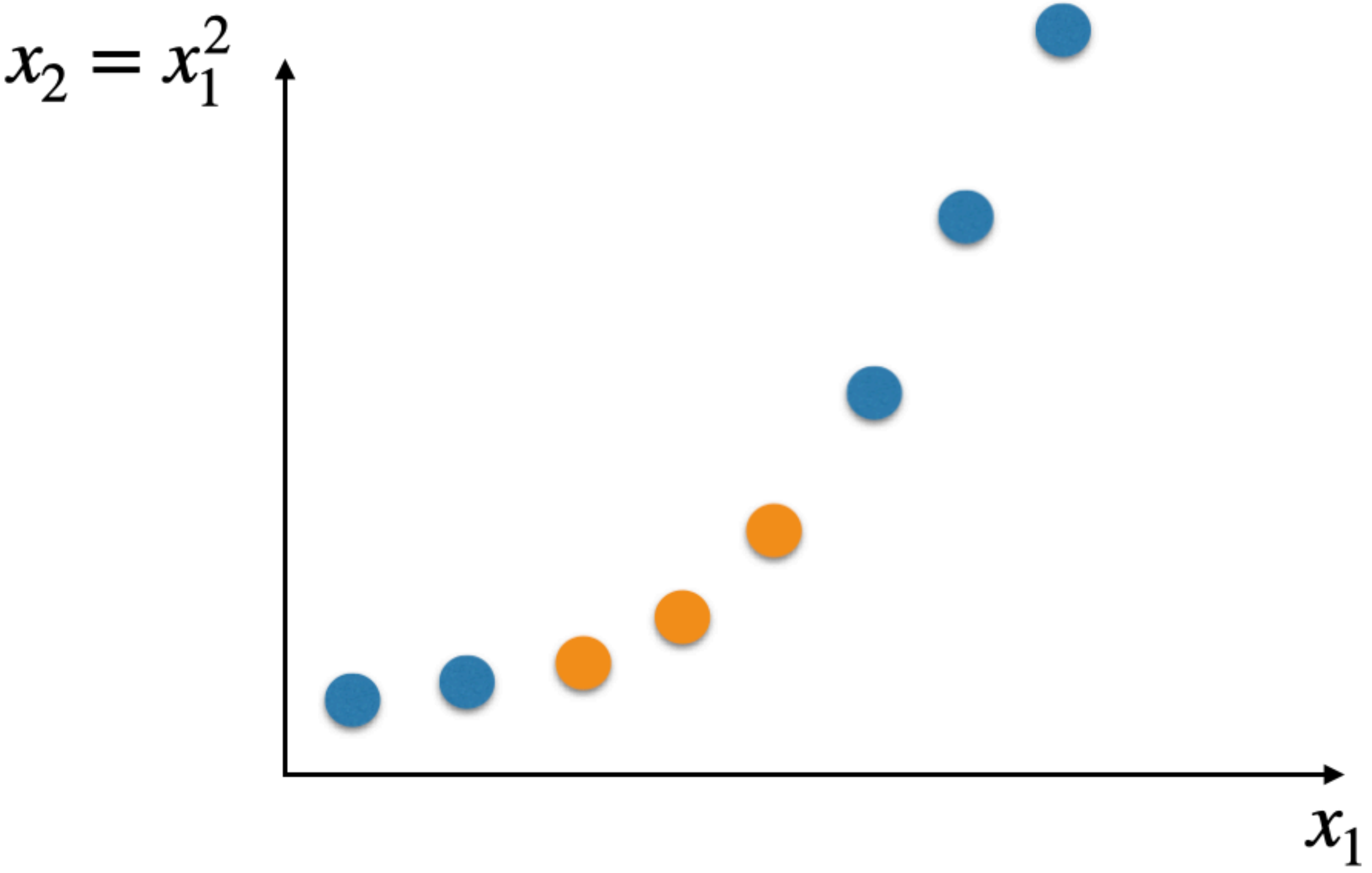


Nonlinear Transformation / Basis Expansion



Higher dimensional embedding / feature space: $\phi(\mathbf{x}) = (x_1, x_1^2)^T$

Nonlinear Transformation / Basis Expansion



feature transform / basis expansion

basis functions

Higher dimensional embedding / feature space: $\phi(\mathbf{x}) = (x_1, x_1^2)^T$

Decision Boundaries Corresponding to Polynomials of Order p in the Original Space

- What feature transform could we use to make the problem linearly separable in the higher dimensional embedding?

- Create a feature transform that includes all terms of order $\leq p$ that can be created based on the input variables $\mathbf{x}$.

- Example for polynomial of order 2 and a problem with 1 input variable:

$$\mathbf{x} = (1, x_1) \rightarrow \phi(\mathbf{x}) = (1, x_1, x_1^2)^T$$

- Example for polynomial of order 2 and a problem with 2 input variables:

$$\mathbf{x} = (1, x_1, x_2)^T \rightarrow \phi(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)^T$$

Decision Boundaries Represented by Polynomials of Order p in the Original Space

- Create a nonlinear transform that includes all terms of order $\leq p$ that can be created based on the input variables $\mathbf{x}$.

- Example for polynomial of order 3 and a problem with 2 input variables:

$$\mathbf{x} = (1, x_1, x_2)^T \rightarrow \phi(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2, x_1^3, x_2^3, x_1 x_2^2, x_1^2 x_2)^T$$

If we follow this idea, any decision boundary that is a polynomial of order p in $\mathbf{x}$ is linear in $\phi(\mathbf{x})$.

So, we can adopt linear models in the higher dimensional embedding formed by $\phi(\mathbf{x})$, to learn decision boundaries corresponding to polynomials of order p in $\mathbf{x}$.

Example

Consider that we need a quadratic decision boundary for a problem with 1 input variable:

$$w_0 x_0 + w_1 x_1 + w_2 x_1^2 = 0 \qquad \text{where } x_0 = 1$$

Nonlinear transform:

$$\mathbf{x} = (1, x_1)^T \rightarrow \phi(\mathbf{x}) = (1, x_1, x_1^2)^T$$

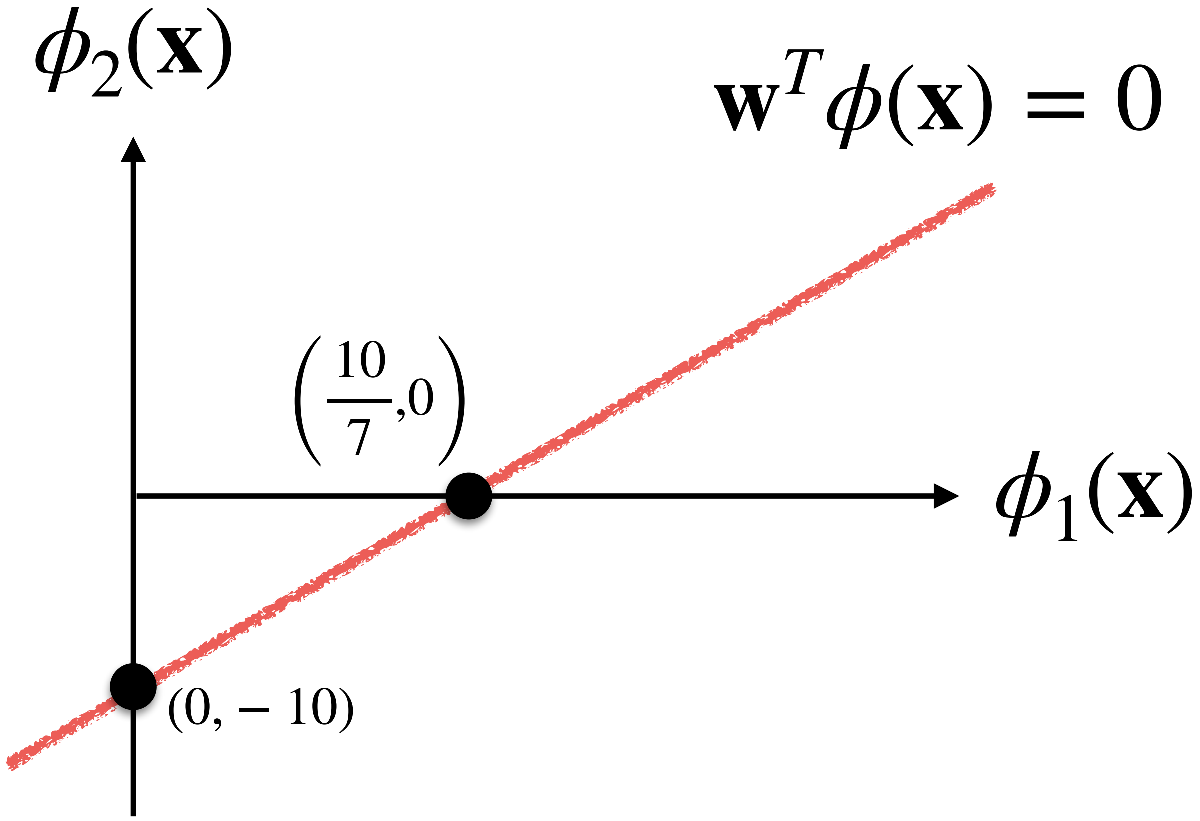
Linear decision boundary in the feature space corresponds to a quadratic decision boundary in the original space:

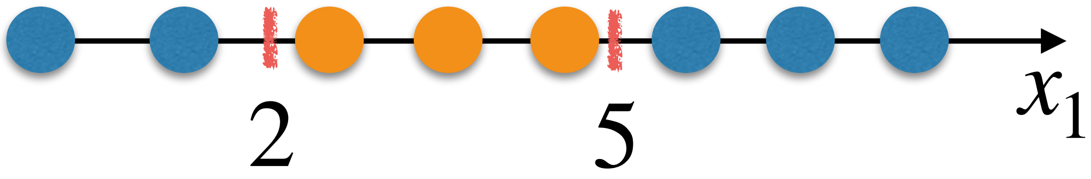
$$\mathbf{w}^T \phi(\mathbf{x}) = 0 \qquad \mathbf{w}^T = (w_0, w_1, w_2)$$

$$w_0 \times 1 + w_1 \phi_1(\mathbf{x}) + w_2 \phi_2(\mathbf{x}) = 0 \qquad w_0 \times 1 + w_1 x_1 + w_2 x_1^2 = 0$$

Illustration for

$$\mathbf{w}^T = (10, -7, 1), \phi(\mathbf{x}) = (1, x_1, x_1^2)^T$$





$$w_0 \times 1 + w_1\phi_1(\mathbf{x}) + w_2\phi_2(\mathbf{x}) = 0$$

$$10 \times 1 - 7\phi_1(\mathbf{x}) + 1\phi_2(\mathbf{x}) = 0$$

$$10 - 7\phi_1(\mathbf{x}) + 1\phi_2(\mathbf{x}) = 0$$

$$w_2 x_1^2 + w_1 x_1 + w_0 \times 1 = 0$$

$$1x_1^2 - 7x_1 + 10 = 0$$

$$x_1 = \frac{7 \pm \sqrt{(-7)^2 - 4 \times 1 \times 10}}{2 \times 1}$$

Adopting Nonlinear Transformations in Logistic Regression

$$\text{logit}(p_1) = \mathbf{w}^T\mathbf{x} \qquad p_1 = p(1\,|\,\mathbf{x},\mathbf{w}) = \frac{e^{(\mathbf{w}^T\mathbf{x})}}{1+e^{(\mathbf{w}^T\mathbf{x})}}$$

$$\Big\downarrow$$

$$\text{logit}(p_1) = \mathbf{w}^T\phi(\mathbf{x}) \qquad p_1 = p(1\,|\,\phi(\mathbf{x}),\mathbf{w}) = \frac{e^{(\mathbf{w}^T\phi(\mathbf{x}))}}{1+e^{(\mathbf{w}^T\phi(\mathbf{x}))}}$$

Adopting Nonlinear Transformations in Logistic Regression

Given $\mathscr{T} = \{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \cdots, (\mathbf{x}^{(N)}, y^{(N)})\}$, $\underset{\mathbf{w}}{\operatorname{argmin}}\, E(\mathbf{w})$

$$E(\mathbf{w}) = -\sum_{i=1}^{N} y^{(i)} \ln p(1 \,|\, \mathbf{x}^{(i)}, \mathbf{w}) + (1 - y^{(i)}) \ln (1 - p(1 \,|\, \mathbf{x}^{(i)}, \mathbf{w}))$$

↓

Given $\mathscr{T} = \{(\phi(\mathbf{x}^{(1)}), y^{(1)}), (\phi(\mathbf{x}^{(2)}), y^{(2)}), \cdots, (\phi(\mathbf{x}^{(N)}), y^{(N)})\}$, $\underset{\mathbf{w}}{\operatorname{argmin}}\, E(\mathbf{w})$

$$E(\mathbf{w}) = -\sum_{i=1}^{N} y^{(i)} \ln p(1 \,|\, \phi(\mathbf{x}^{(i)}), \mathbf{w}) + (1 - y^{(i)}) \ln (1 - p(1 \,|\, \phi(\mathbf{x}^{(i)}), \mathbf{w}))$$

Adopting Nonlinear Transformations in Logistic Regression

$$\nabla_E(\mathbf{w}) = \sum_{i=1}^{N} (p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}) - y^{(i)})\mathbf{x}^{(i)}$$

$$H_E(\mathbf{w}) = \sum_{i=1}^{N} p(1 \mid \mathbf{x}^{(i)}, \mathbf{w})(1 - p(1 \mid \mathbf{x}^{(i)}, \mathbf{w}))\mathbf{x}^{(i)}{\mathbf{x}^{(i)}}^T$$

↓

$$\nabla_E(\mathbf{w}) = \sum_{i=1}^{N} (p(1 \mid \phi(\mathbf{x}^{(i)}), \mathbf{w}) - y^{(i)})\phi(\mathbf{x}^{(i)})$$

$$H_E(\mathbf{w}) = \sum_{i=1}^{N} p(1 \mid \phi(\mathbf{x}^{(i)}), \mathbf{w})(1 - p(1 \mid \phi(\mathbf{x}^{(i)}), \mathbf{w}))\phi(\mathbf{x}^{(i)})\phi(\mathbf{x}^{(i)})^T$$

Adopting Nonlinear Transformations

1. Choose a nonlinear transformation.

2. Apply it to the training examples so that they have the format $(\phi(\mathbf{x}), y)$.

3. Create a linear model $h'(\phi(\mathbf{x}))$ based on the transformed training examples.

4. Determine the (nonlinear) model $h(\mathbf{x})$ by replacing $\phi_i(\mathbf{x})$ with the corresponding value that depends on $\mathbf{x}$.

Advantages of Linear Models

- Linear models are often associated to relatively efficient learning algorithms.
- They can be robust and have good generalisation properties.

Caveats of Nonlinear Transforms

- The number of dimensions may become very high.
- Choosing a nonlinear transformation that fits the training examples well does not necessarily mean that there will be good generalisation.

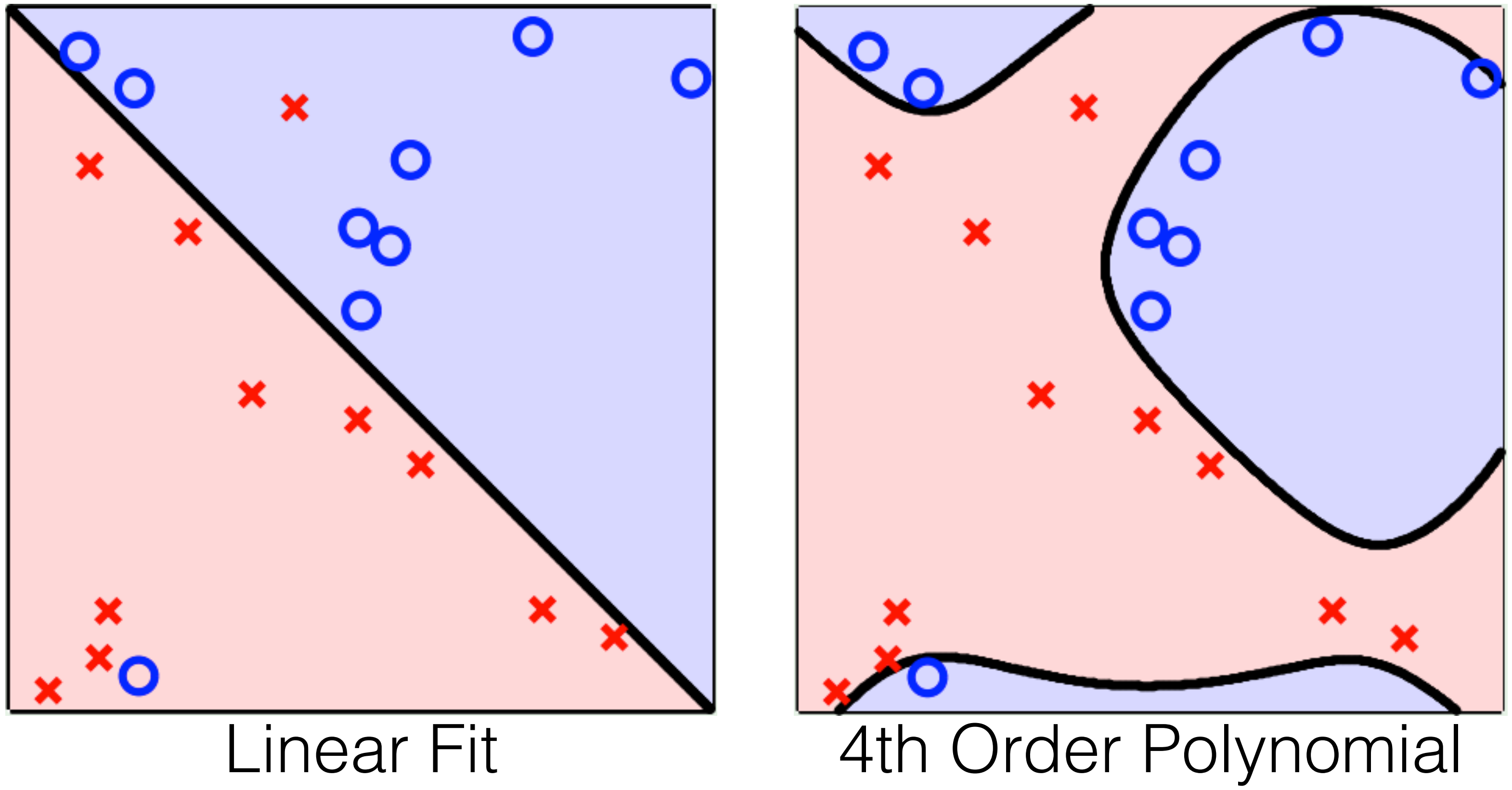


Figure from: Abu-Mostafa et al's Learning from Data: A Short Course.

Summary

- We can create nonlinear transformations to obtain a higher dimensional embedding where our problems become linearly separable, even if they were not linearly separable in the original space.

- We can then adopt our original logistic regression to create a linear decision boundary in this higher dimensional embedding.

- This idea can is also applicable to other linear models.

Further Reading

- Essential:
    - Abu-Mostafa et al.'s Learning from Data: A Short Course. Section 3.4 (Nonlinear Transformation) pages 99 to 101.
- Recommended:
    - Bishop's book on "Machine Learning and Pattern Recognition", Section 4.3.1 (Fixed Basis Functions).
- Optional:
    - You may wish to read the whole of Section 3.4 of Abu-Mostafa et al.'s Learning from Data: A Short Course. However, it involves certain concepts that we will discuss only later in the module. It's ok to ignore those concepts for now. You may not fully understand the chapter as a whole now, but you will understand it later once these concepts are covered in the module.