TECHNISCHE UNIVERSITÄT
CHEMNITZ

Neurocomputing

Learning theory

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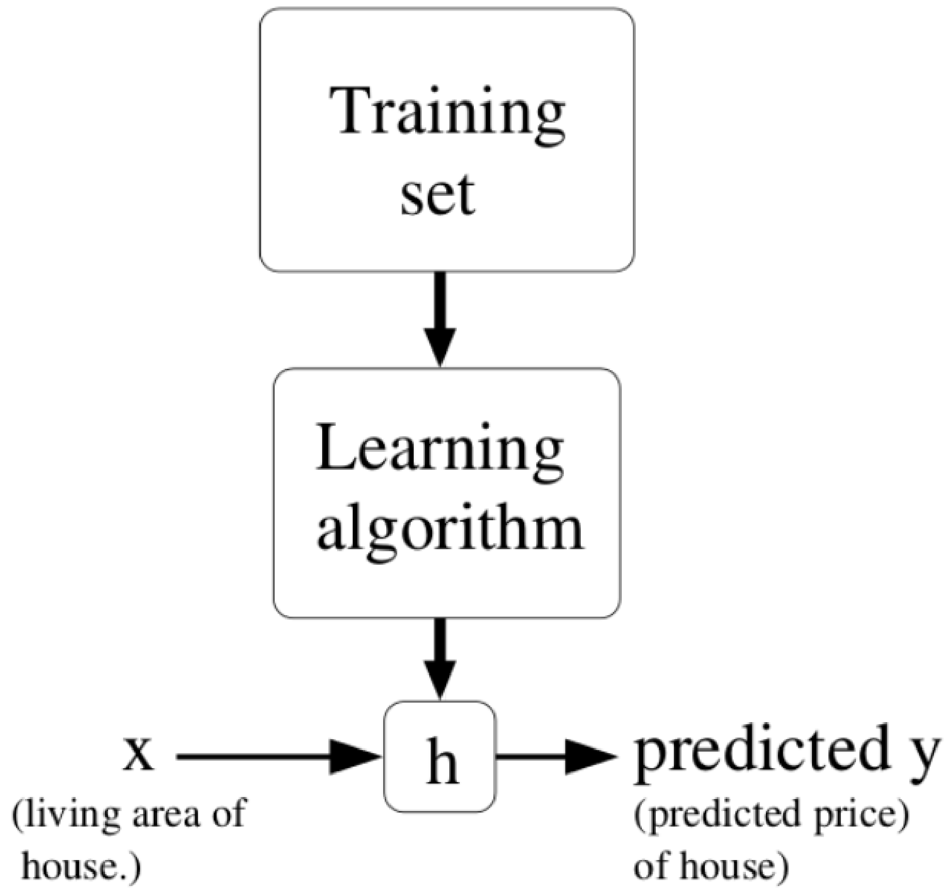
https://tu-chemnitz.de/informatik/KI/edu/neurocomputing

1 - Error measurements

Training vs. Generalization error



- The **training error** is the error made on the training set.
  - Easy to measure for classification: number of misclassified examples divided by the total number.

$$\epsilon_{\mathcal{D}} = \frac{\text{\# misclassifications}}{\text{\# examples}}$$

  - For regression, the mse is generally used.
  - Totally irrelevant on usage: reading the training set has a training error of 0%.

- What matters is the **generalization error**, which is the error that will be made on new examples (not used during learning).
  - Much harder to measure (potentially infinite number of new examples, what is the correct answer?).
  - Often approximated by the **empirical error**: one keeps a number of training examples out of the learning phase and one tests the performance on them.

Classification errors

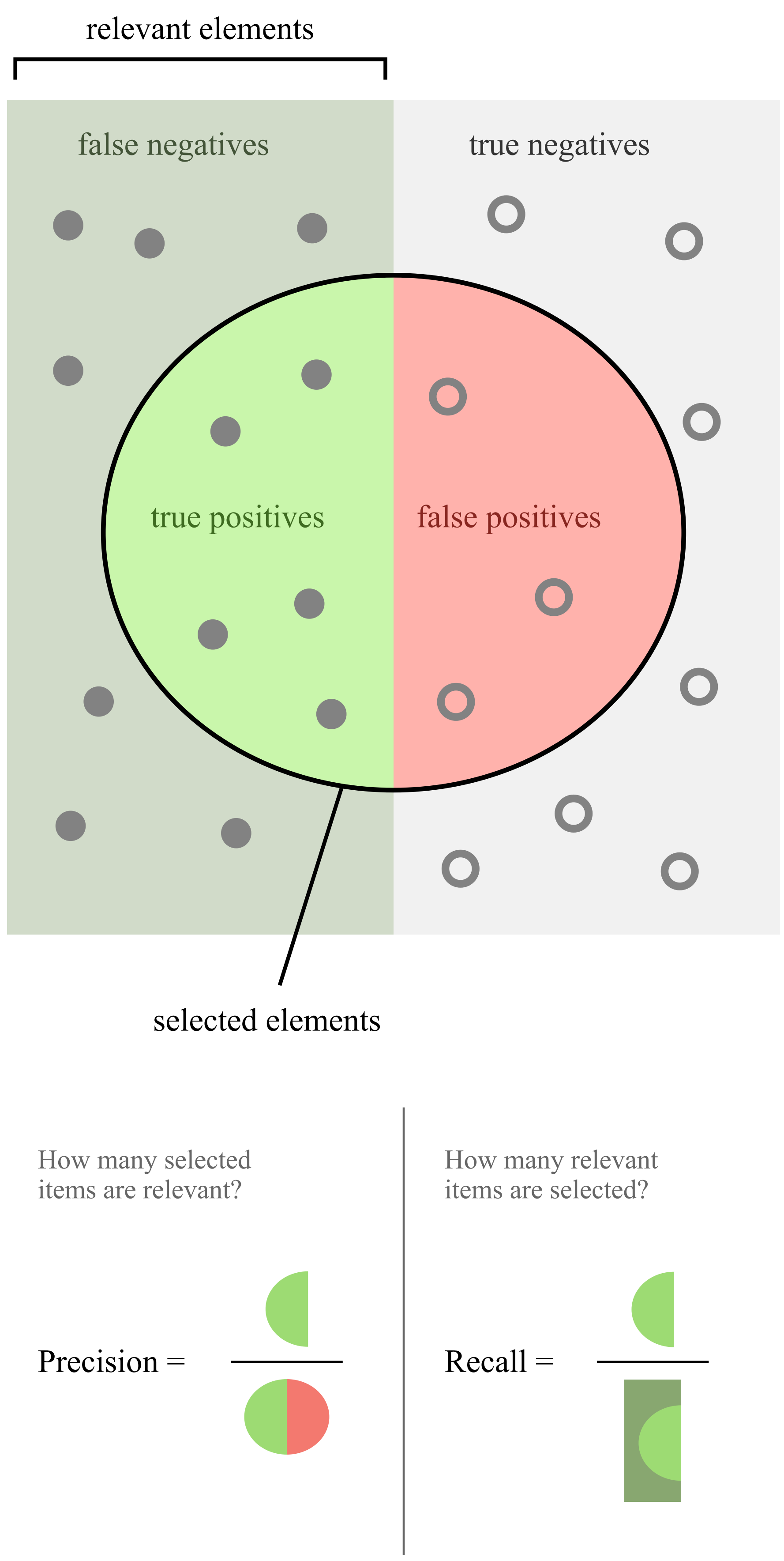
Confusion matrix

		actual value		
		p	***n***	**total**
prediction outcome	***p'***	True Positive	False Positive	P'
	n'	False Negative	True Negative	N'
	total	P	N	

- Classification errors can also depend on the class:
    - **False Positive** errors (FP, false alarm, type I) is when the classifier predicts a positive class for a negative example.
    - **False Negative** errors (FN, miss, type II) is when the classifier predicts a negative class for a positive example.
- **True Positive** (TP) and **True Negative** (TN) are correctly classified examples.
- Is it better to fail to detect a cancer (FN) or to incorrectly predict one (FP)?

Source: https://alliance.seas.upenn.edu/~cis520/dynamic/2017/wiki/index.php?n=Lectures.PrecisionRecall

Classification errors



- Error

$$\epsilon = \frac{\mathrm{FP} + \mathrm{FN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{TN} + \mathrm{FN}}$$

- Accuracy (1 - error)

$$\mathrm{acc} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{TN} + \mathrm{FN}}$$

- Recall (hit rate, sensitivity) and Precision (specificity)

$$R = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} \quad P = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

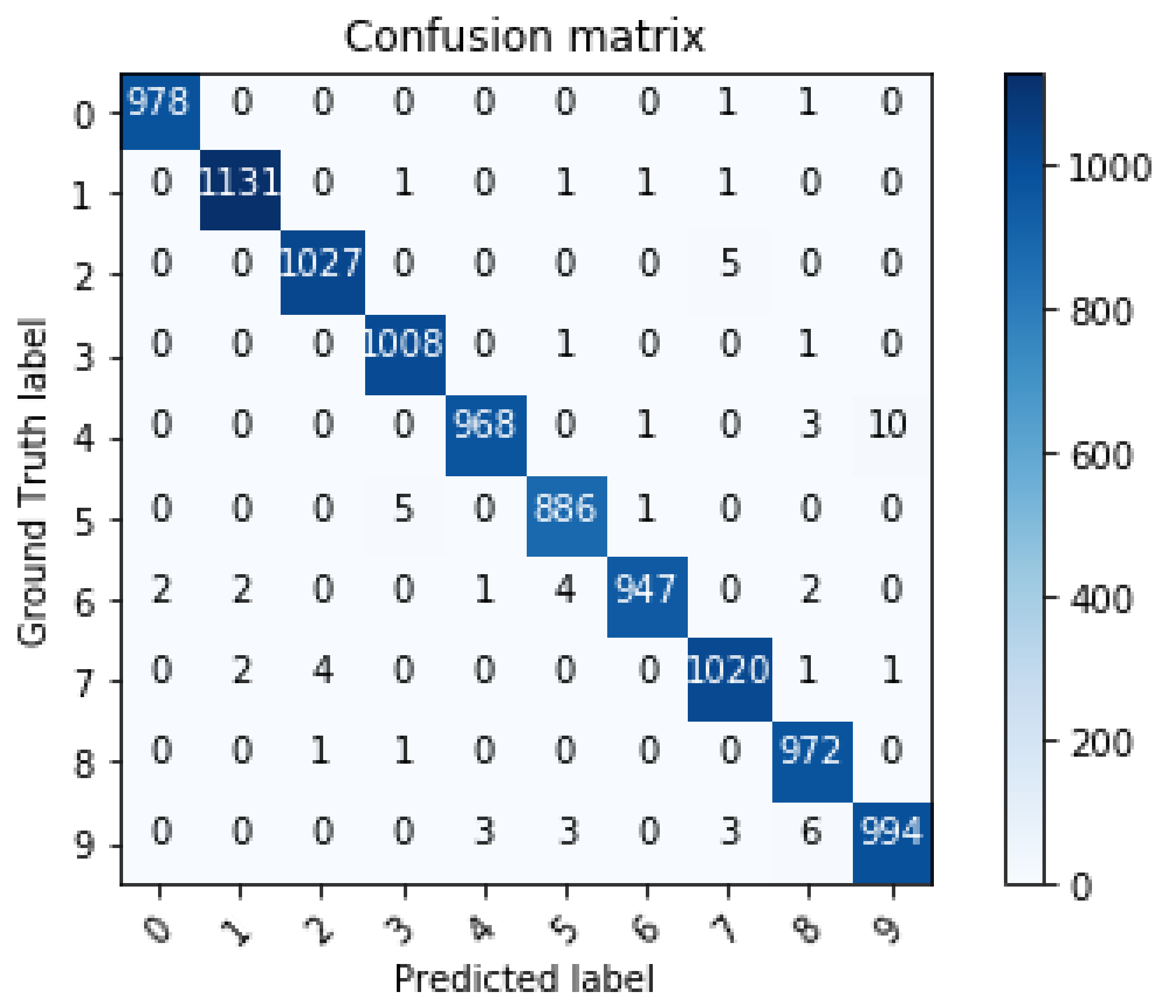
- F1 score = harmonic mean of precision and recall

$$\mathrm{F1} = \frac{2\,P\,R}{P + R}$$

Source:
https://upload.wikimedia.org/wikipedia/commons/2/26/Precisionrecall.svg

Confusion matrix

- For multiclass classification problems, the **confusion matrix** tells how many examples are correctly classified and where confusion happens.
- One axis is the predicted class, the other is the target class.
- Each element of the matrix tells how many examples are classified or misclassified.
- The matrix should be as diagonal as possible.

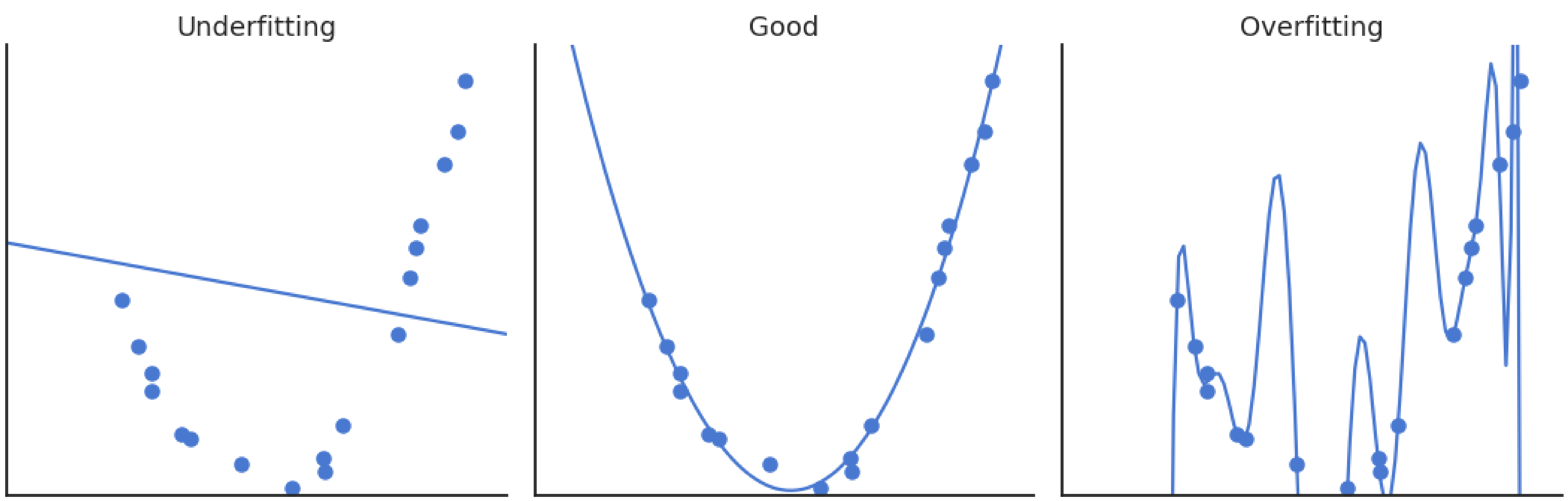


- Using `scikit-learn`:

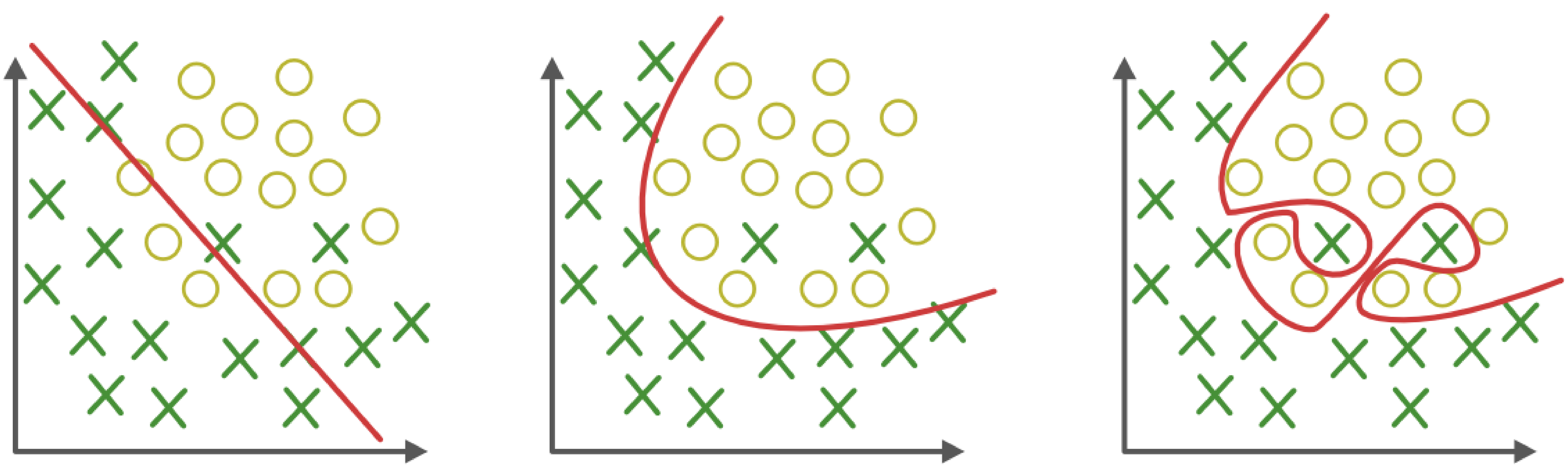
```python
from sklearn.metrics import confusion_matrix

m = confusion_matrix(t, y)
```

Overfitting in regression

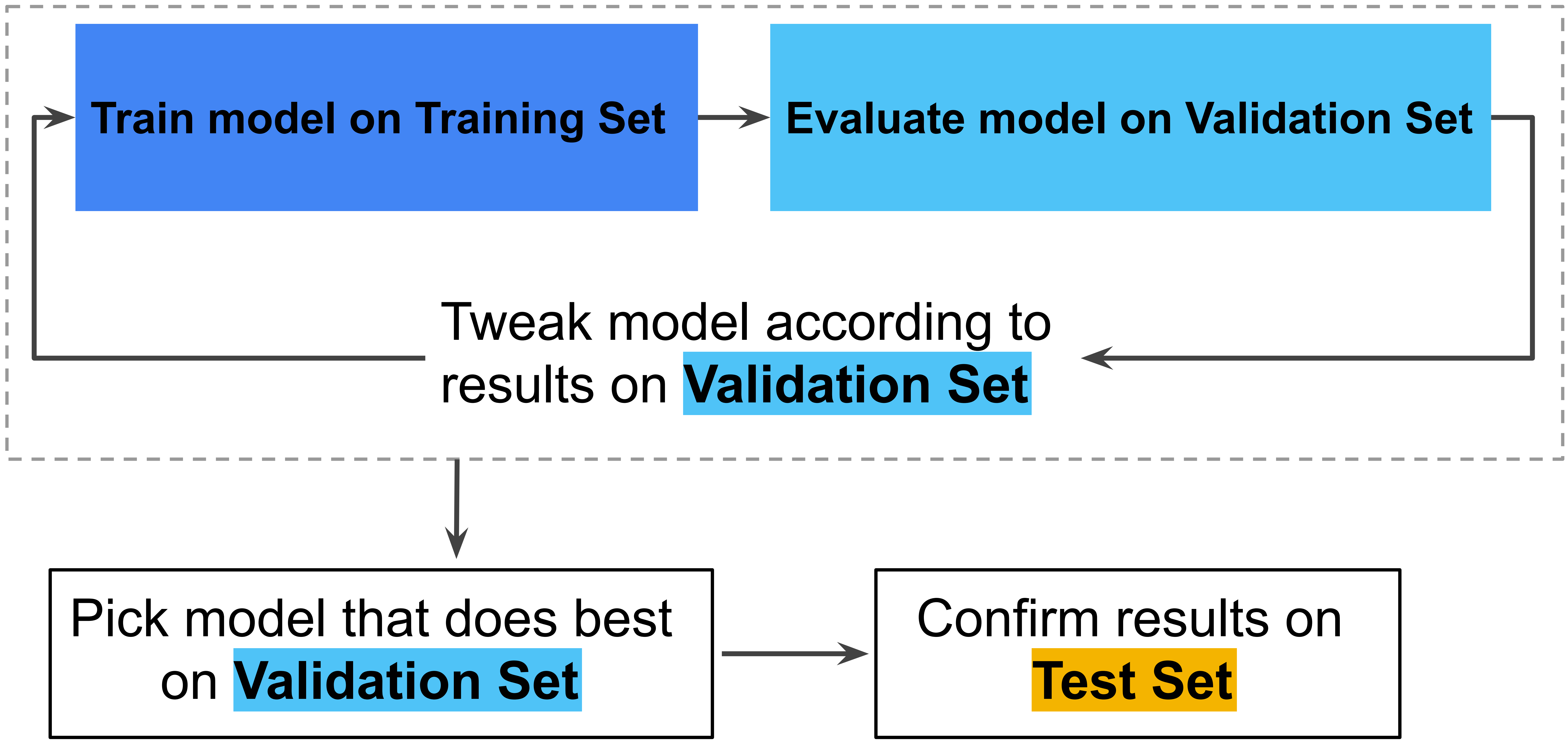


Overfitting in classification



Cross-validation

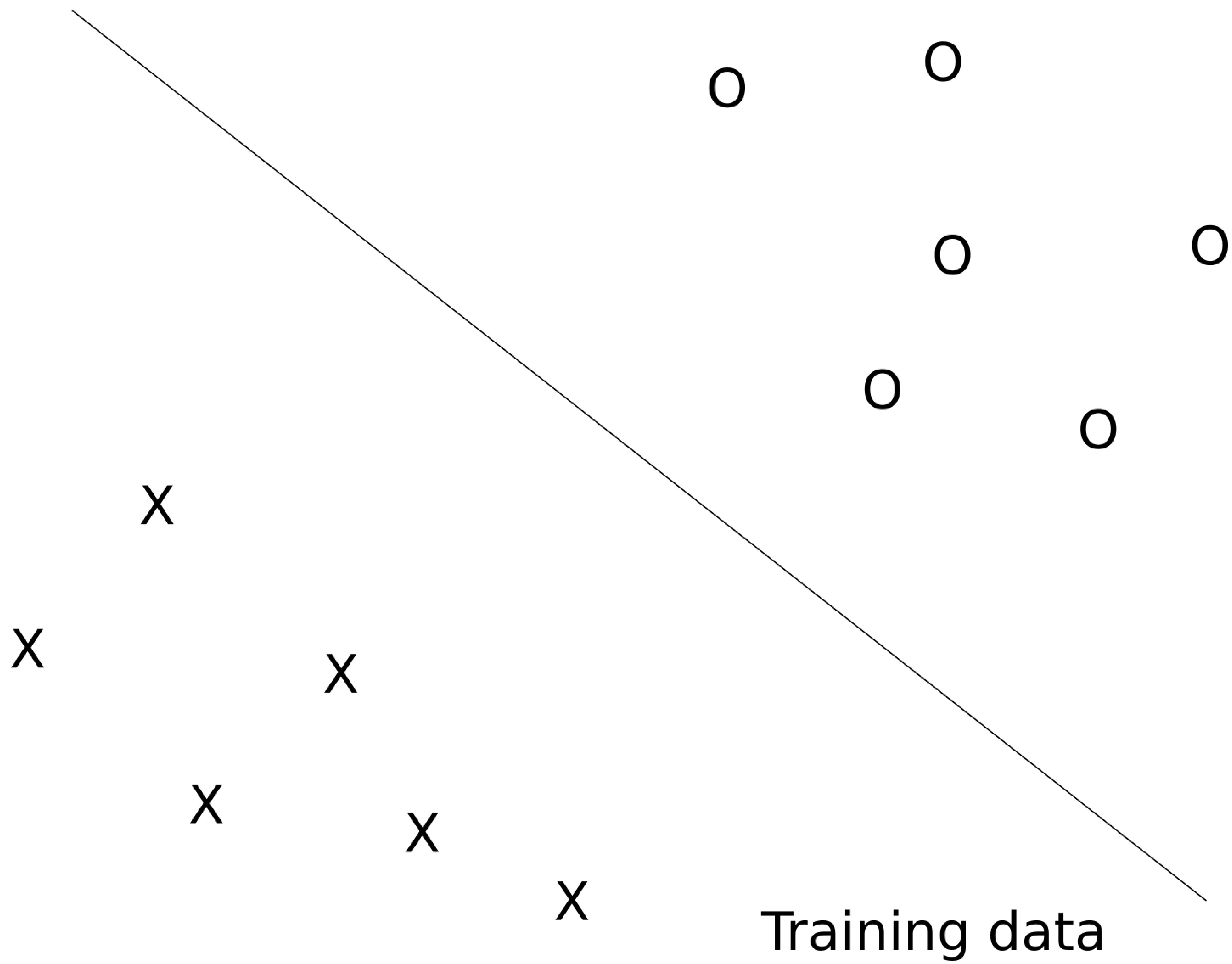
- In classification too, **cross-validation** has to be used to prevent overfitting.
- The classifier is trained on the **training set** and tested on the **test set**.
- Optionally, a third **validation set** can be used to track overfitting during training.



Source: https://developers.google.com/machine-learning/crash-course/validation/another-partition

Training and test data distribution

- Beware: the test data must come from the same distribution as the training data, otherwise it makes no sense.



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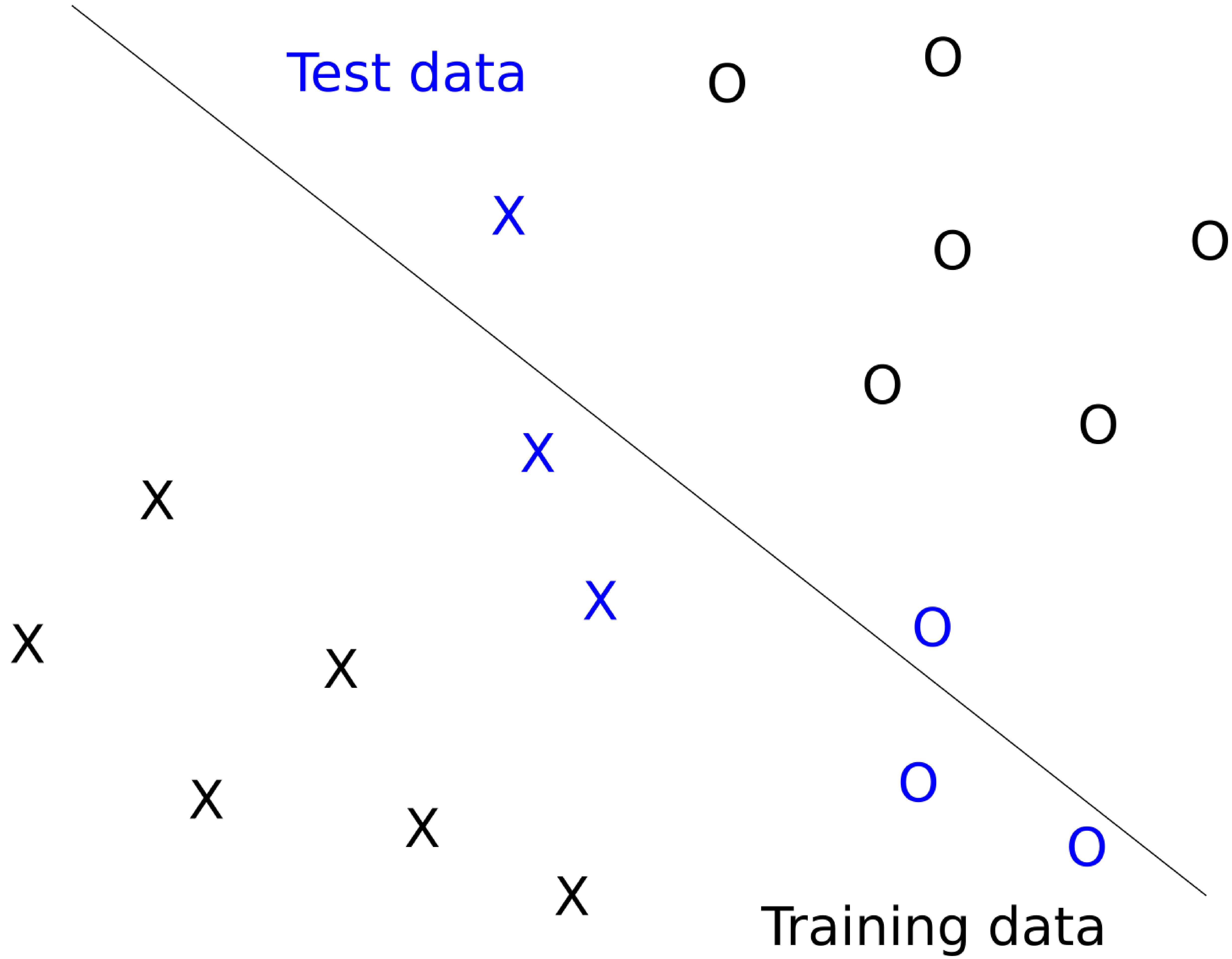
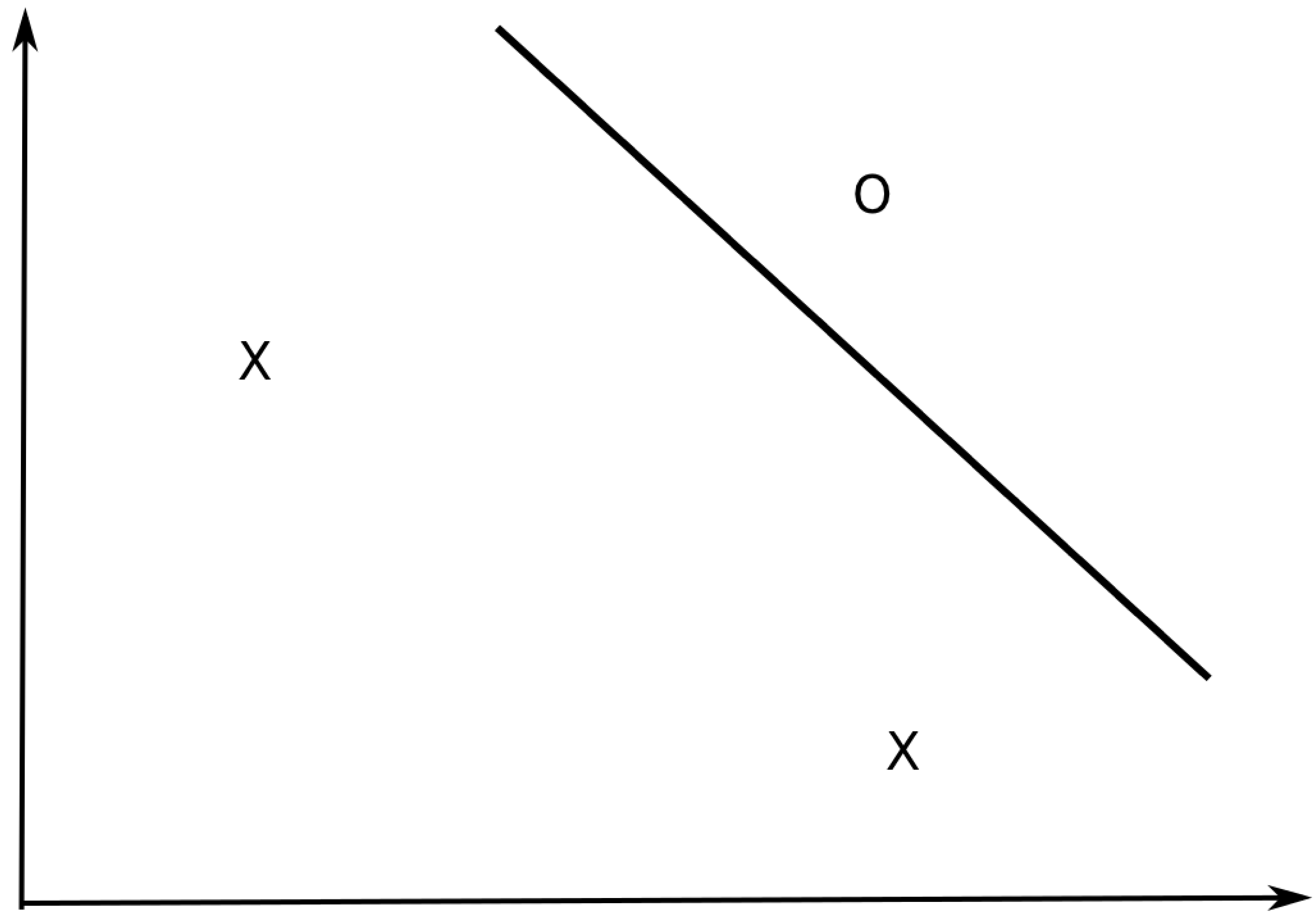


2 - VC dimension

Vapnik-Chervonenkis dimension of an hypothesis class

How many data examples can be correctly classified by a linear model in $\Re^d$?



In $\Re^2$, all dichotomies of three non-aligned examples can be correctly classified by a linear model ($y = w_o + w_1 \cdot x_1 + w_2 \cdot x_2$).

Vapnik-Chervonenkis dimension of an hypothesis class

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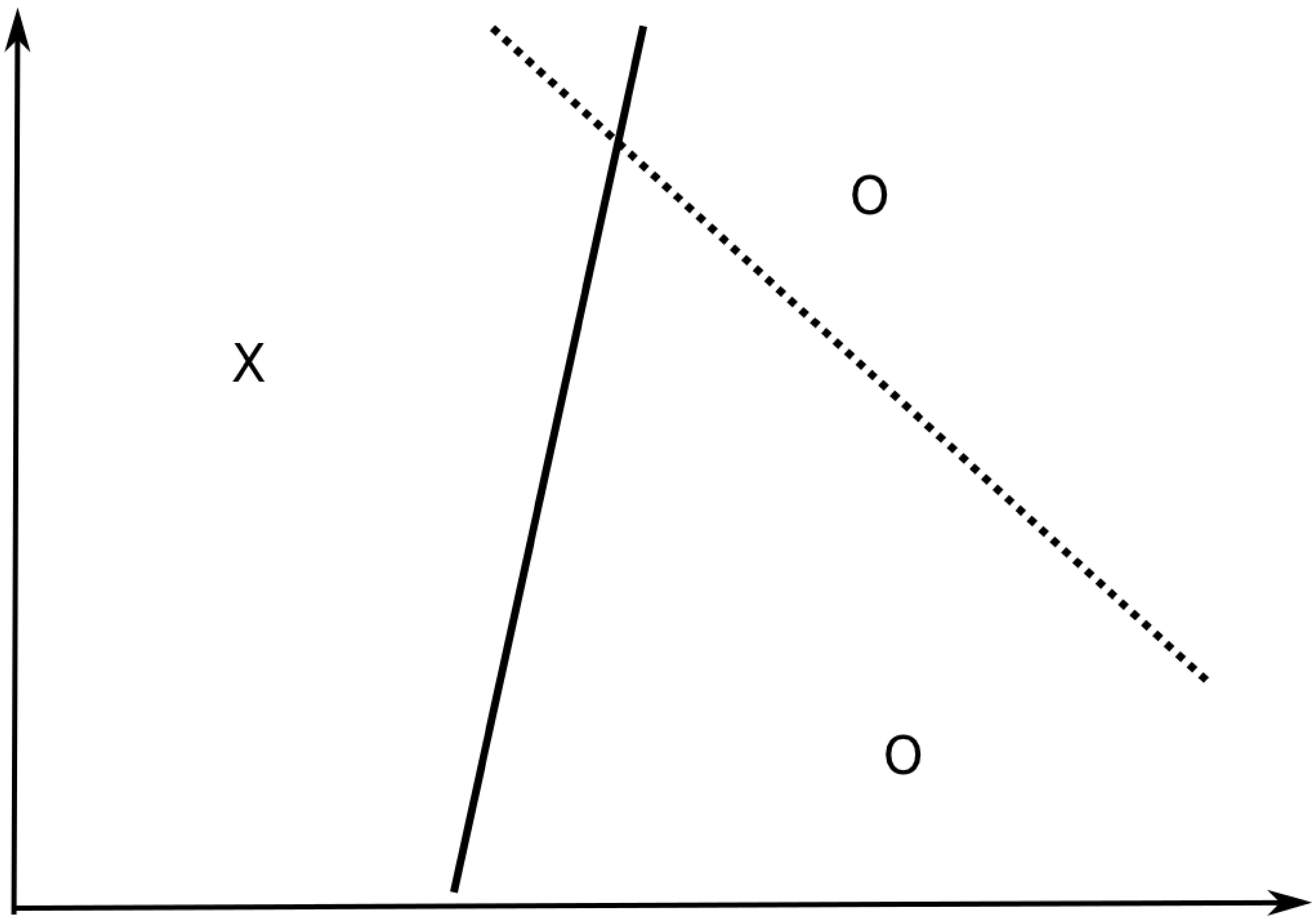

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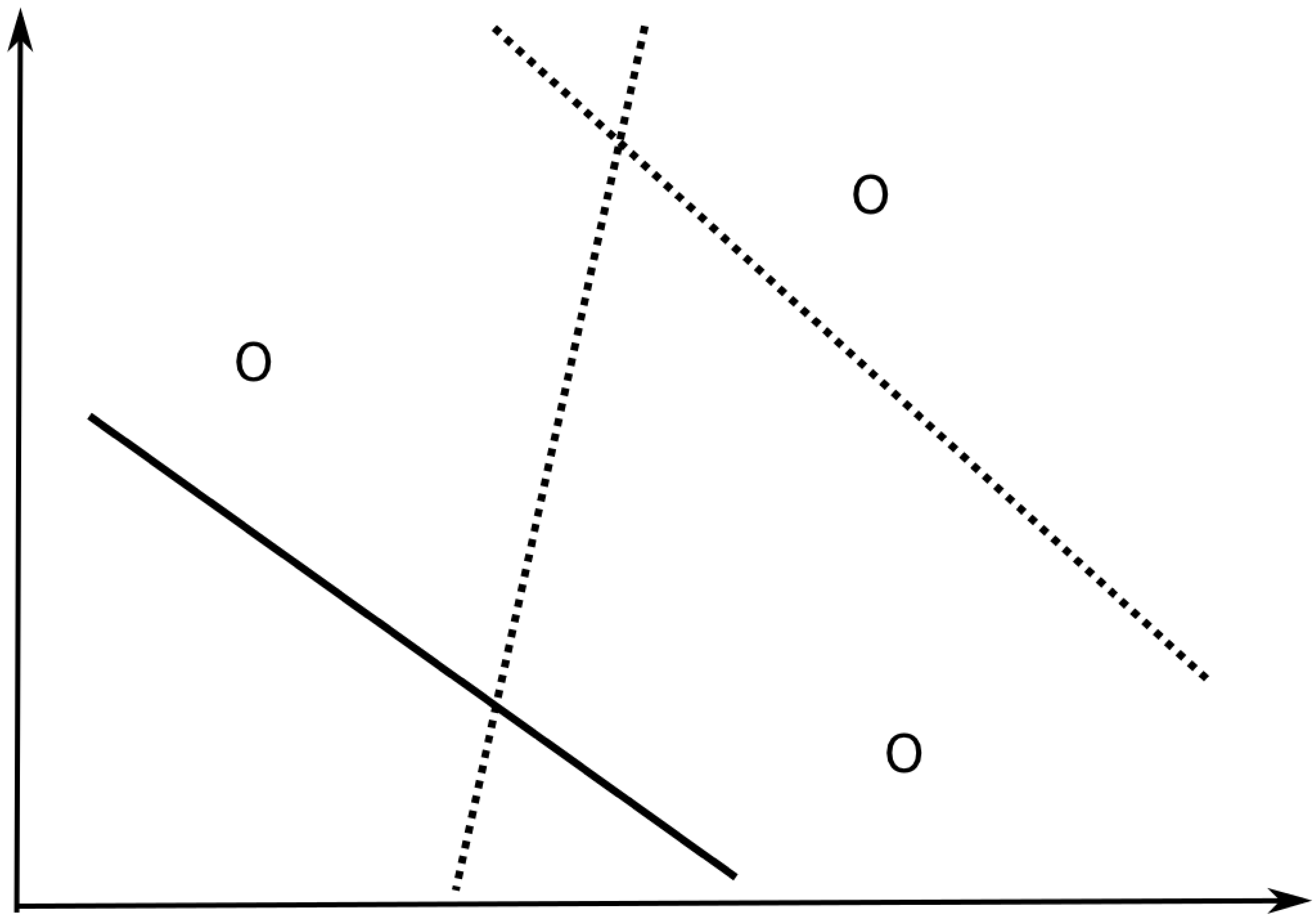

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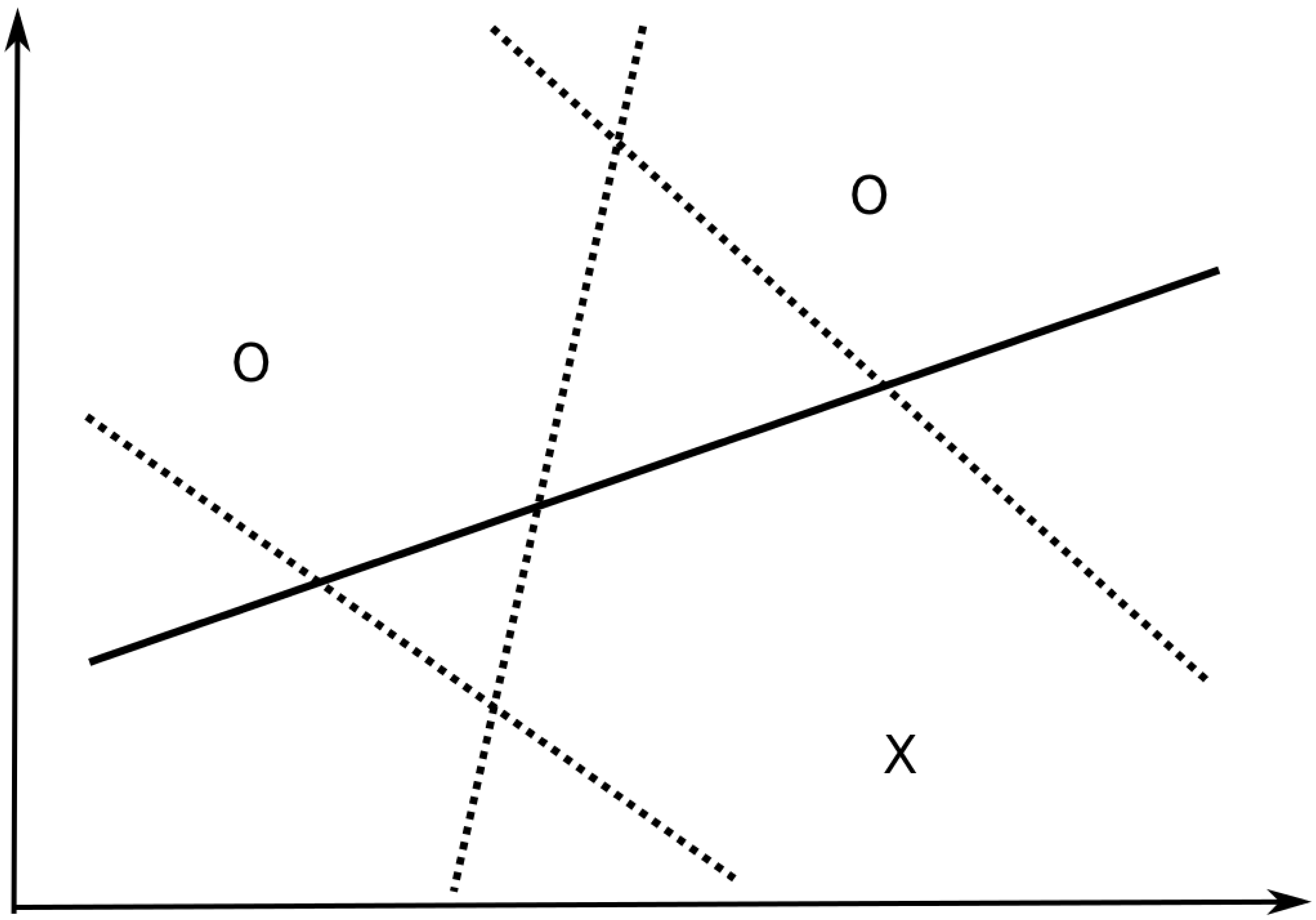

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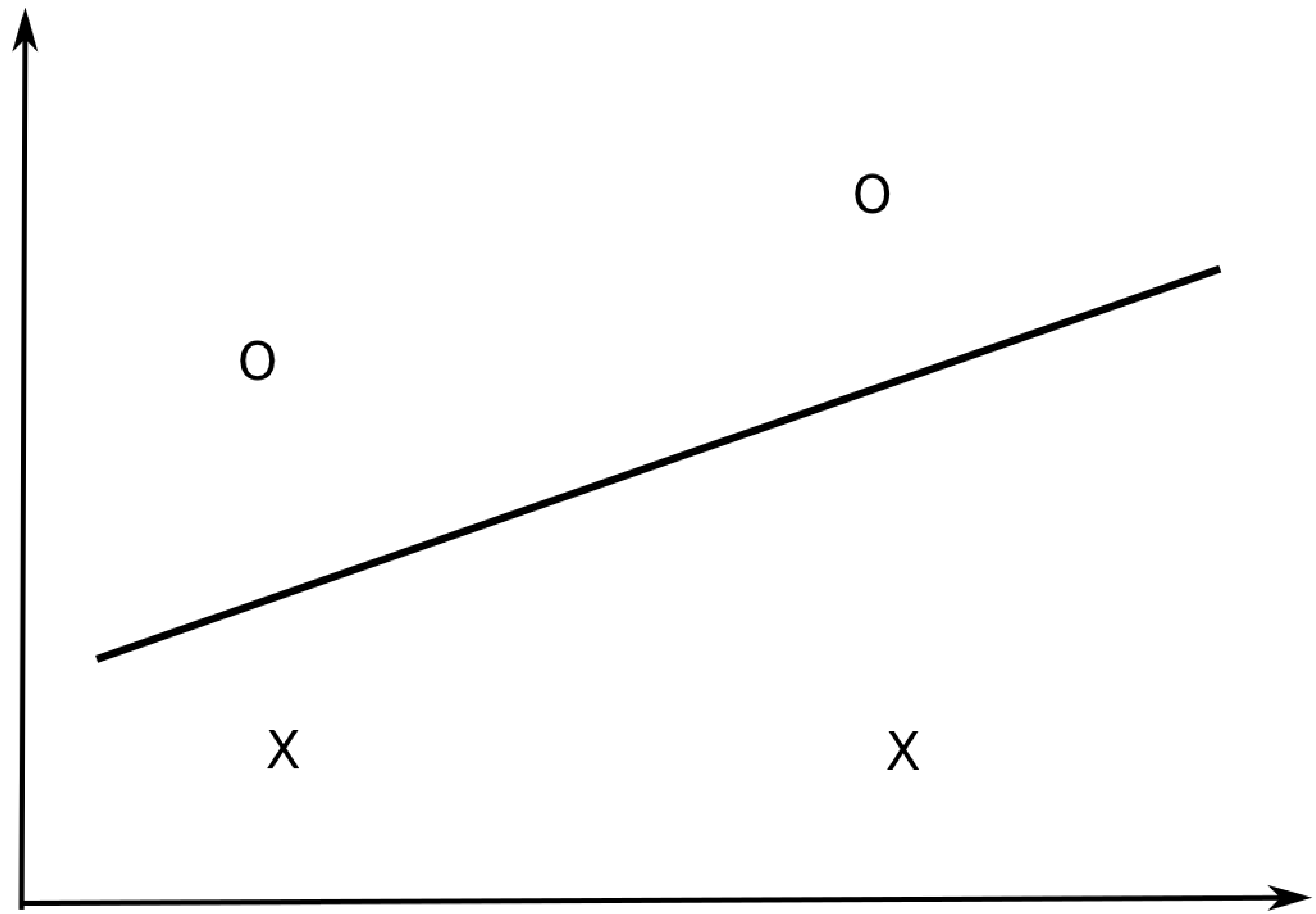

However, there exists sets of four examples in $\Re^2$ which can NOT be correctly classified by a linear model, i.e. they are not linearly separable.

Vapnik-Chervonenkis dimension of an hypothesis class

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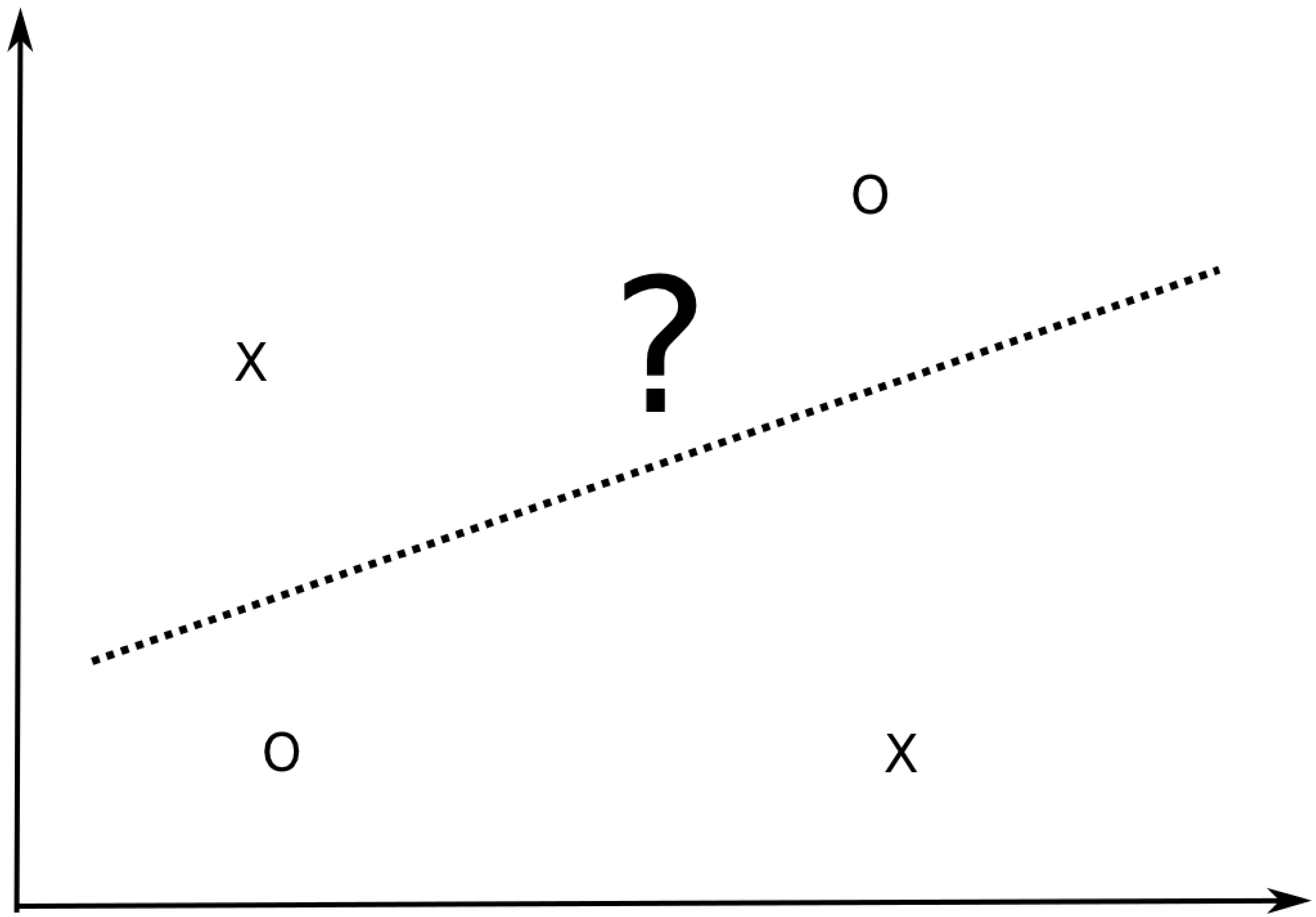
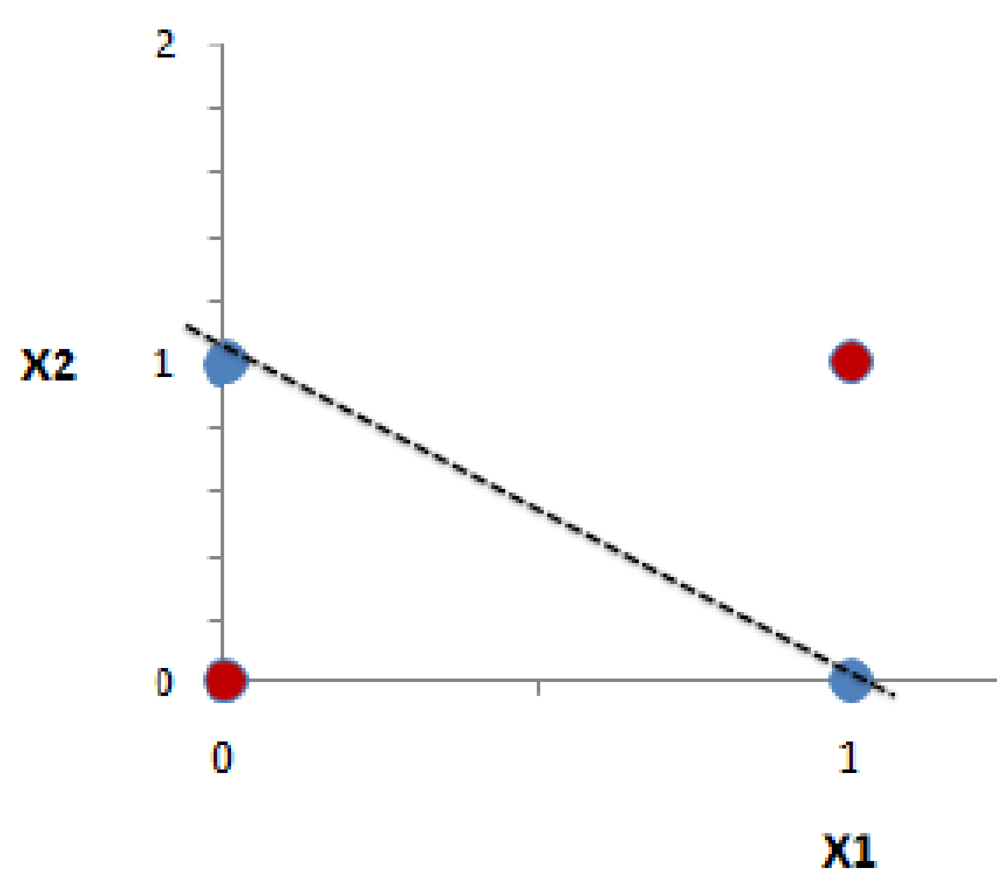


However, there exists sets of four examples in $\Re^2$ which can NOT be correctly classified by a linear model, i.e. they are not linearly separable.

Non-linearly separable data

- The XOR function in $\Re^2$ is for example not linearly separable, i.e. the Perceptron algorithm can not converge.



x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0

- The probability that a set of 3 (non-aligned) points in $\Re^2$ is linearly separable is 1, but the probability that a set of four points is linearly separable is smaller than 1 (but not zero).
- When a class of hypotheses $\mathcal{H}$ can correctly classify all points of a training set $\mathcal{D}$, we say that $\mathcal{H}$ **shatters** $\mathcal{D}$.

Vapnik-Chervonenkis dimension of an hypothesis class

- The **Vapnik-Chervonenkis dimension** $\text{VC}_\text{dim}(\mathcal{H})$ of an hypothesis class $\mathcal{H}$ is defined as the maximal number of training examples that $\mathcal{H}$ can shatter.
- We saw that in $\Re^2$, this dimension is 3:

$$\text{VC}_\text{dim}(\text{Linear}(\Re^2)) = 3$$

- This can be generalized to linear classifiers in $\Re^d$:

$$\text{VC}_\text{dim}(\text{Linear}(\Re^d)) = d + 1$$

- This corresponds to the number of **free parameters** of the linear classifier:
  - d parameters for the weight vector, 1 for the bias.
- Given any set of $(d+1)$ examples in $\Re^d$, there exists a linear classifier able to classify them perfectly.
- For other types of (non-linear) hypotheses, the VC dimension is generally proportional to the **number of free parameters**.
- But **regularization** reduces the VC dimension of the classifier.

Vapnik-Chervonenkis theorem

- The generalization error $\epsilon(h)$ of an hypothesis h taken from a class $\mathcal{H}$ of finite VC dimension and trained on N samples of $\mathcal{S}$ is bounded by the sum of the training error $\hat{\epsilon}_{\mathcal{S}}(h)$ and the VC complexity term:

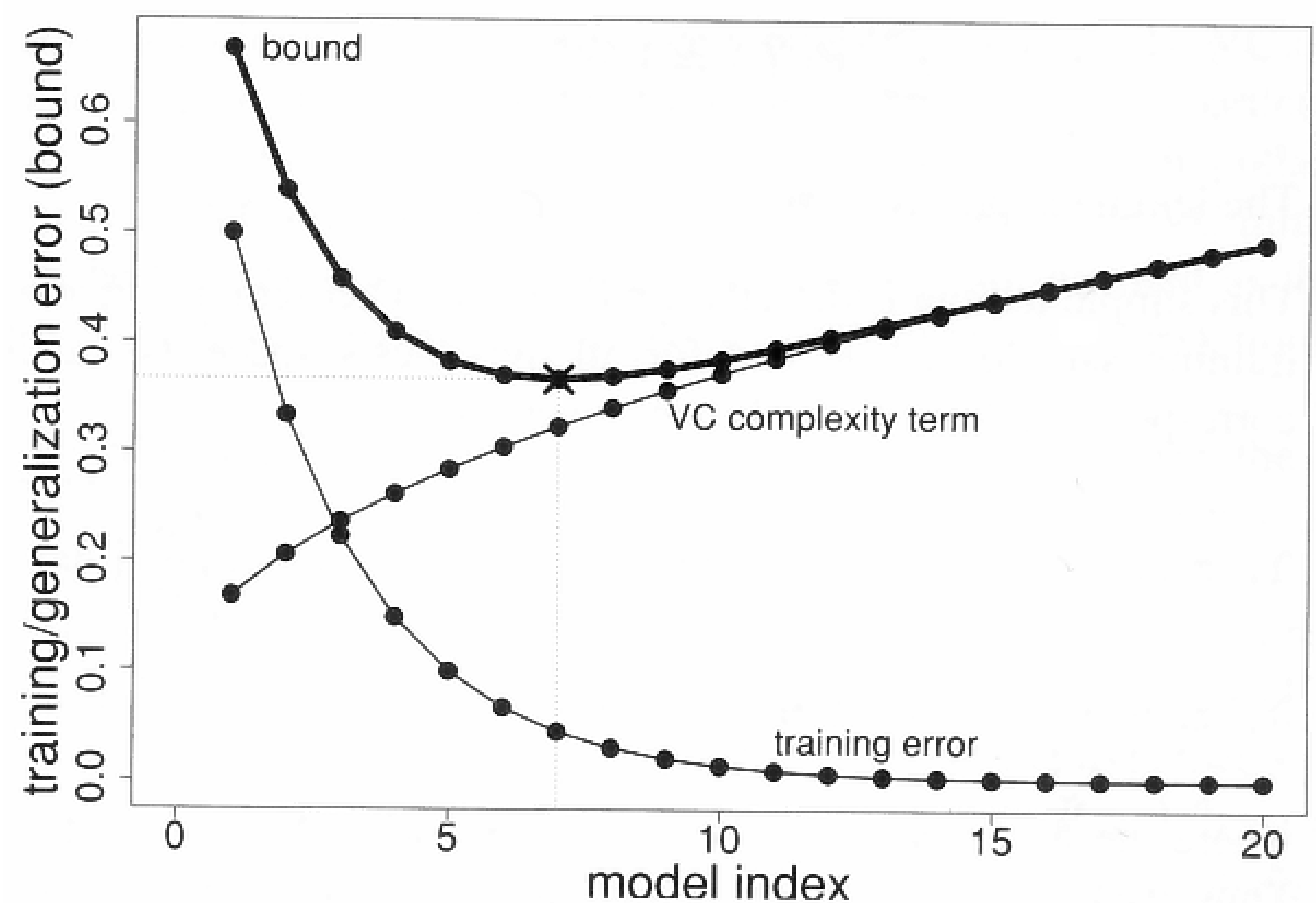
$$\epsilon(h) \leq \hat{\epsilon}_{\mathcal{S}}(h) + \sqrt{\frac{\text{VC}_{\text{dim}}(\mathcal{H}) \cdot (1 + \log(\frac{2 \cdot N}{\text{VC}_{\text{dim}}(\mathcal{H})})) - \log(\frac{\delta}{4})}{N}}$$

with probability $1 - \delta$, if $\text{VC}_{\text{dim}}(\mathcal{H}) << N$.

Vapnik, Vladimir (2000). The nature of statistical learning theory. Springer.

Structural risk minimization

$$\epsilon(h) \leq \hat{\epsilon}_{\mathcal{S}(h)} + \sqrt{\frac{\mathrm{VC}_{\mathrm{dim}}(\mathcal{H}) \cdot (1 + \log(\frac{2 \cdot N}{\mathrm{VC}_{\mathrm{dim}}(\mathcal{H})})) - \log(\frac{\delta}{4})}{N}}$$



Structural risk minimization

$$\epsilon(h) \leq \hat{\epsilon}_{\mathcal{S}(h)} + \sqrt{\frac{\text{VC}_{\text{dim}} (\mathcal{H}) \cdot (1 + \log(\frac{2 \cdot N}{\text{VC}_{\text{dim}} (\mathcal{H})})) - \log(\frac{\delta}{4})}{N}}$$

- The generalization error increases with the VC dimension, while the training error decreases.
- Structural risk minimization is an alternative method to cross-validation.
- The VC dimensions of various classes of hypothesis are already known (~ number of free parameters).
- This bounds tells how many training samples are needed by a given hypothesis class in order to obtain a satisfying generalization error.
    - **The more complex the model, the more training data you will need to get a good generalization error!**

$$\epsilon(h) \approx \frac{\text{VC}_{\text{dim}} (\mathcal{H})}{N}$$

- A learning algorithm should only try to minimize the training error, as the VC complexity term only depends on the model.
- This term is only an upper bound: most of the time, the real bound is usually 100 times smaller.

Implication for non-linear classifiers

- The VC dimension of linear classifiers in $\Re^d$ is:

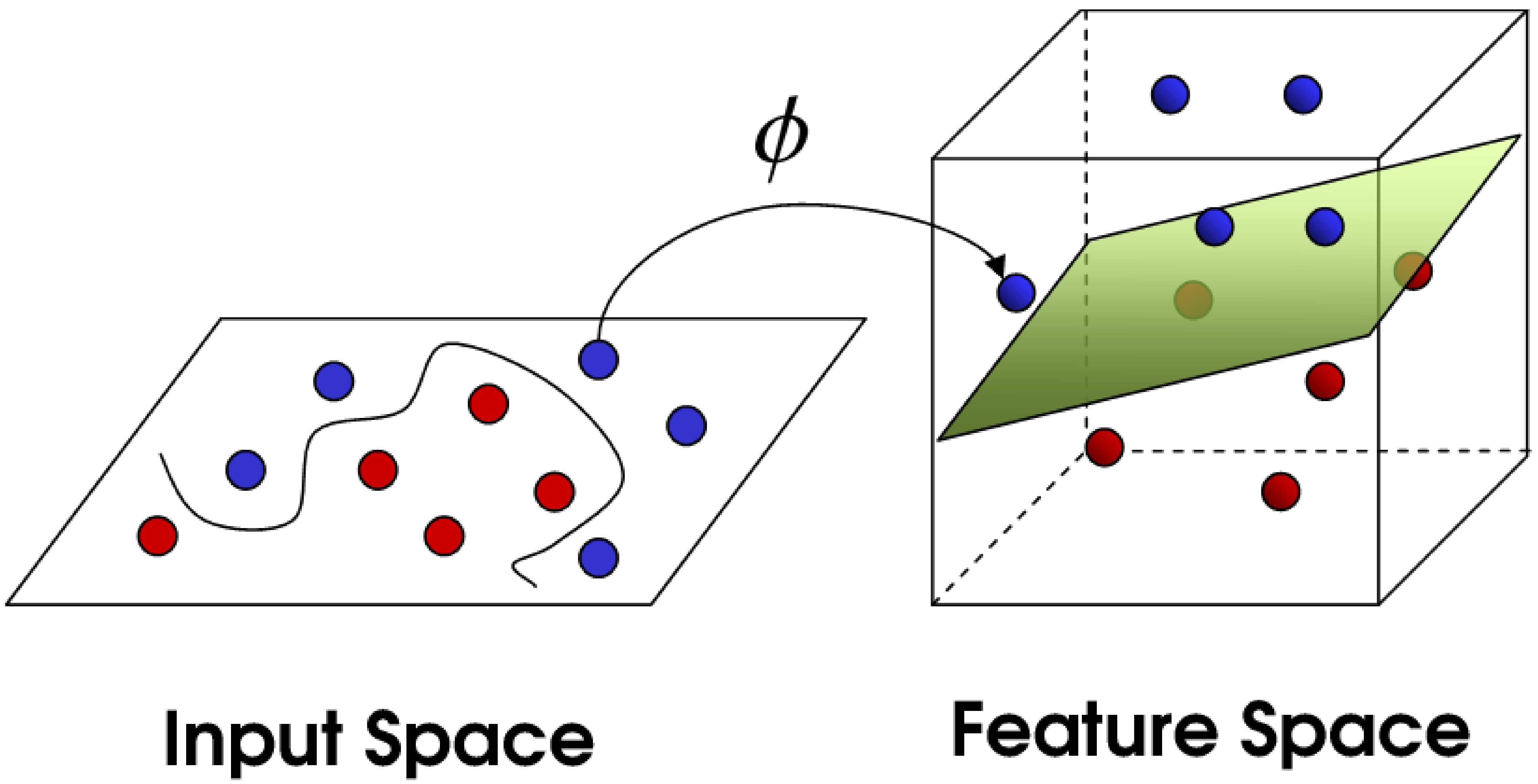
$$\text{VC}_{\text{dim}} (\text{Linear}(\Re^d)) = d + 1$$

- Given any set of $(d+1)$ examples in $\Re^d$, there exists a linear classifier able to classify them perfectly.
- For $N >> d$ the probability of having training errors becomes huge (the data is generally not linearly separable).
    - **If we project the input data onto a space with sufficiently high dimensions, it becomes then possible to find a linear classifier on this projection space that is able to classify the data!**
- However, if the space has too many dimensions, the VC dimension will increase and the generalization error will increase.
- Basic principle of all non-linear methods: multi-layer perceptron, radial-basis-function networks, support-vector machines…

3 - Feature space

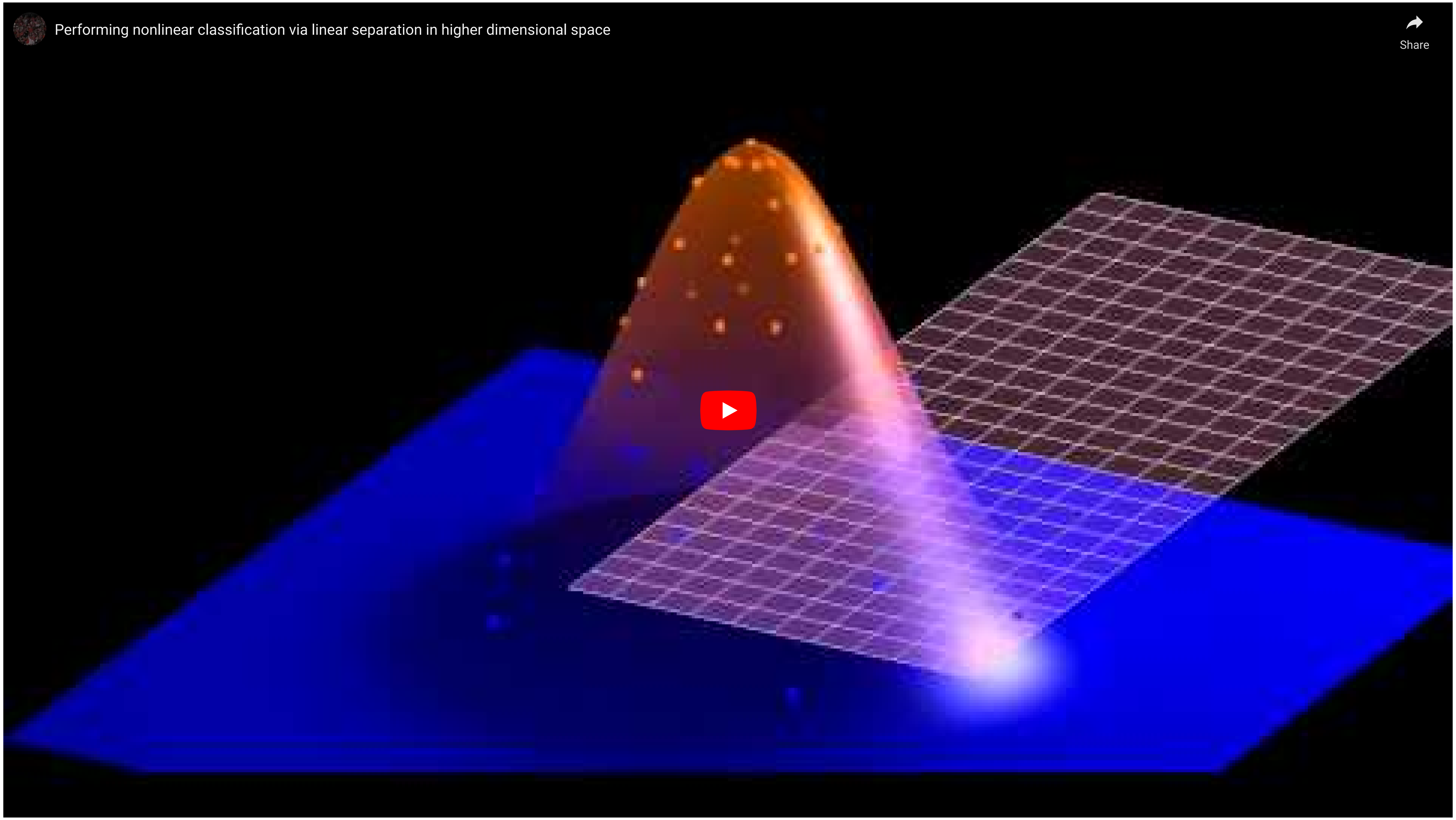
Cover's theorem on the separability of patterns (1965)

A complex pattern-classification problem, cast in a high dimensional space non-linearly, is more likely to be linearly separable than in a low-dimensional space, provided that the space is not densely populated.



- The highly dimensional space where the input data is projected is called the **feature space**.
- When the number of dimensions of the feature space increases:
  - the training error decreases (the pattern is more likely linearly separable);
  - the generalization error increases (the VC dimension increases).

Feature space

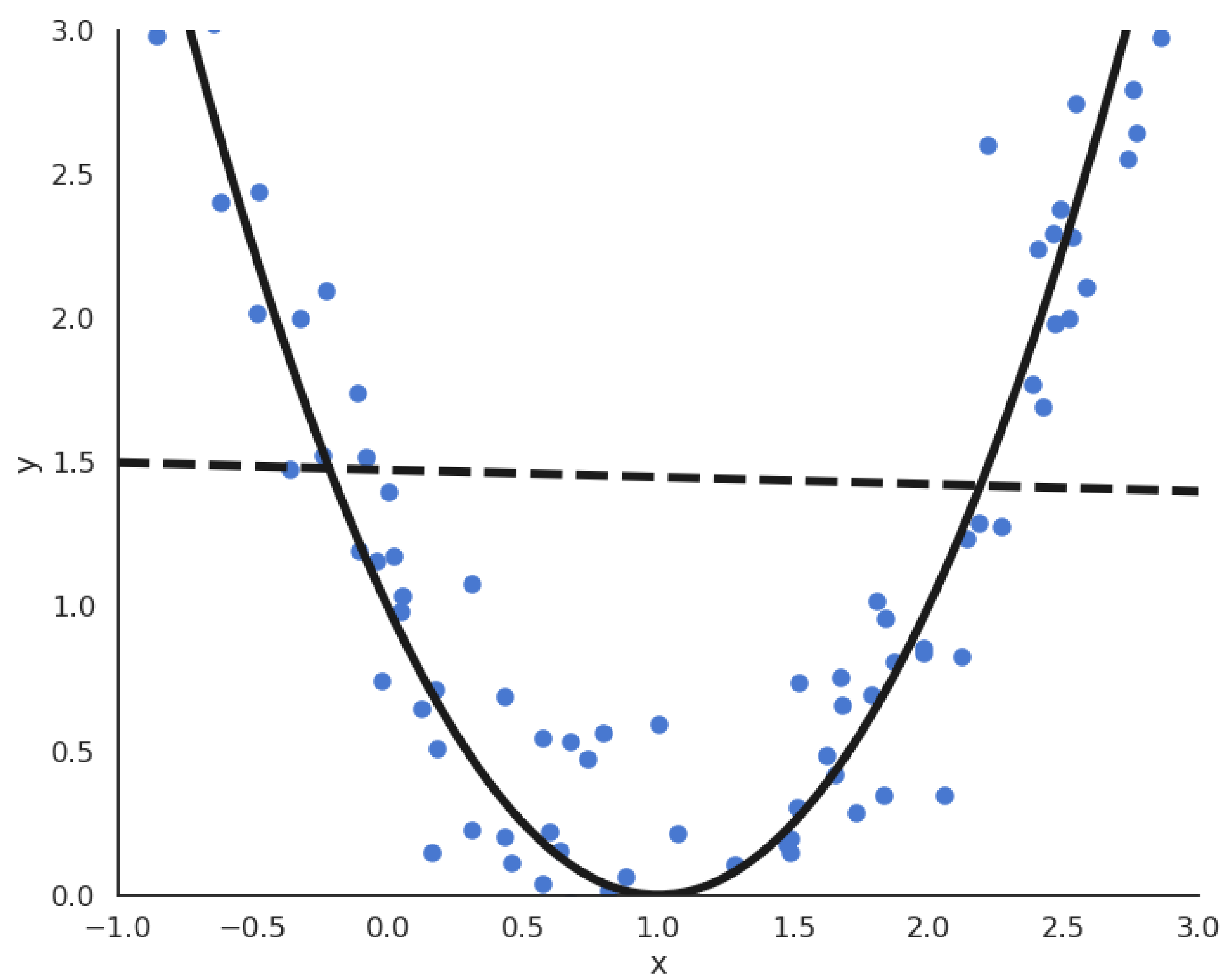


Polynomial features

- For the polynomial regression of order p:

$$y = f_{\mathbf{w}, b}(x) = w_1 \, x + w_2 \, x^2 + \ldots + w_p \, x^p + b$$

the vector $\mathbf{x} = \begin{bmatrix} x \\ x^2 \\ \ldots \\ x^p \end{bmatrix}$ defines a feature space for the input x.



- The elements of the feature space are called **polynomial features**.
- We can define polynomial features of more than one variable, e.g. $x^2 \, y$, $x^3 \, y^4$, etc.
- We then apply multiple **linear** regression (MLR) on the polynomial feature space to find the parameters:

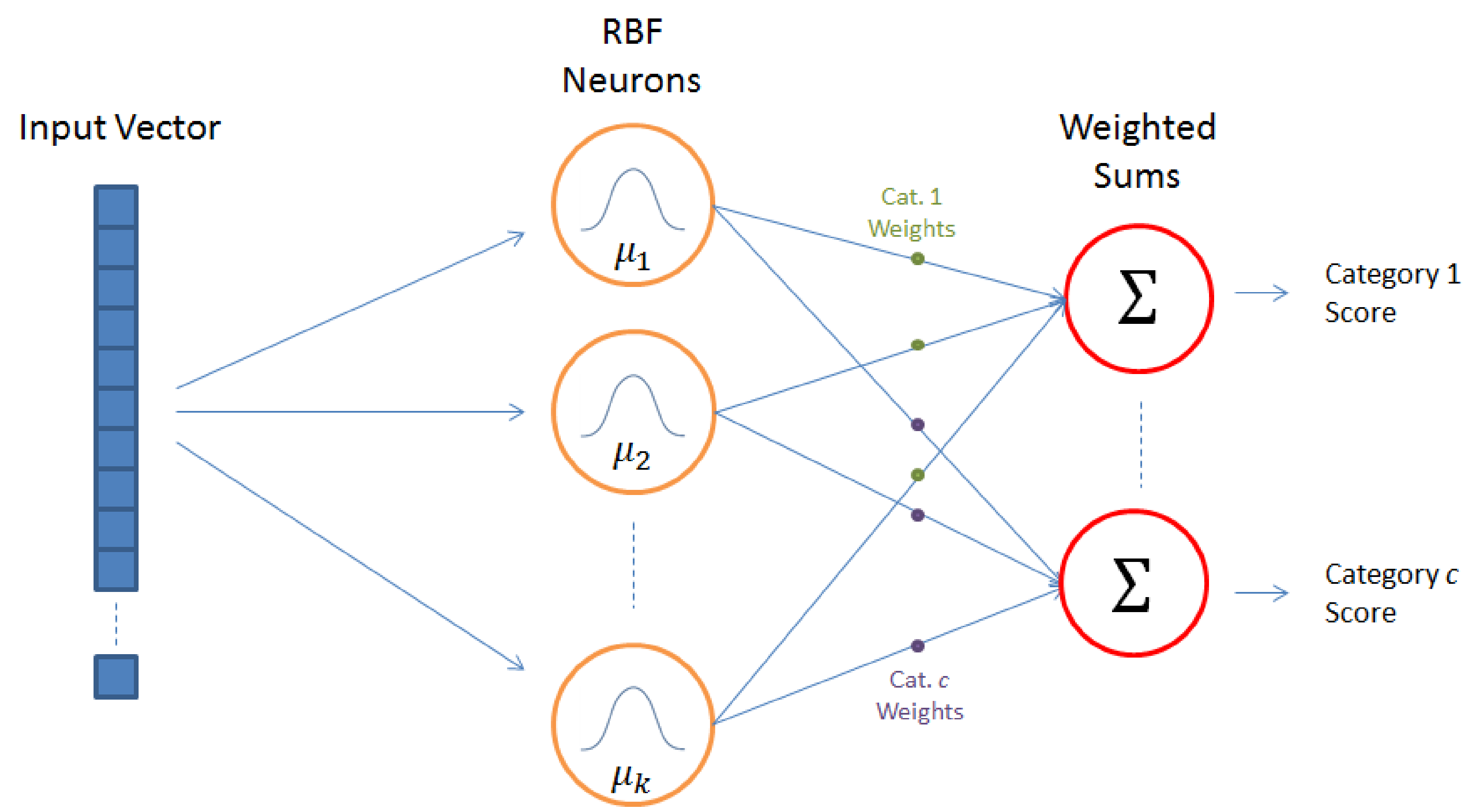
$$\Delta \mathbf{w} = \eta \, (t - y) \, \mathbf{x}$$

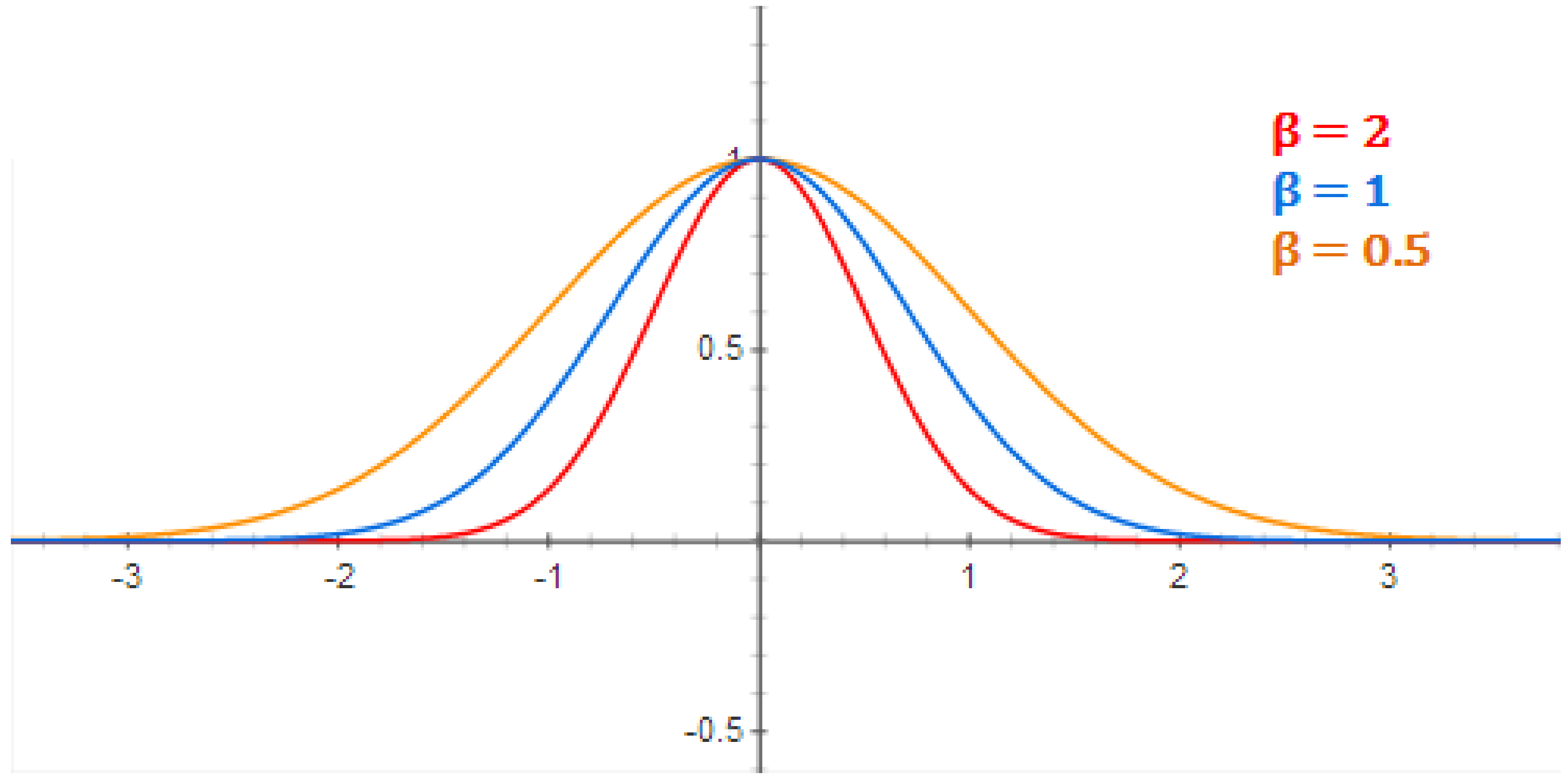
Radial-basis function networks

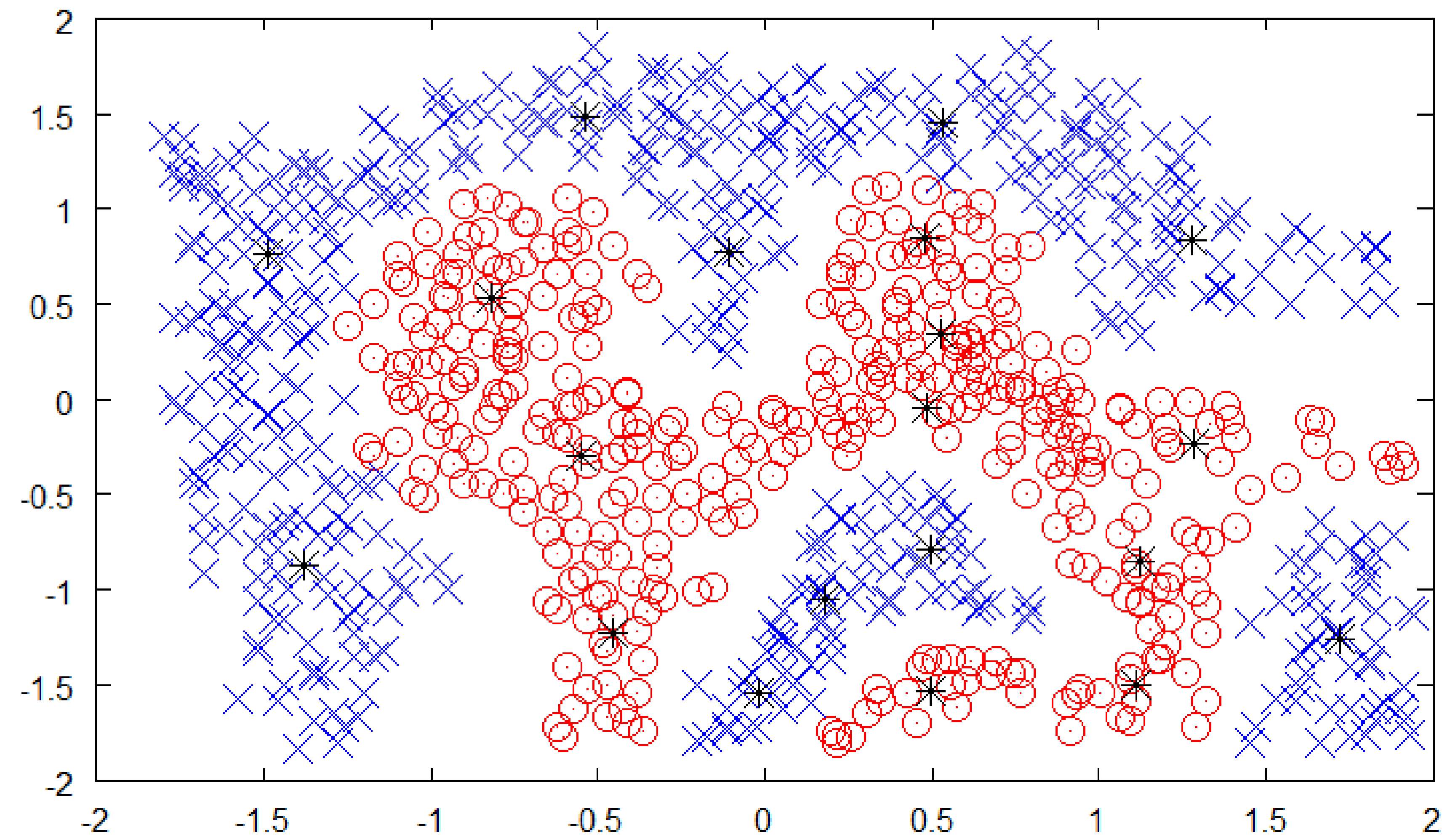
- Radial-basis function (**RBF**) networks samples a subset of K training examples and form the feature space using a **gaussian kernel**:

$$\phi(\mathbf{x}) = \begin{bmatrix} \varphi(\mathbf{x} - \mathbf{x}_1) \\ \varphi(\mathbf{x} - \mathbf{x}_2) \\ \dots \\ \varphi(\mathbf{x} - \mathbf{x}_K) \end{bmatrix}$$

with $\varphi(\mathbf{x} - \mathbf{x}_i) = \exp -\beta \, ||\mathbf{x} - \mathbf{x}_i||^2$ decreasing with the distance between the vectors.







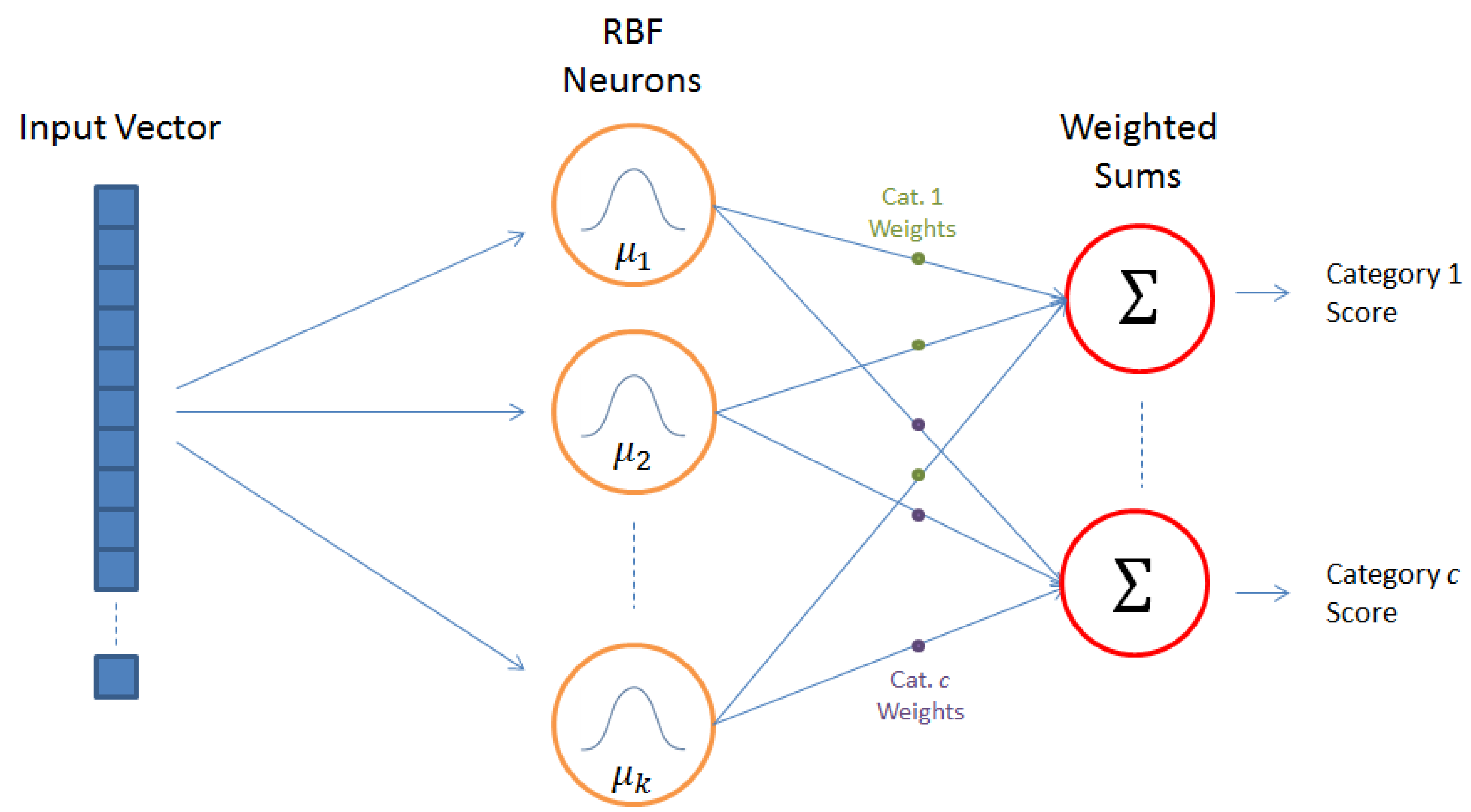
Radial-basis function networks

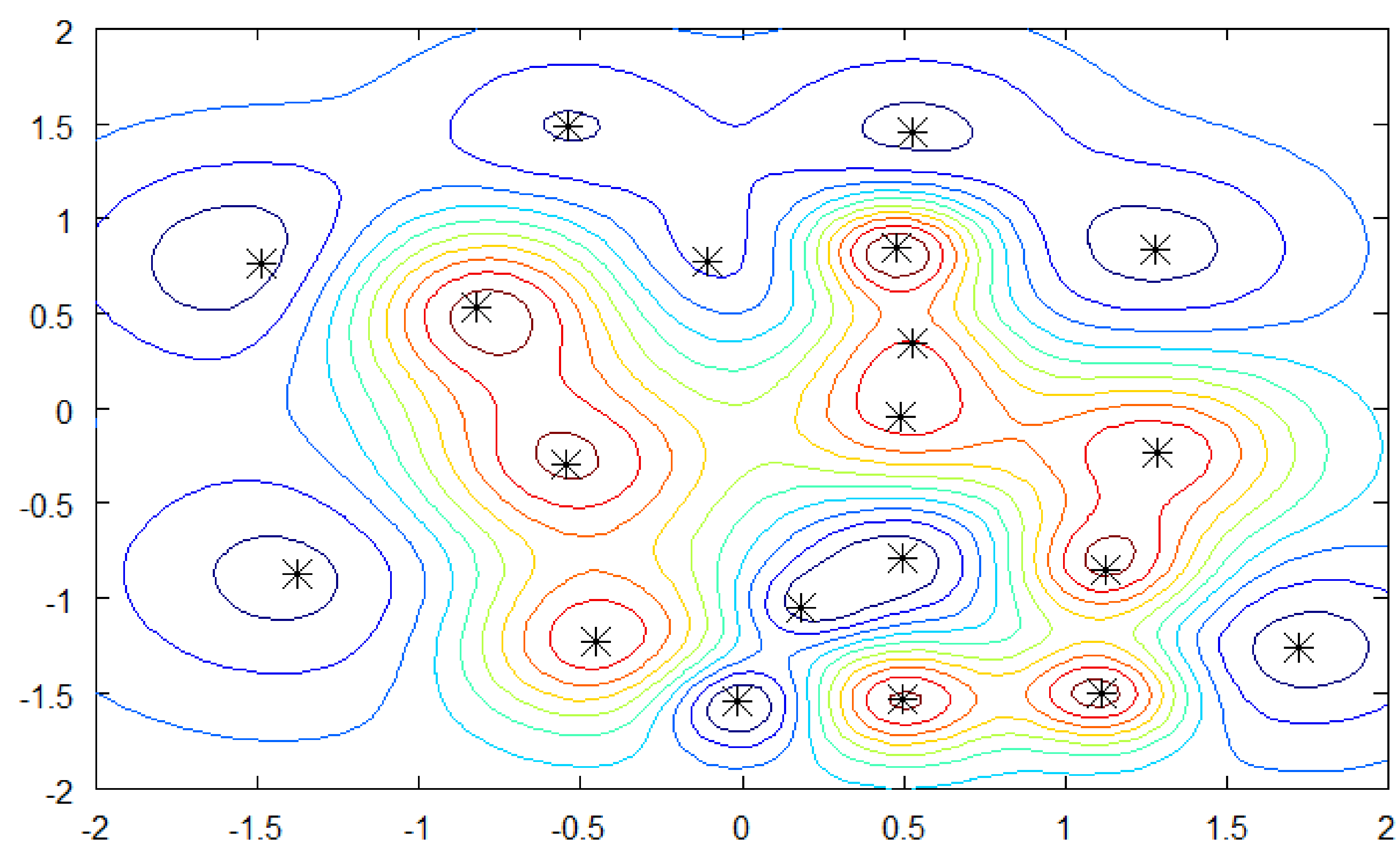
- By applying a linear classification algorithm on the RBF feature space:

$$\mathbf{y} = f(W \times \phi(\mathbf{x}) + \mathbf{b})$$

we obtain a smooth **non-linear** partition of the input space.

- The width of the gaussian kernel allows distance-based **generalization**.





Source: https://mccormickml.com/2013/08/15/radial-basis-function-network-rbfn-tutorial/

Kernel perceptron

- What happens during online Perceptron learning?
- If an example $\mathbf{x}_i$ is correctly classified ($y_i = t_i$), the weight vector does not change.

$$\mathbf{w} \leftarrow \mathbf{w}$$

- If an example $\mathbf{x}_i$ is miscorrectly classified ($y_i \neq t_i$), the weight vector is increased from $t_i \, \mathbf{x}_i$.

$$\mathbf{w} \leftarrow \mathbf{w} + 2 \, \eta \, t_i \, \mathbf{x}_i$$

Primal form of the online Perceptron algorithm

- **for** M epochs:
  - **for** each sample $(\mathbf{x}_i, t_i)$:
    - $y_i = \text{sign}(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b)$
    - $\Delta \mathbf{w} = \eta \, (t_i - y_i) \, \mathbf{x}_i$
    - $\Delta b = \eta \, (t_i - y_i)$

- If you initialize the weight vector to 0, its final value will therefore be a **linear combination** of the input samples:

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

- The coefficients α_i represent the **embedding strength** of each example, i.e. how often they were misclassified.

Kernel perceptron

- With $\mathbf{w} = \sum_{i=1}^N \alpha_i \, t_i \, \mathbf{x}_i$, the prediction for an input $\mathbf{x}$ only depends on the training samples and their α_i value:

$$y = \text{sign}(\sum_{i=1}^N \alpha_i \, t_i \, \langle \mathbf{x}_i \cdot \mathbf{x} \rangle)$$

- To make a prediction y, we need the dot product between the input $\mathbf{x}$ and all training examples $\mathbf{x}_i$.
- We ignore the bias here, but it can be added back.

Dual form of the online Perceptron algorithm

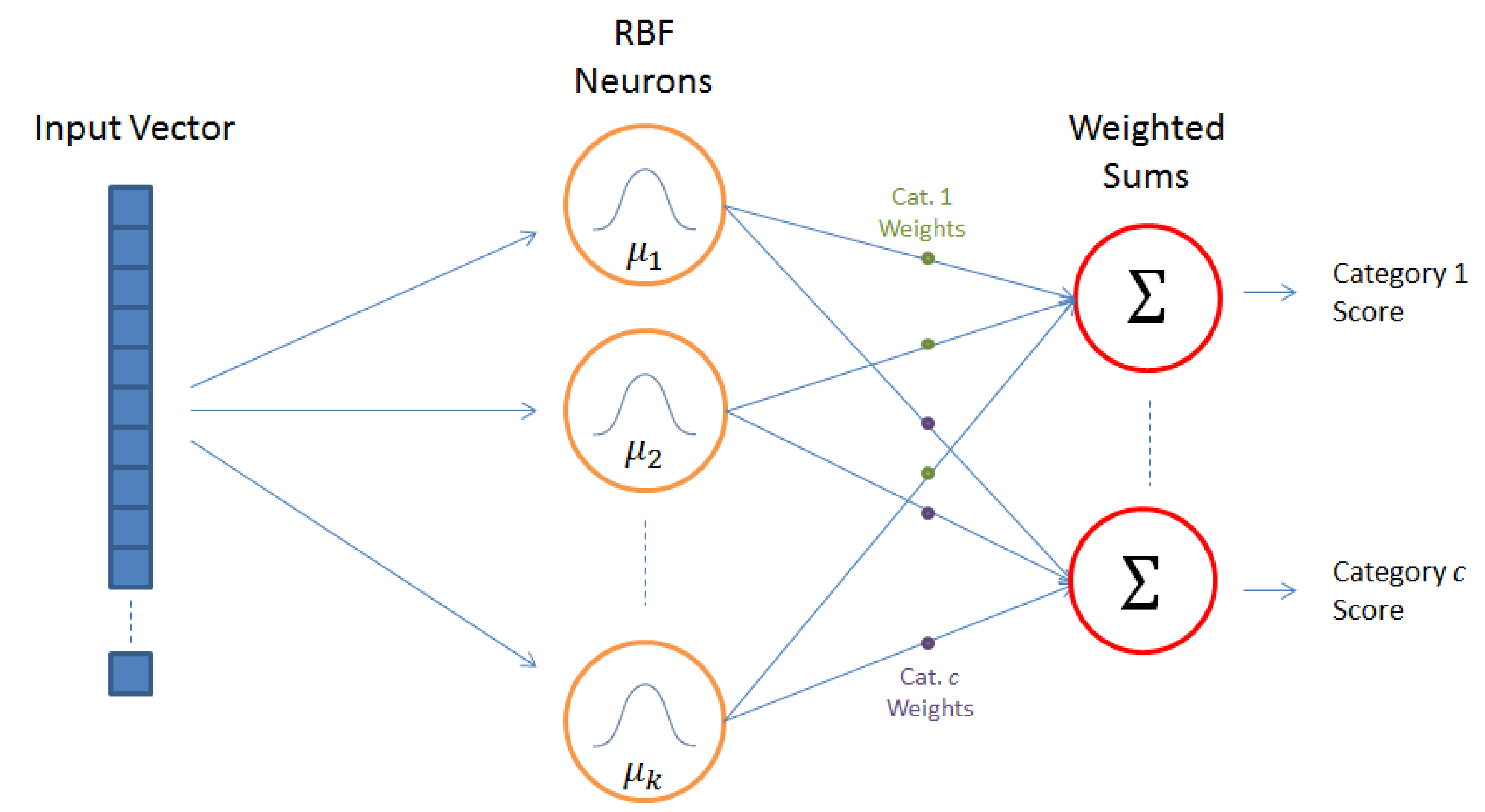
- **for** M epochs:
  - **for** each sample $(\mathbf{x}_i, t_i)$:
    - $y_i = \text{sign}(\sum_{j=1}^N \alpha_j \, t_j \, \langle \mathbf{x}_j \cdot \mathbf{x}_i \rangle)$
    - **if** $y_i \neq t_i$:
      - $\alpha_i \leftarrow \alpha_i + 1$

- This **dual form** of the Perceptron algorithm is strictly equivalent to its primal form.
- It needs one parameter α_i per training example instead of a weight vector ($N >> d$), but relies on dot products between vectors.

Kernel perceptron

- Why is it interesting to have an algorithm relying on dot products?

$$y = \text{sign}(\sum_{i=1}^N \alpha_i \, t_i \, \langle \mathbf{x}_i \cdot \mathbf{x} \rangle)$$



- You can project the inputs $\mathbf{x}$ to a **feature space** $\phi(\mathbf{x})$ and apply the same algorithm:

$$y = \text{sign}(\sum_{i=1}^N \alpha_i \, t_i \, \langle \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}) \rangle)$$

- But you do not need to compute the dot product in the feature space, all you need to know is its result.

$$K(\mathbf{x}_i, \mathbf{x}) = \langle \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}) \rangle$$

- **Kernel trick:** A kernel $K(\mathbf{x}, \mathbf{z})$ allows to compute the dot product between the feature space representation of two vectors without ever computing these representations!

Example of the polynomial kernel

- Let's consider the quadratic kernel in $\Re^3$:

$$\forall (\mathbf{x}, \mathbf{z}) \in \Re^3 \times \Re^3$$

$$\begin{aligned} K(\mathbf{x}, \mathbf{z}) &= (\langle \mathbf{x} \cdot \mathbf{z} \rangle)^2 \\ &= (\sum_{i=1}^{3} x_i \cdot z_i) \cdot (\sum_{j=1}^{3} x_j \cdot z_j) \\ &= \sum_{i=1}^{3} \sum_{j=1}^{3} (x_i \cdot x_j) \cdot (z_i \cdot z_j) \\ &= \langle \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \rangle \end{aligned}$$

$$\text{with:} \qquad \phi(\mathbf{x}) = \begin{bmatrix} x_1 \cdot x_1 \\ x_1 \cdot x_2 \\ x_1 \cdot x_3 \\ x_2 \cdot x_1 \\ x_2 \cdot x_2 \\ x_2 \cdot x_3 \\ x_3 \cdot x_1 \\ x_3 \cdot x_2 \\ x_3 \cdot x_3 \end{bmatrix}$$

- The quadratic kernel implicitely transforms an input space with three dimensions into a feature space of 9 dimensions.

Example of the polynomial kernel

- More generally, the polynomial kernel in $\Re^d$ of degree p:

$$\forall (\mathbf{x}, \mathbf{z}) \in \Re^d \times \Re^d \qquad \begin{aligned} K(\mathbf{x}, \mathbf{z}) &= (\langle \mathbf{x} \cdot \mathbf{z} \rangle)^p \\ &= \langle \phi(\mathbf{x}) \cdot \phi(\mathbf{z}) \rangle \end{aligned}$$

transforms the input from a space with d dimensions into a feature space of d^p dimensions.

- While the inner product in the feature space would require $O(d^p)$ operations, the calculation of the kernel directly in the input space only requires $O(d)$ operations.
- This is called the **kernel trick**: when a linear algorithm only relies on the dot product between input vectors, it can be safely projected into a higher dimensional feature space through a kernel function, without increasing too much its computational complexity, and without ever computing the values in the feature space.

Kernel perceptron

- The **kernel perceptron** is the dual form of the Perceptron algorithm using a kernel.

Kernel Perceptron

- **for** M epochs:
    - **for** each sample $(\mathbf{x}_i, t_i)$:
        - $y_i = \text{sign}(\sum_{j=1}^N \alpha_j \, t_j \, K(\mathbf{x}_j, \mathbf{x}_i))$
        - **if** $y_i \neq t_i$:
            - $\alpha_i \leftarrow \alpha_i + 1$

- Depending on the kernel, the implicit dimensionality of the feature space can even be infinite!

- **Linear kernel**: dimension of the feature space = d.

$$K(\mathbf{x}, \mathbf{z}) = \langle \mathbf{x} \cdot \mathbf{z} \rangle$$

- **Polynomial kernel**: dimension of the feature space = d^p.

$$K(\mathbf{x}, \mathbf{z}) = (\langle \mathbf{x} \cdot \mathbf{z} \rangle)^p$$

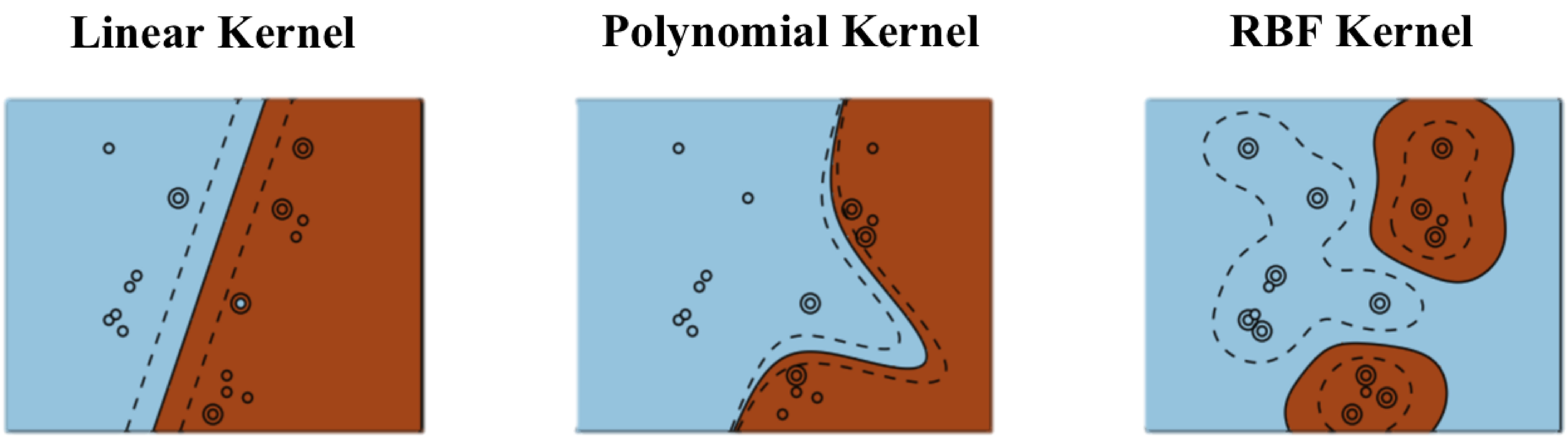
- **Gaussian kernel** (or RBF kernel): dimension of the feature space= ∞.

$$K(\mathbf{x}, \mathbf{z}) = \exp(-\frac{\| \mathbf{x} - \mathbf{z} \|^2}{2\sigma^2})$$

- **Hyperbolic tangent kernel**: dimension of the feature space = ∞

$$k(\mathbf{x}, \mathbf{z}) = \tanh(\langle \kappa \mathbf{x} \cdot \mathbf{z} \rangle + c)$$

Examples of kernels

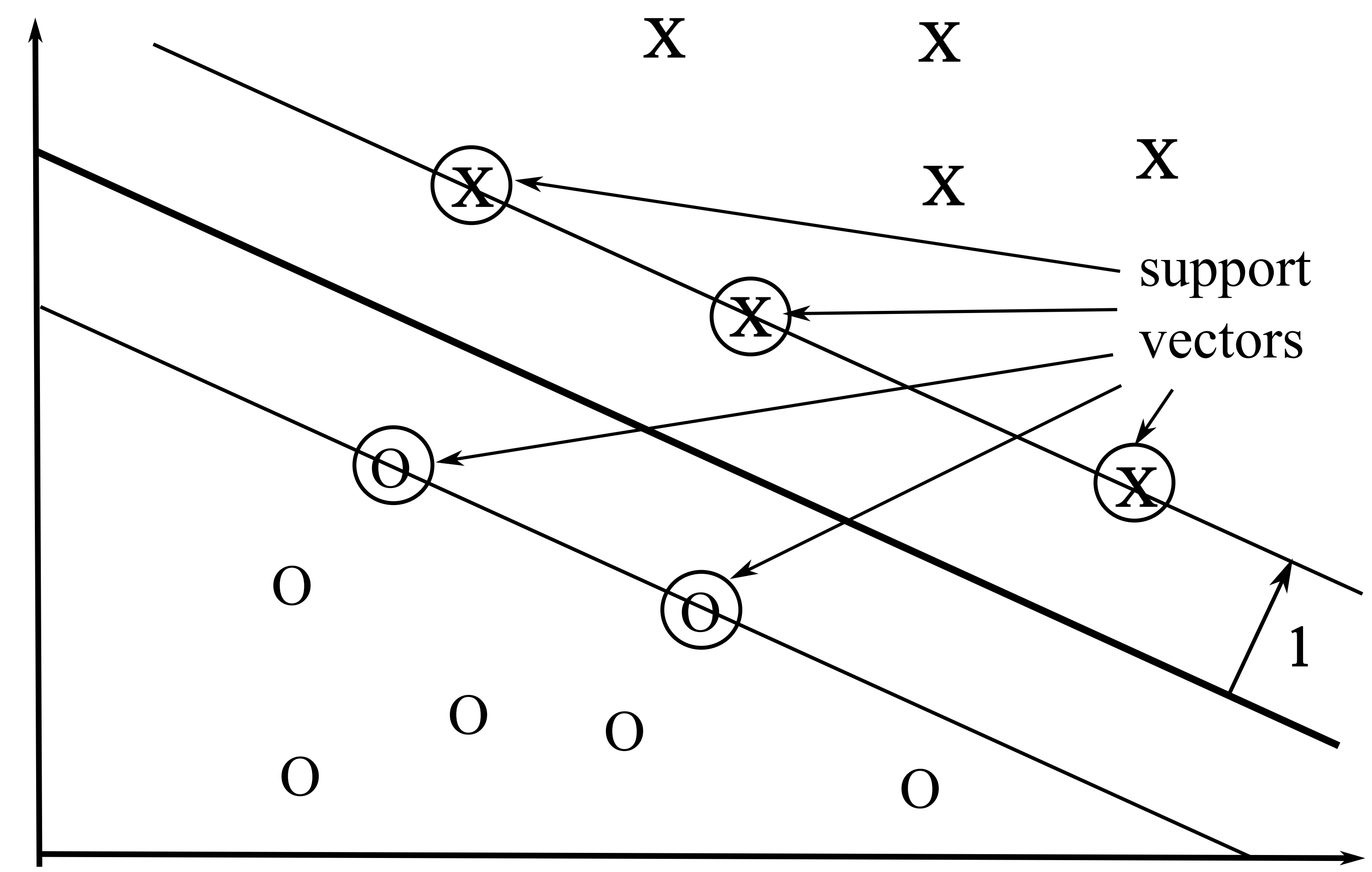


- In practice, the choice of the kernel family depends more on the nature of data (text, image…) and its distribution than on the complexity of the learning problem.
- RBF kernels tend to “group” positive examples together.
- Polynomial kernels are more like “distorted” hyperplanes.
- Kernels have parameters (p, σ…) which have to found using cross-validation.

Source: http://beta.cambridgespark.com/courses/jpm/05-module.html

Support vector machines

- **Support vector machines** (SVM) extend the idea of a kernel perceptron using a different linear learning algorithm, the maximum margin classifier.
- Using Lagrange optimization and regularization, the maximal margin classifer tries to maximize the "safety zone" (geometric margin) between the classifier and the training examples.
- It also tries to reduce the number of non-zero α_i coefficients to keep the complexity of the classifier bounded, thereby improving the generalization:



$$\mathbf{y} = \text{sign}(\sum_{i=1}^{N_{SV}} \alpha_i \, t_i \, K(\mathbf{x}_i, \mathbf{x}) + b)$$

- Coupled with a good kernel, a SVM can efficiently solve non-linear classification problems without overfitting.
- SVMs were the weapon of choice before the deep learning era, which deals better with huge datasets.