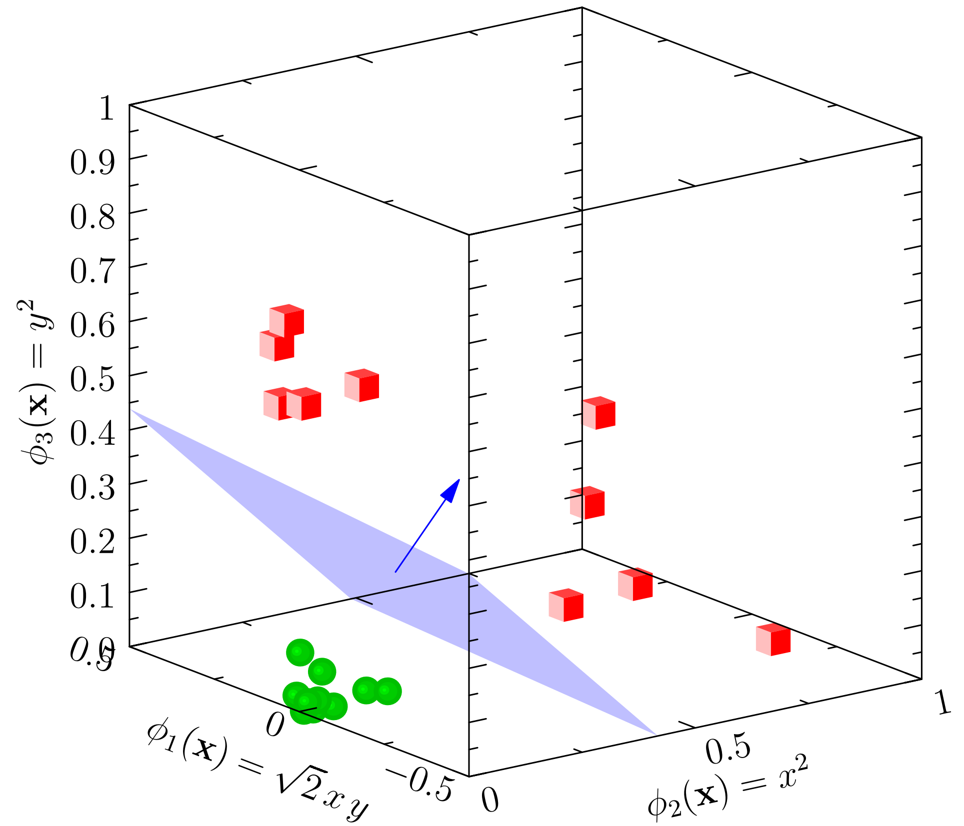
Advanced Machine Learning

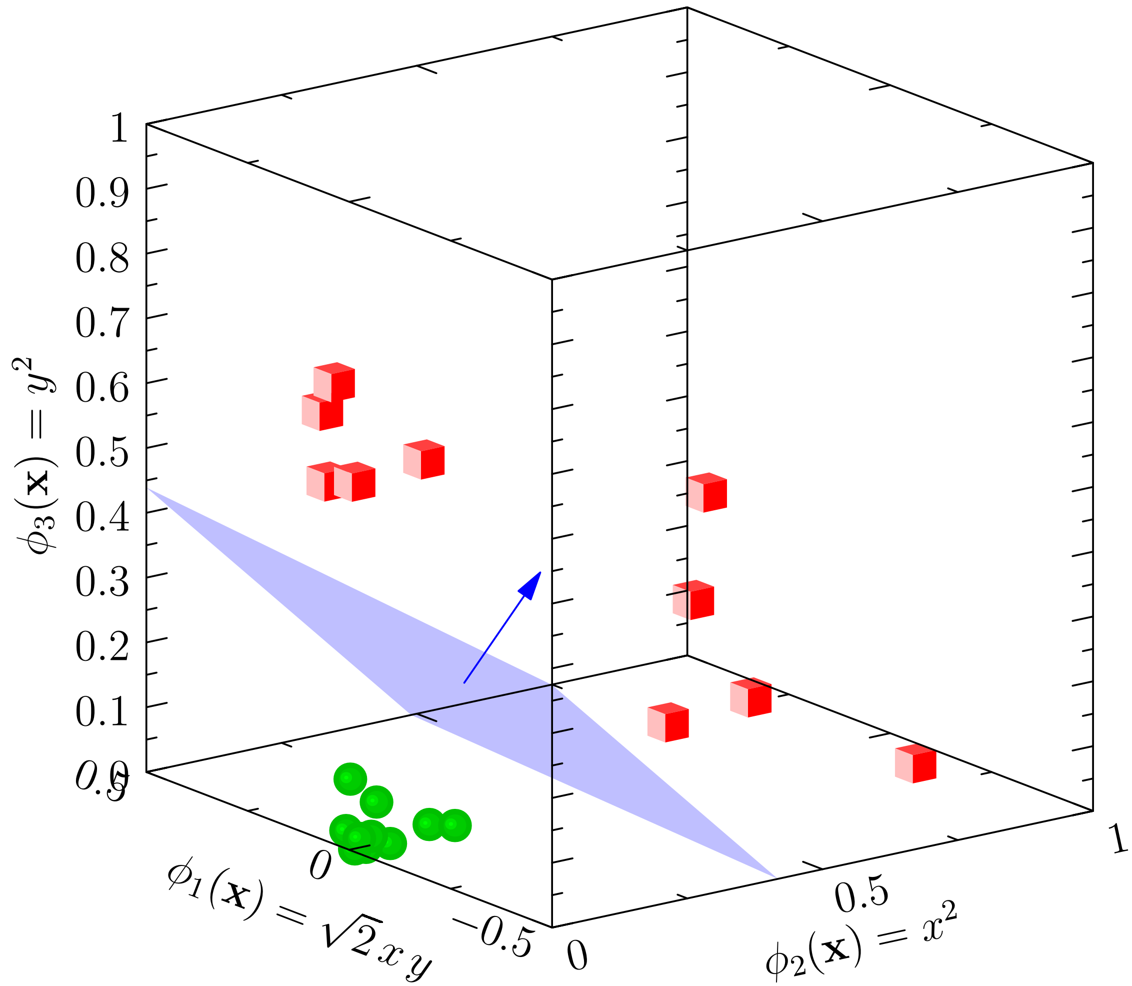
Support Vector Machines



Support Vector Machines, maximum margins

Outline

1. **The Big Picture**
2. Maximum Margins
3. Duality
4. Practice



Support Vector Machines

- Support vector machines, when used right, often have the best generalisation results
- They are typically used on numerical data, but can and have been adapted to text, sequences, etc.
- Although not as trendy as deep learning, they will often be the method of choice on small data sets
- They subtly regularise themselves, choosing a solution that generalises well from a host of different solutions

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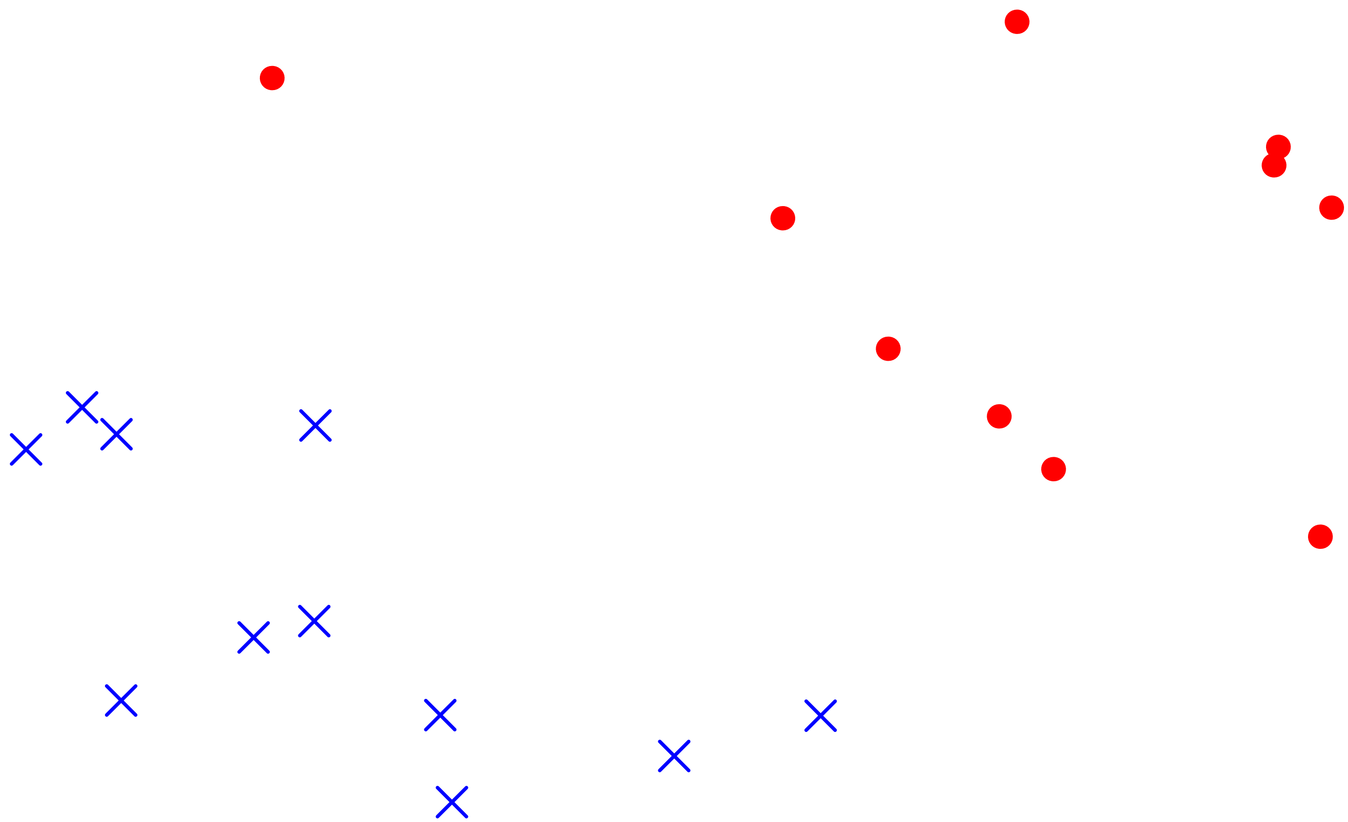
Linear Separation of Data

- SVMs classify linearly separable data



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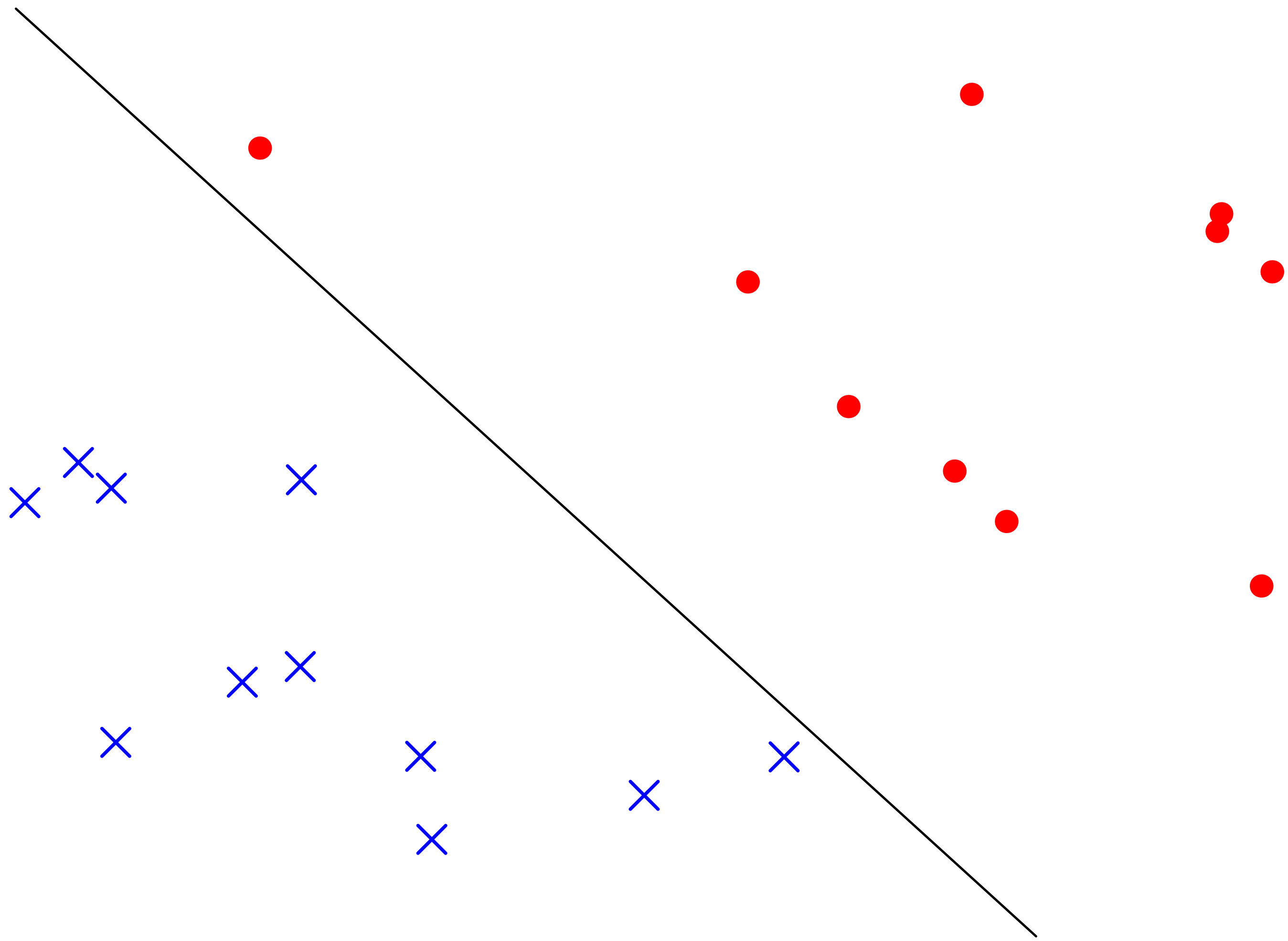

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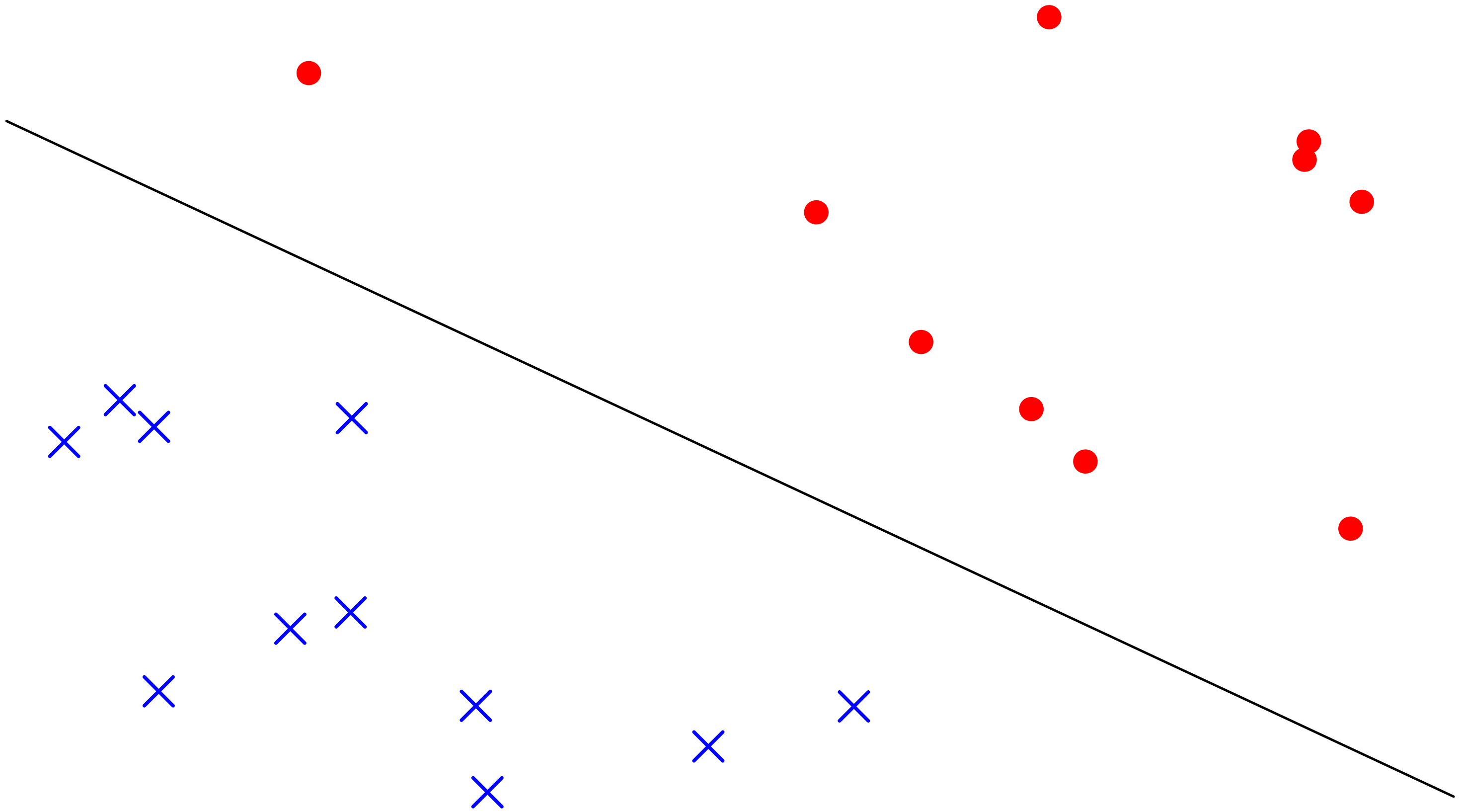

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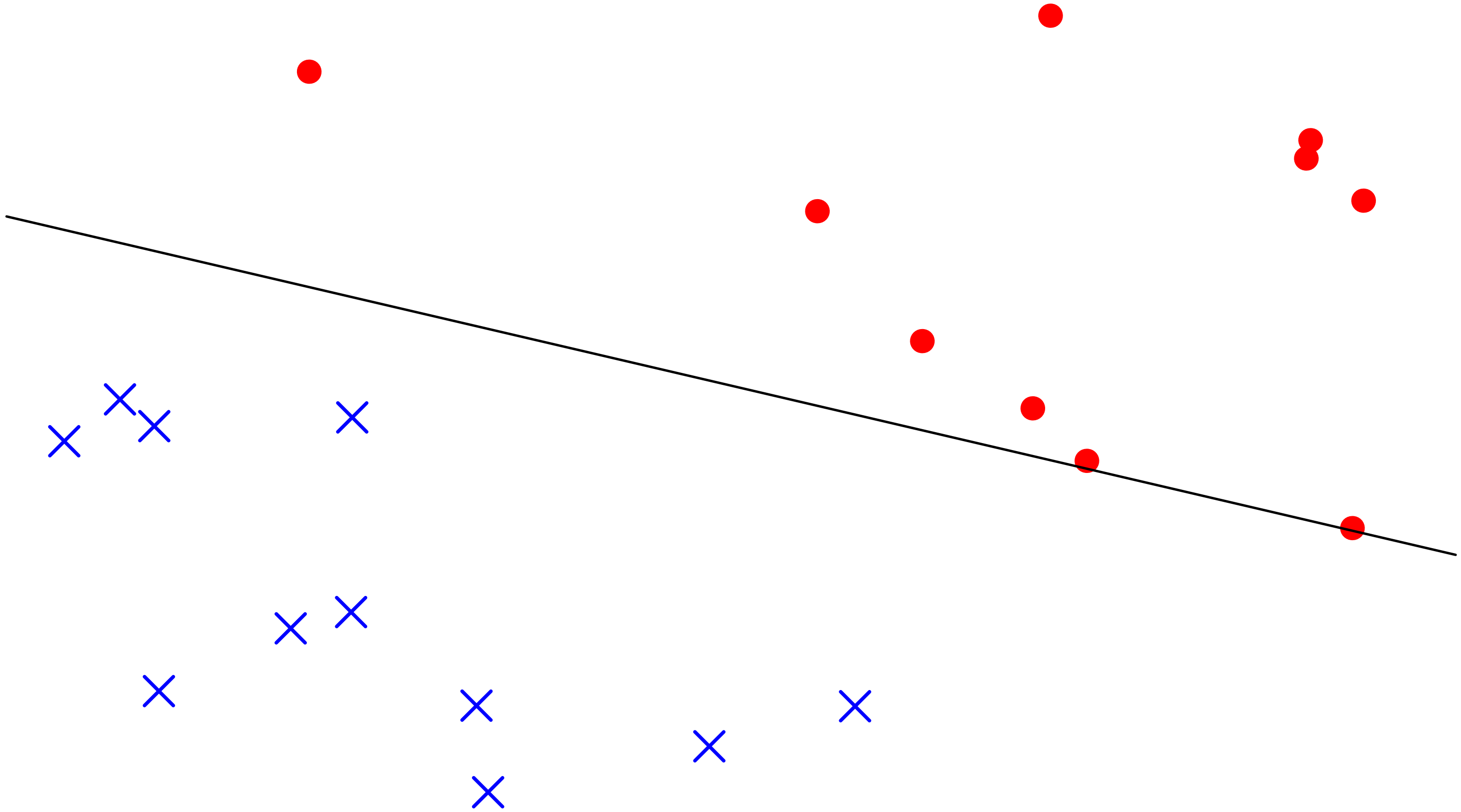

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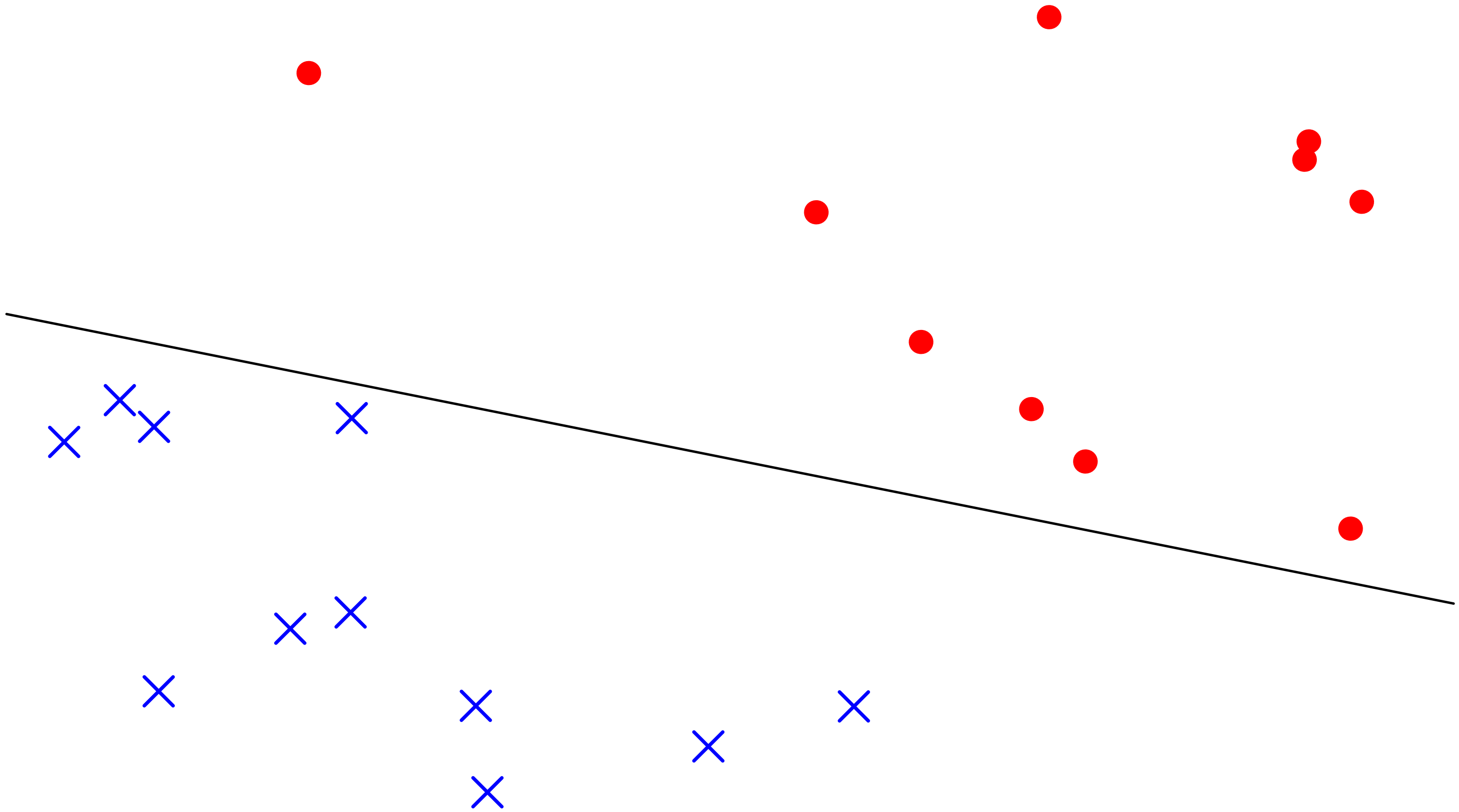

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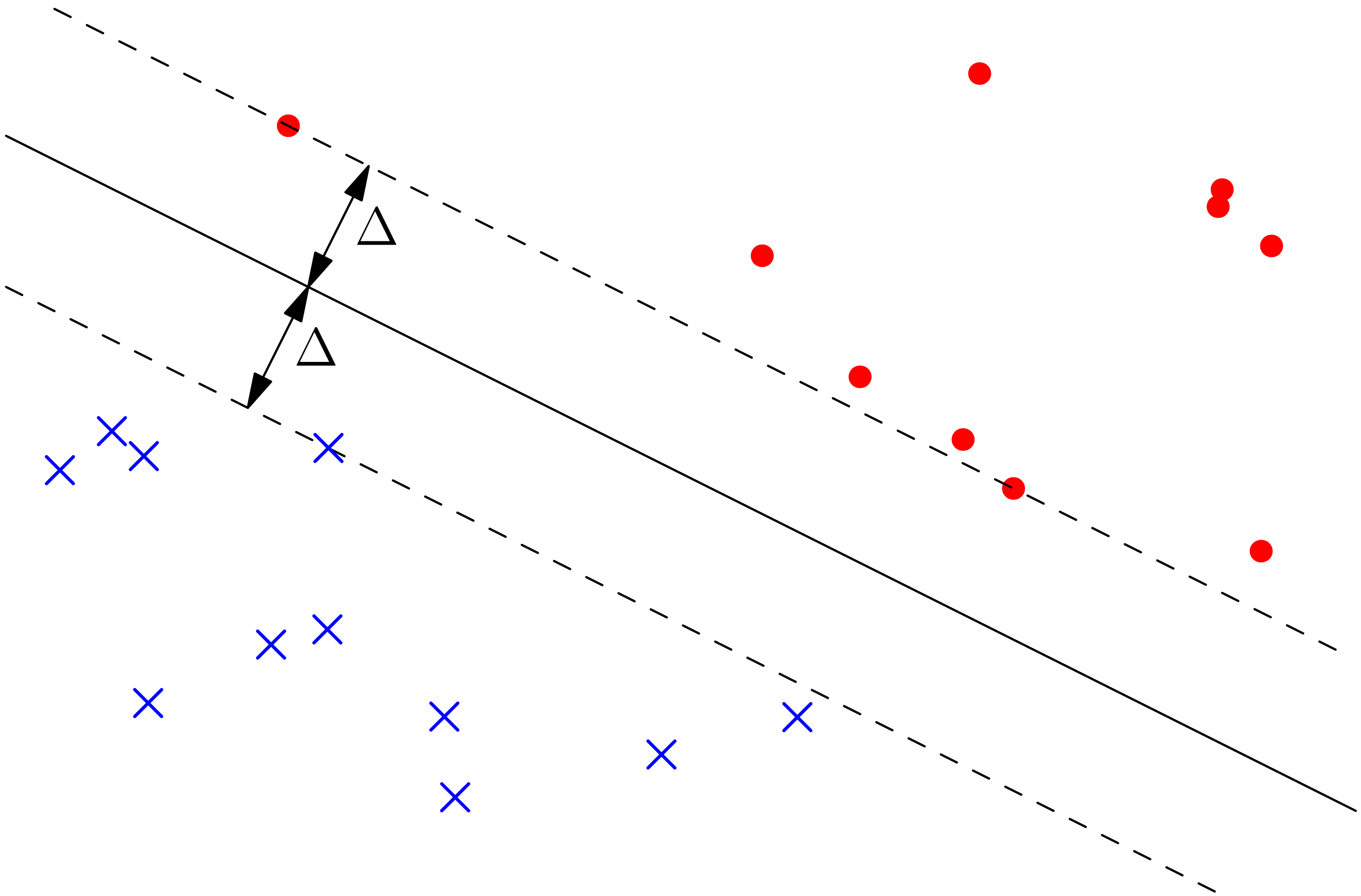

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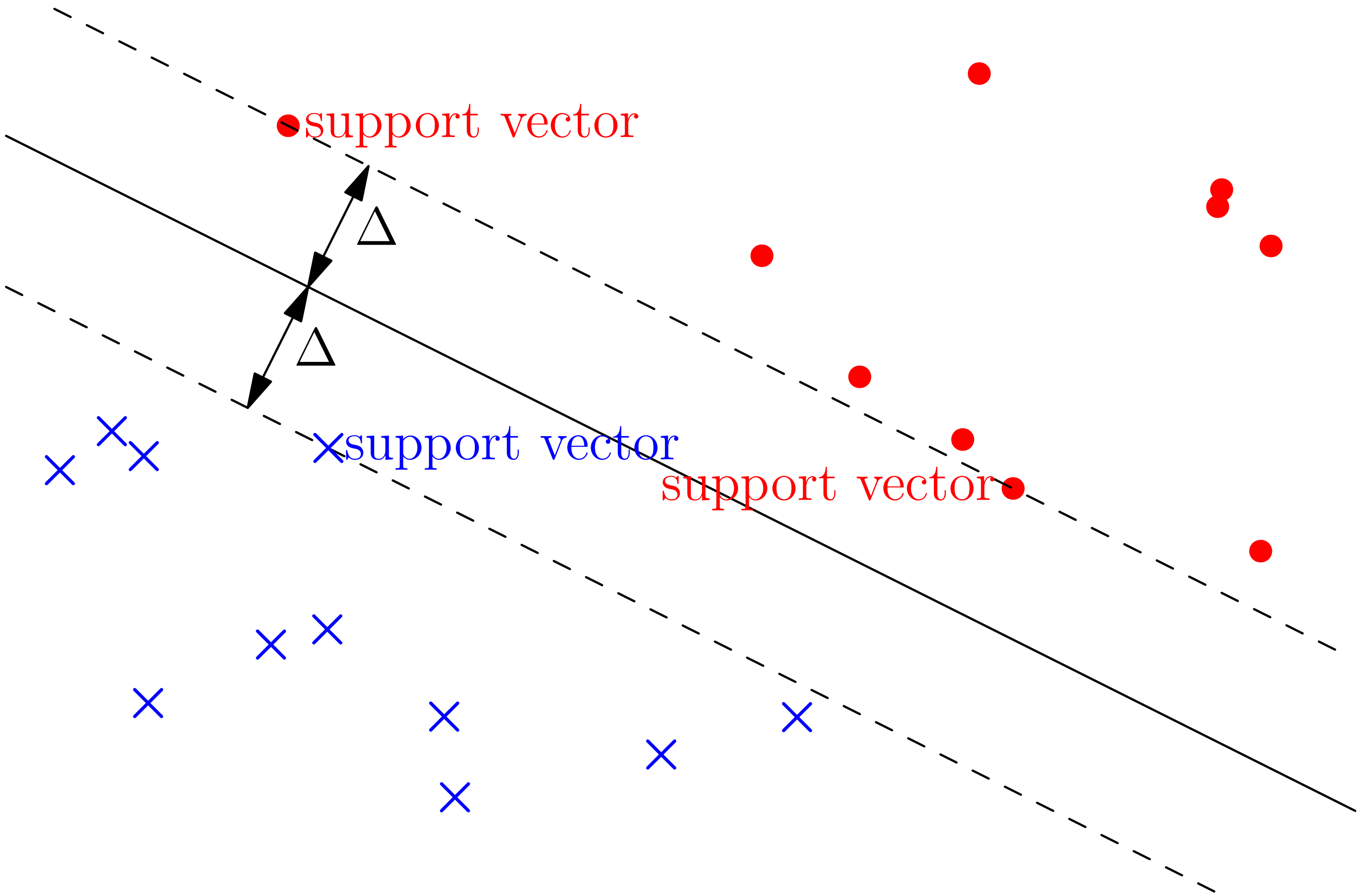

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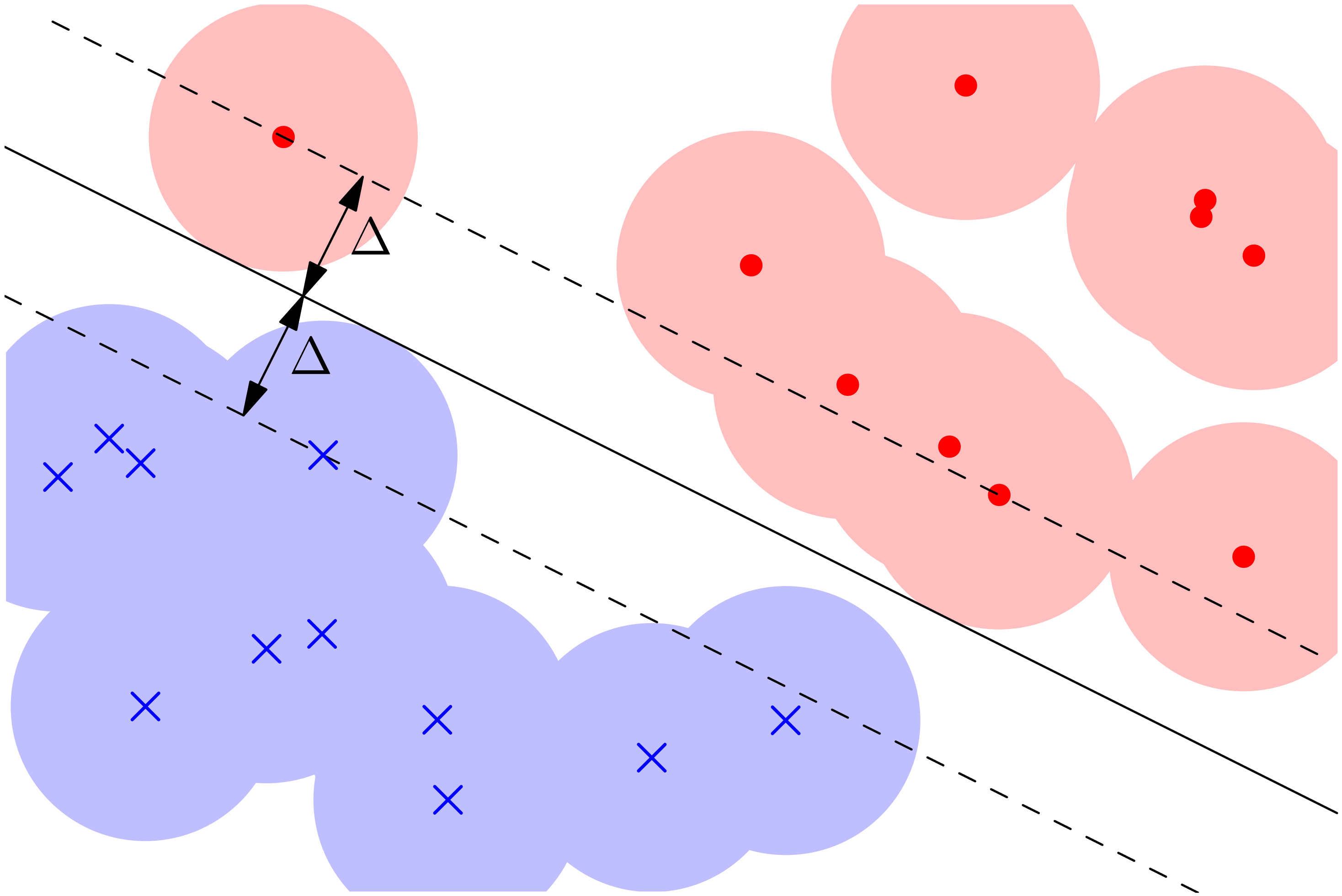

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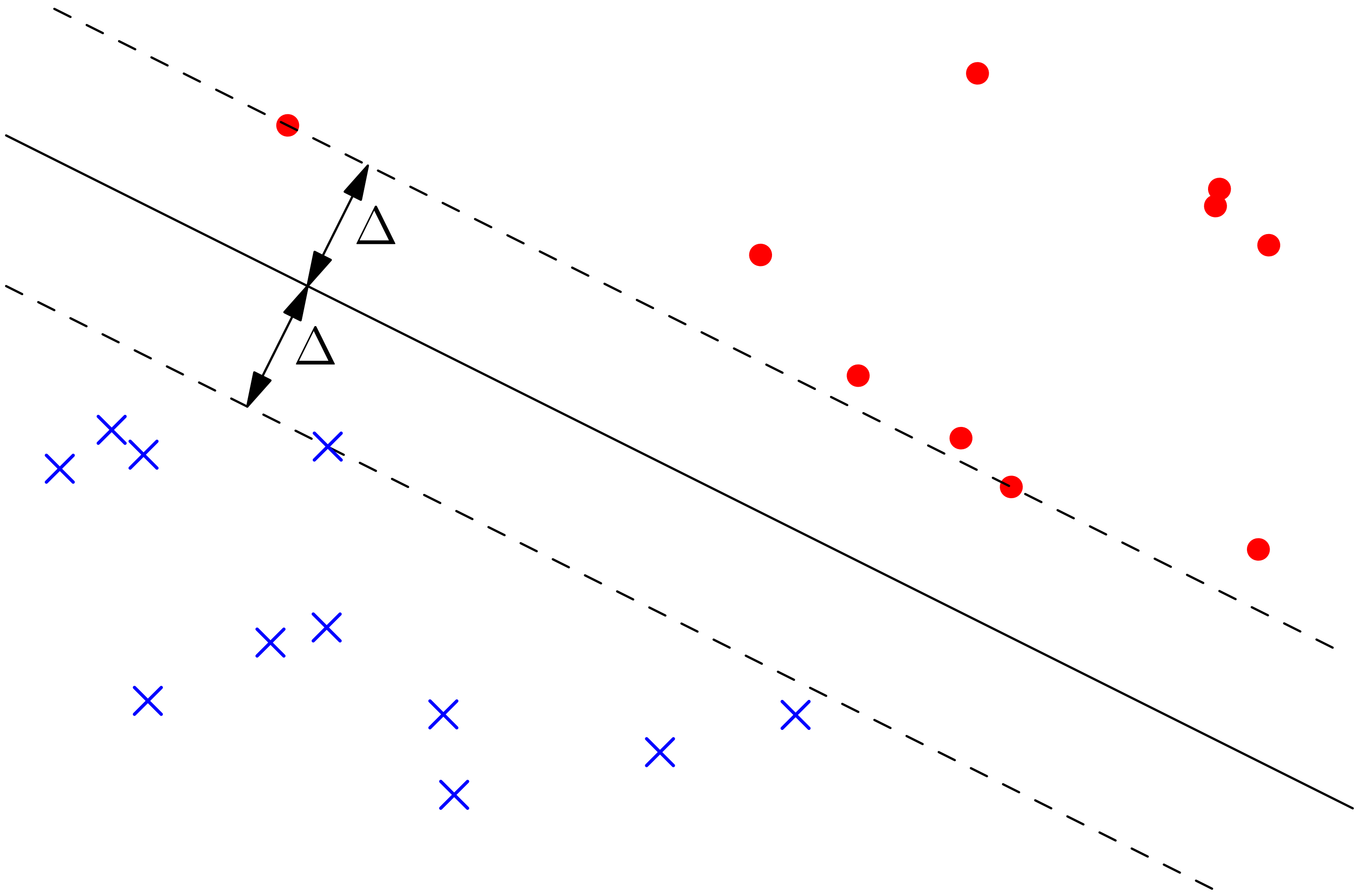

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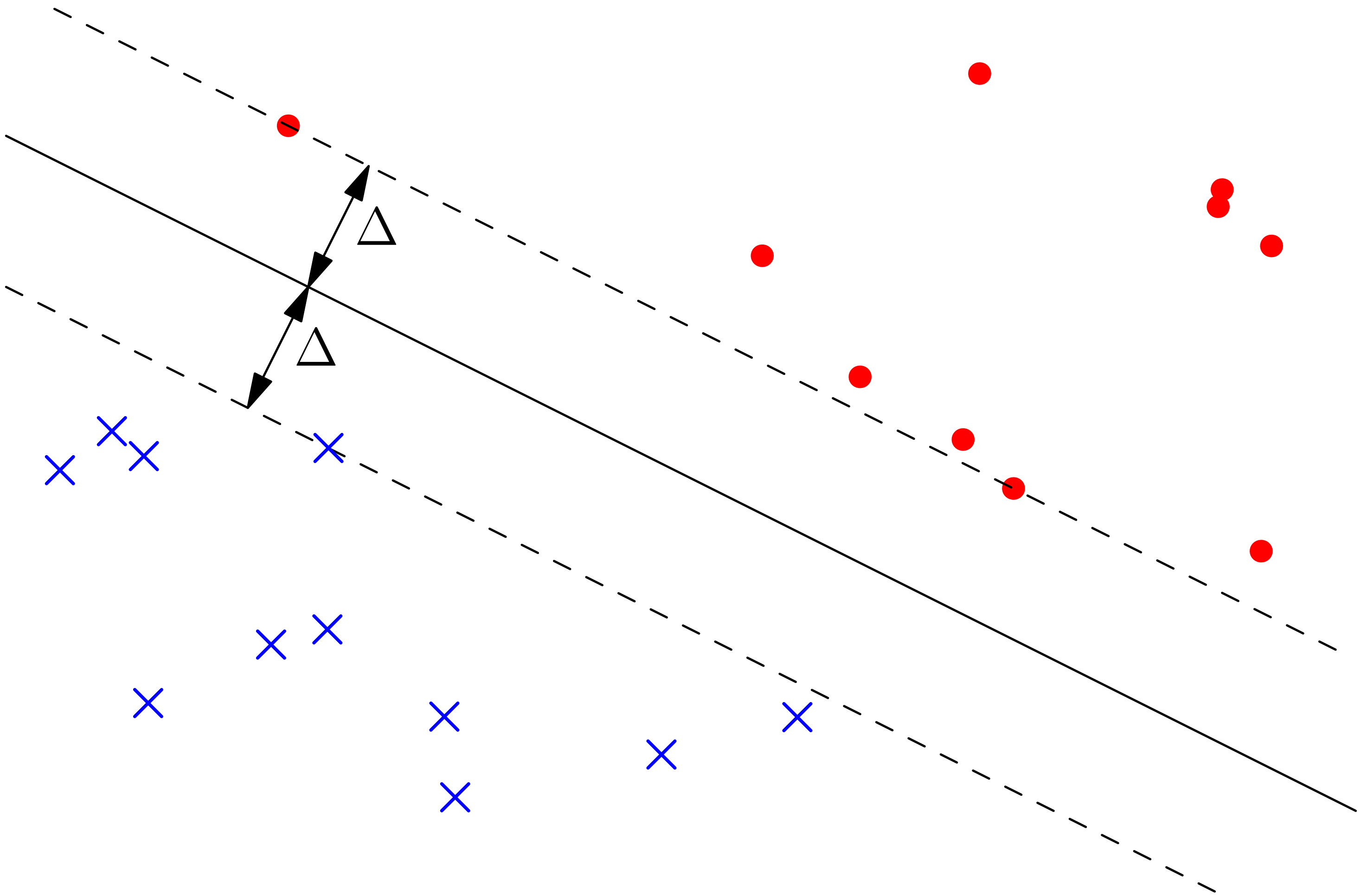

- Finds maximum-margin separating plane

Extended Feature Space

- To increase the likelihood of linear-separability we often use a high-dimensional mapping

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_p)^\mathsf{T} \rightarrow \boldsymbol{\phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \ldots, \phi_r(\boldsymbol{x}))^\mathsf{T}$$

  $r \gg p$

- Finding the maximum margin hyper-plane is time consuming in "primal" form if r is large

- We can work in the "dual" space of patterns, then we only need to compute inner-products

$$\langle \boldsymbol{\phi}(\boldsymbol{x}_i), \boldsymbol{\phi}(\boldsymbol{x}_j) \rangle = \boldsymbol{\phi}(\boldsymbol{x}_i)^\mathsf{T} \boldsymbol{\phi}(\boldsymbol{x}_j)$$

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Kernel Trick

- If we choose a **positive semi-definite** kernel function $K(\boldsymbol{x}, \boldsymbol{y})$ then there exists functions $\boldsymbol{\phi}(\boldsymbol{x}) = (\phi_k(\boldsymbol{x}) | k = 1, 2, \ldots, r)$, such that

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \langle \boldsymbol{\phi}(\boldsymbol{x}_i), \boldsymbol{\phi}(\boldsymbol{x}_j) \rangle$$

  (like an eigenvector decomposition of a matrix)

- Never need to compute $\phi_k(\boldsymbol{x}_i)$ explicitly as we only need the inner-product $\langle \boldsymbol{\phi}(\boldsymbol{x}_i), \boldsymbol{\phi}(\boldsymbol{x}_j) \rangle = K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ to compute maximum margin separating hyper-plane

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Kernel Functions

- Kernel functions are symmetric functions of two variable
- Strong restriction: *positive semi-definite*
- Examples

$$\text{Quadratic kernel:} \qquad K(\boldsymbol{x}_1, \boldsymbol{x}_2) = \left(\boldsymbol{x}_1^{\mathsf{T}} \boldsymbol{x}_2\right)^2$$

$$\text{Gaussian (RBF) kernel:} \qquad K(\boldsymbol{x}_1, \boldsymbol{x}_2) = \mathrm{e}^{-\gamma \|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}$$

- Consider the mapping

$$\boldsymbol{x}_i = \begin{pmatrix} x_i \\ y_i \end{pmatrix} \rightarrow \boldsymbol{\phi}(\boldsymbol{x}_i) = \begin{pmatrix} x_i^2 \\ y_i^2 \\ \sqrt{2} x_i y_i \end{pmatrix}$$

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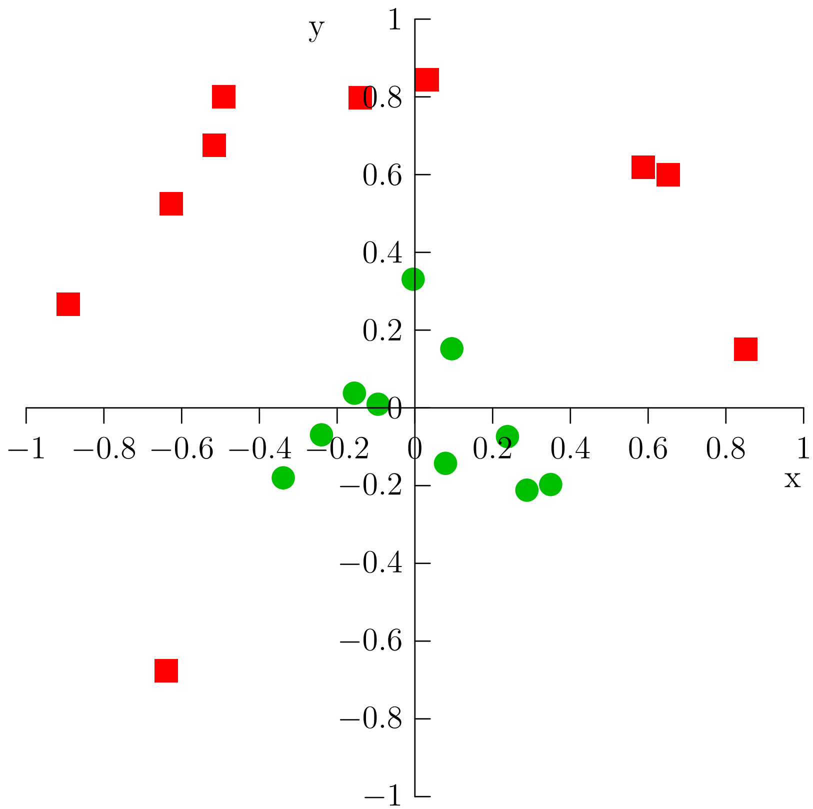

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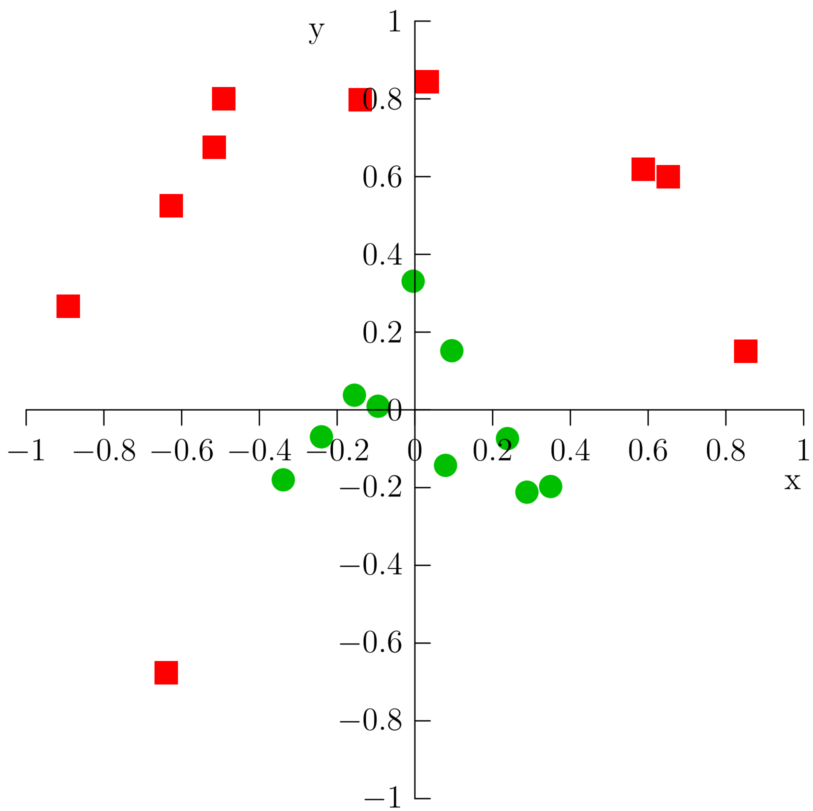

$\boldsymbol{x} \rightarrow \boldsymbol{\phi}(\boldsymbol{x})$

$\longrightarrow$

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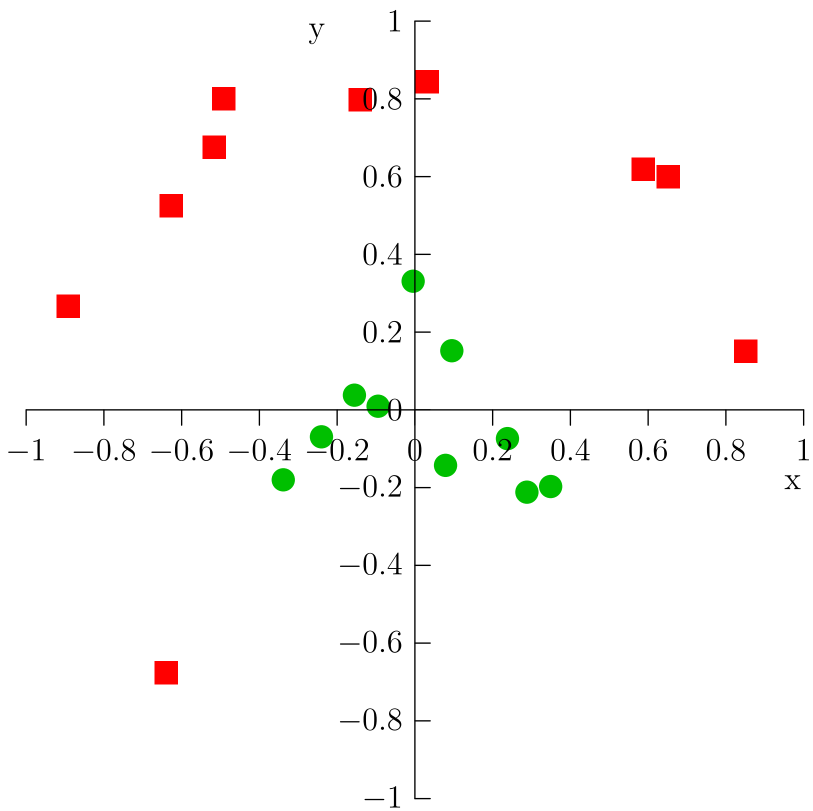
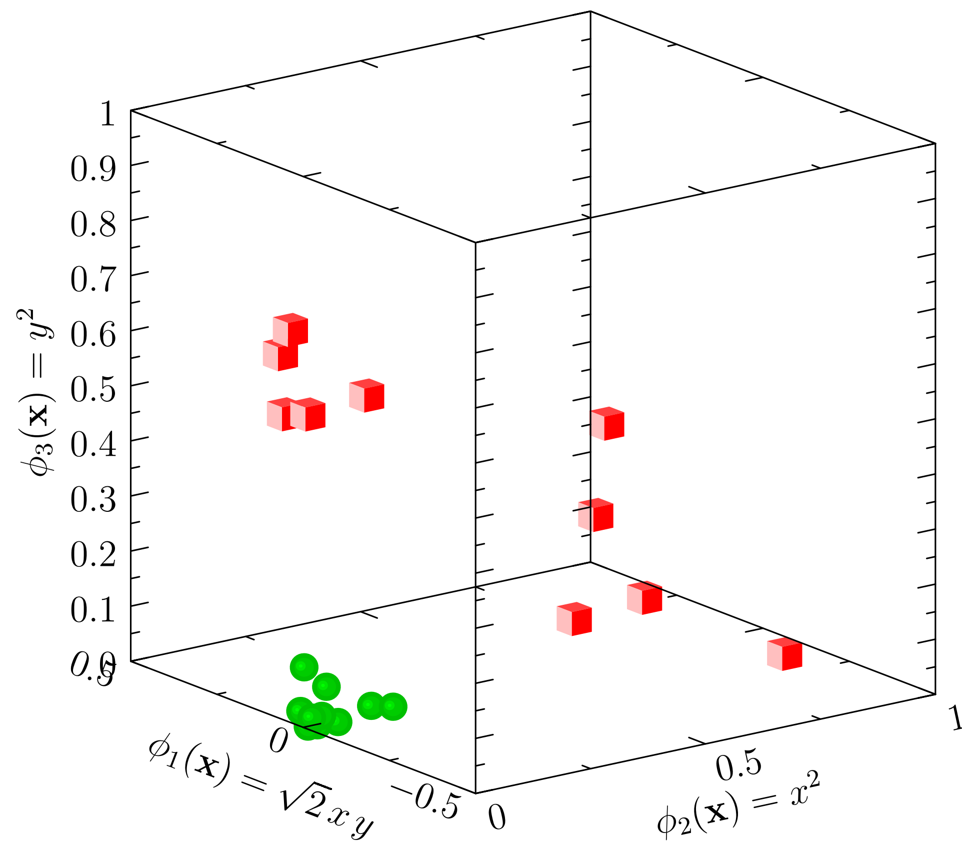


$$\xrightarrow{\boldsymbol{x} \to \boldsymbol{\phi}(\boldsymbol{x})}$$



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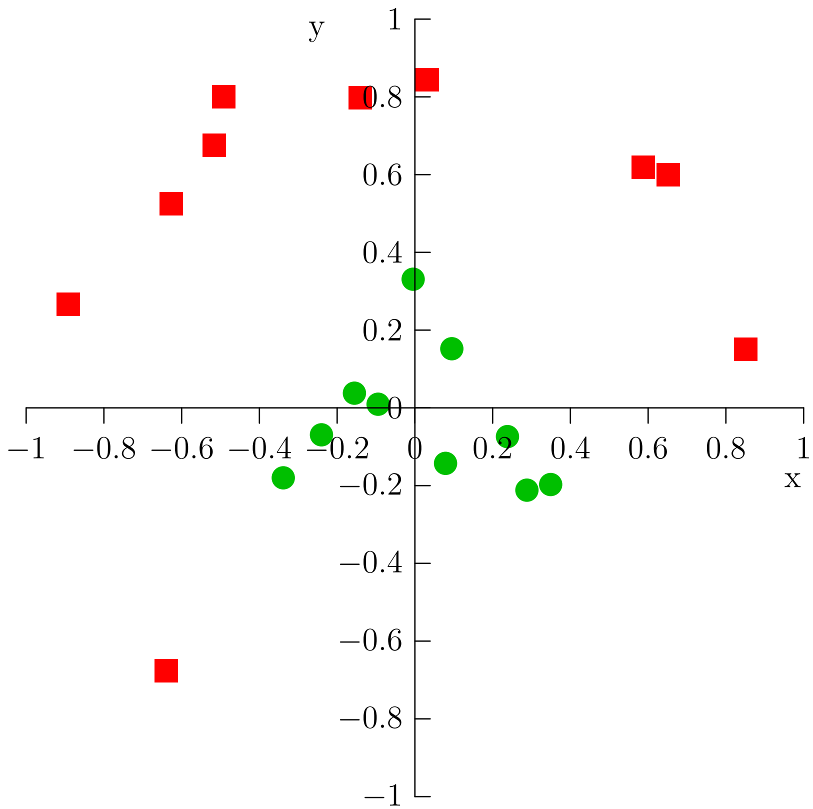

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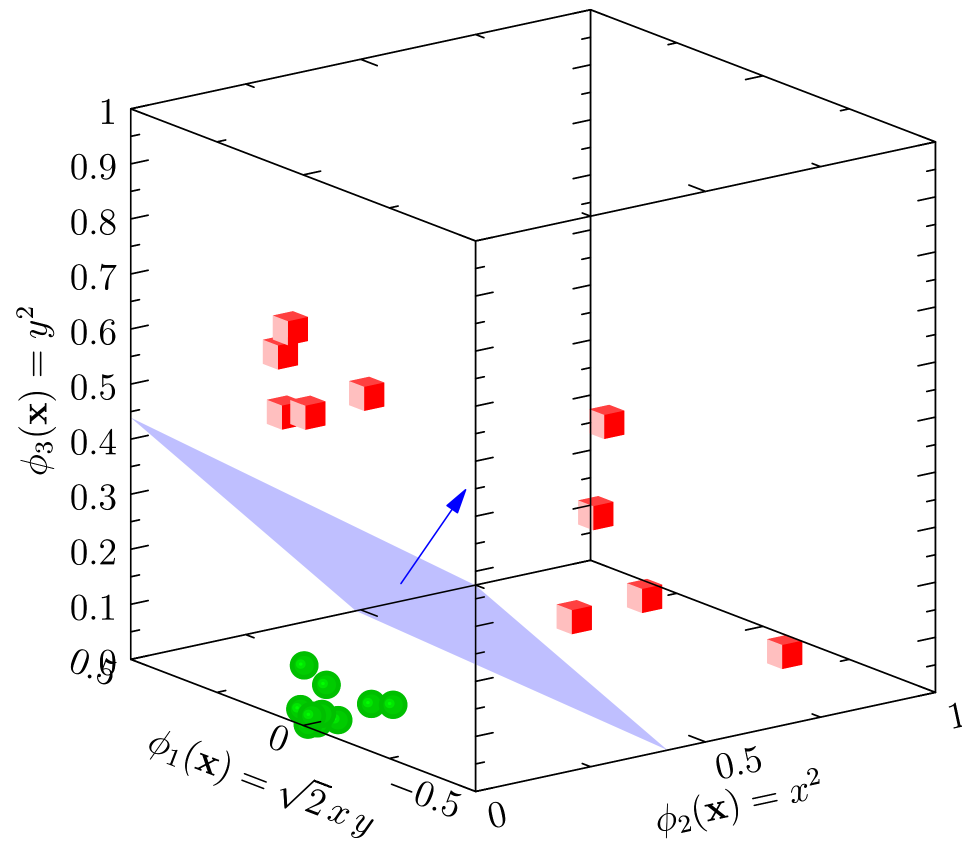

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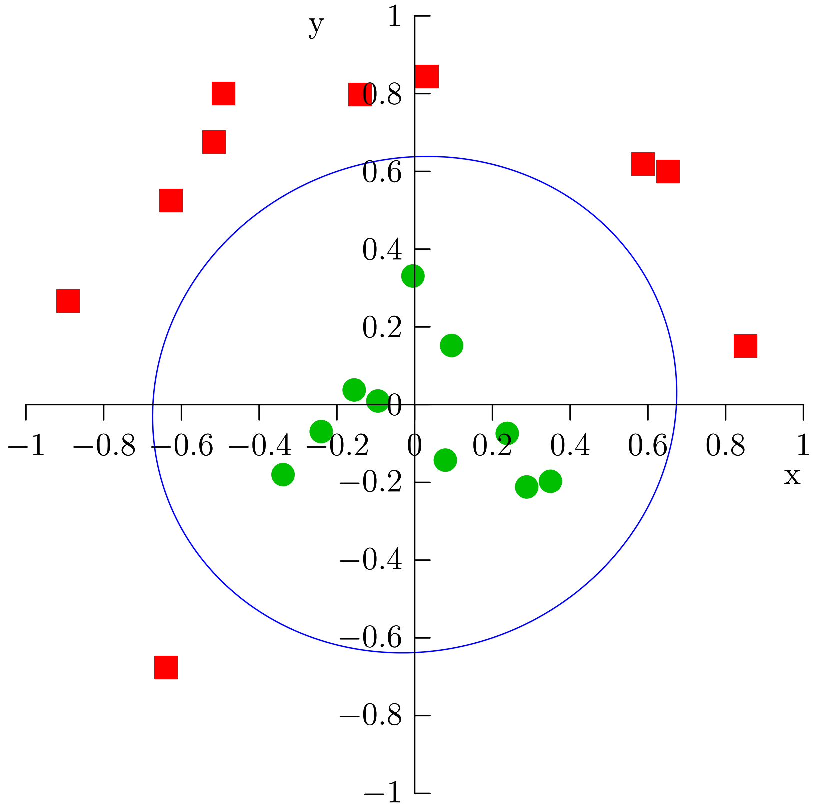

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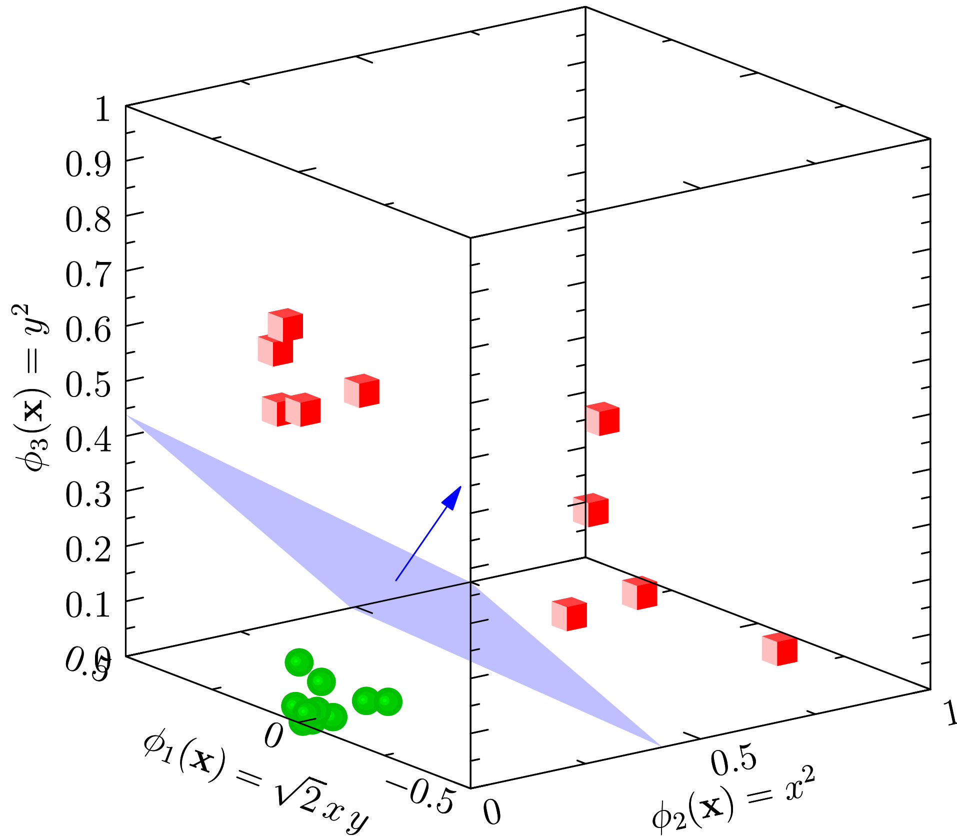

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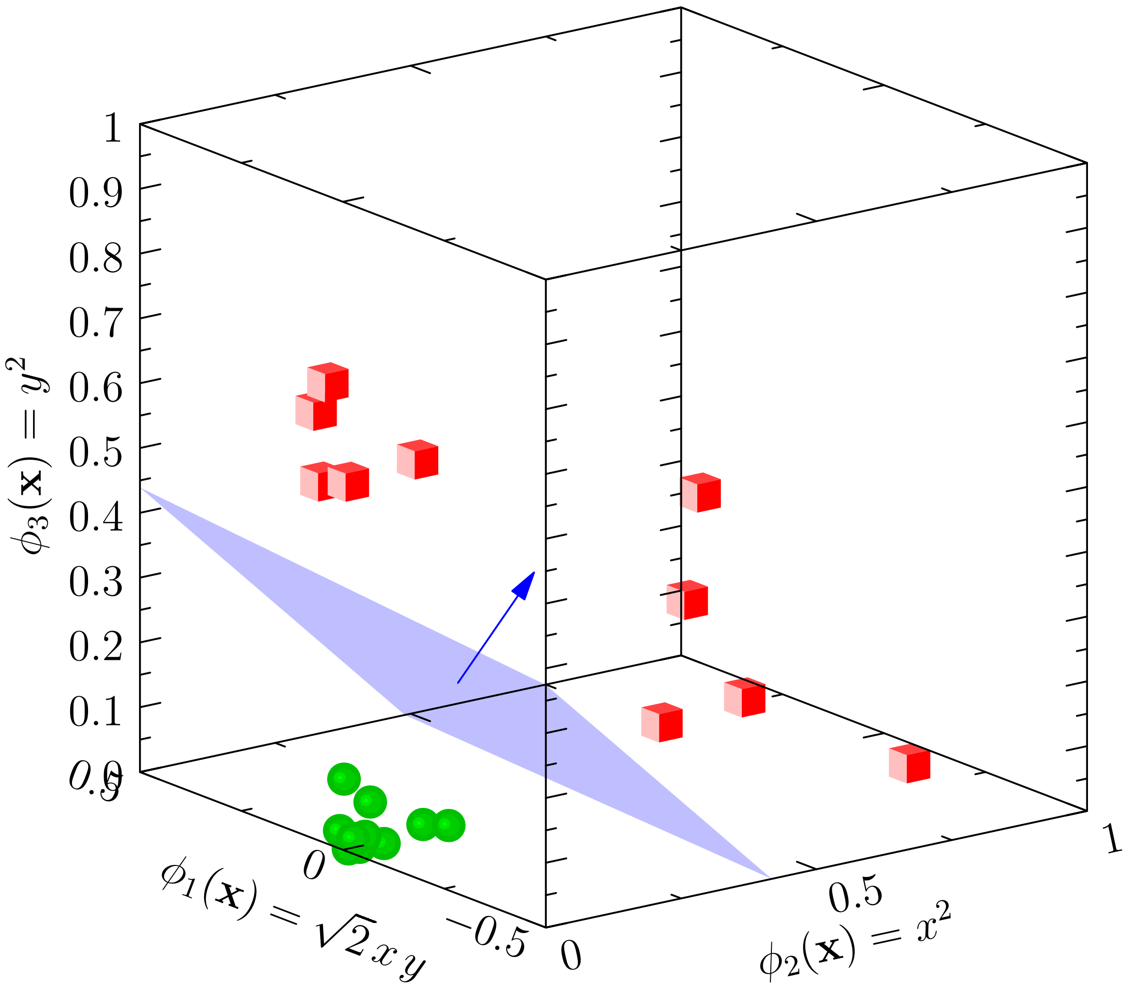
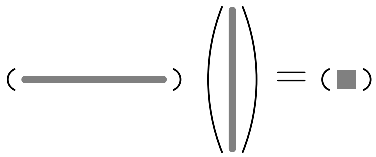


Inner Product

- Recall the inner or dot product in $\mathbb{R}^n$



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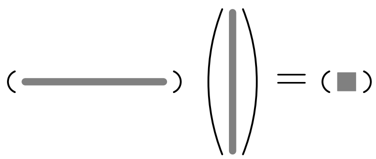

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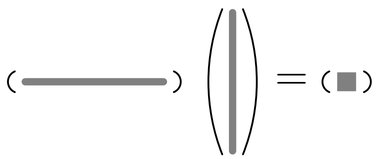

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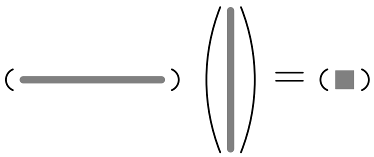

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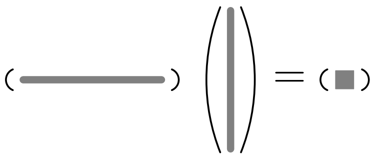

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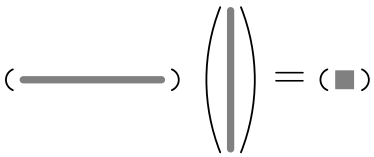

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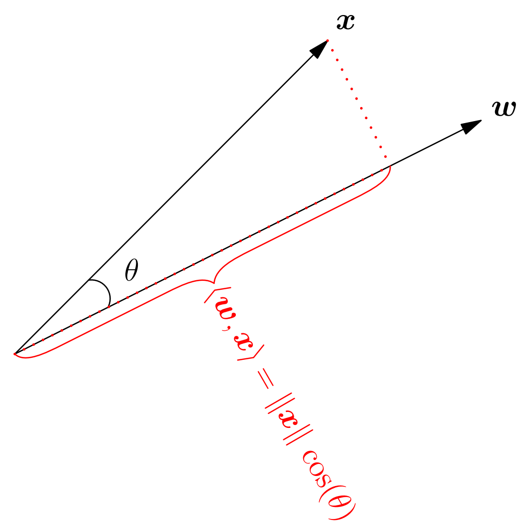

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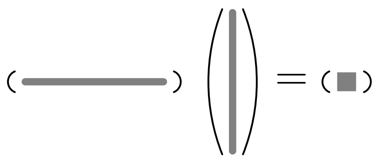

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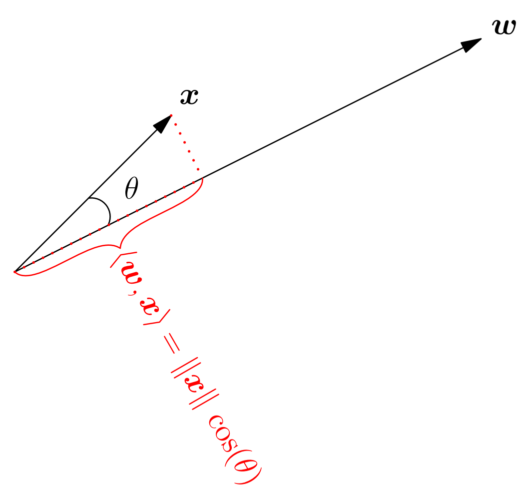

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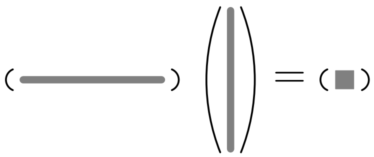

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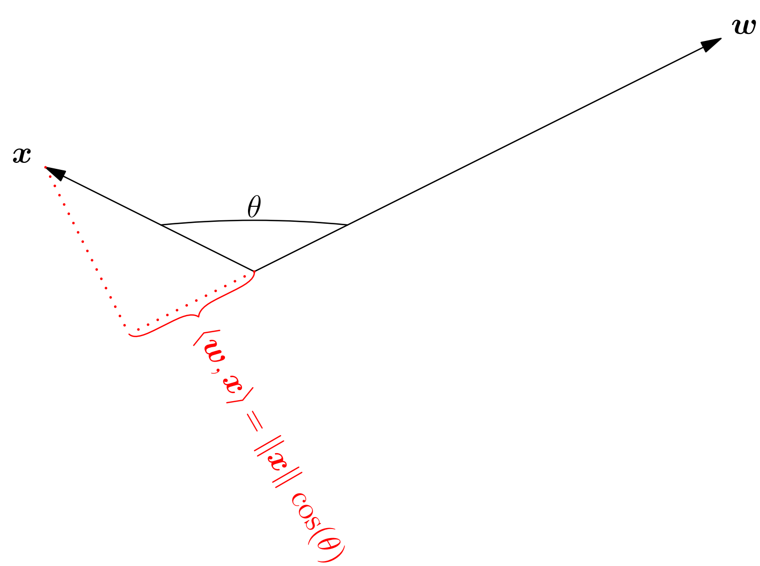

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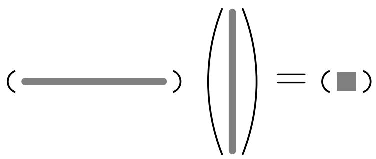

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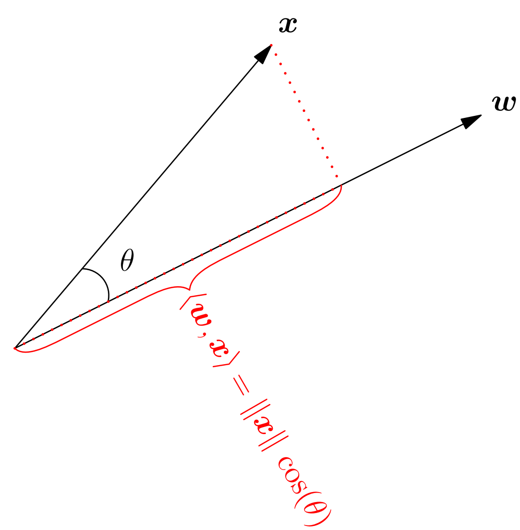

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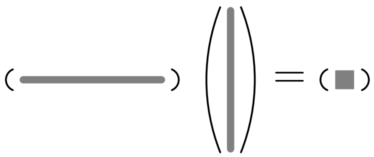

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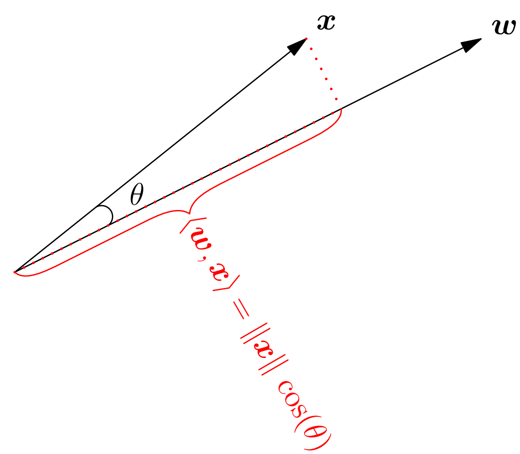

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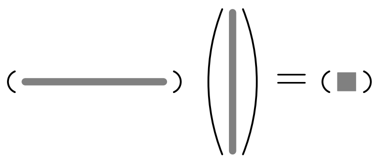

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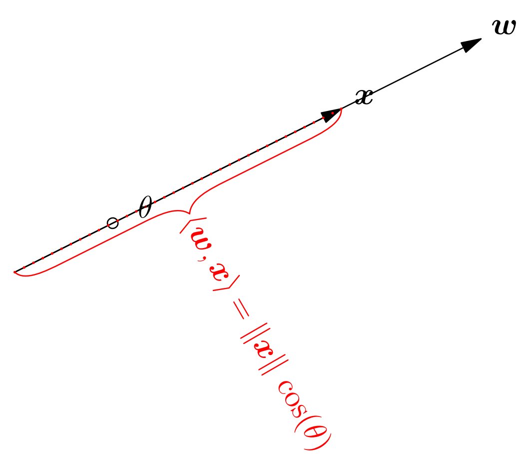

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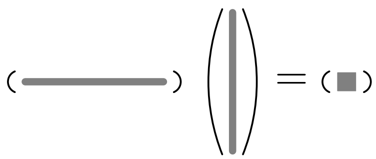

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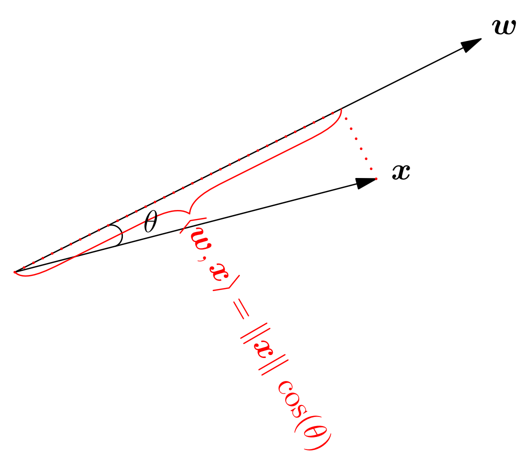

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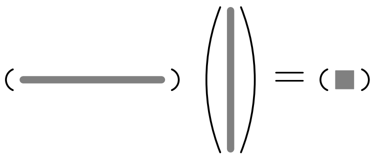

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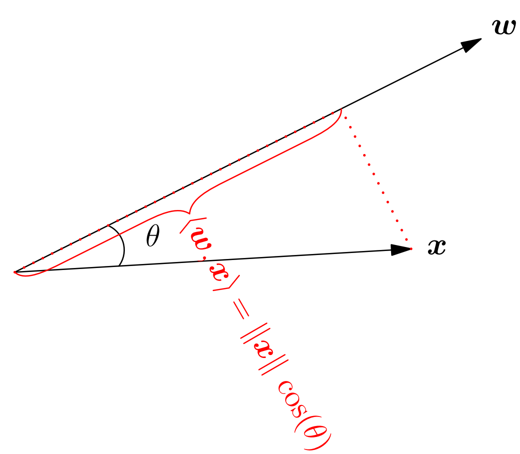

Maximise Margin

- Consider a linearly separable set of data
  - $\mathcal{D} = \{(\boldsymbol{x}_k, y_k)\}_{k=1}^{m}$
  - $y_k \in \{-1,1\}$
- Our task is to find a separating plane defined by the orthogonal vector $\boldsymbol{w}$ and a threshold b such that

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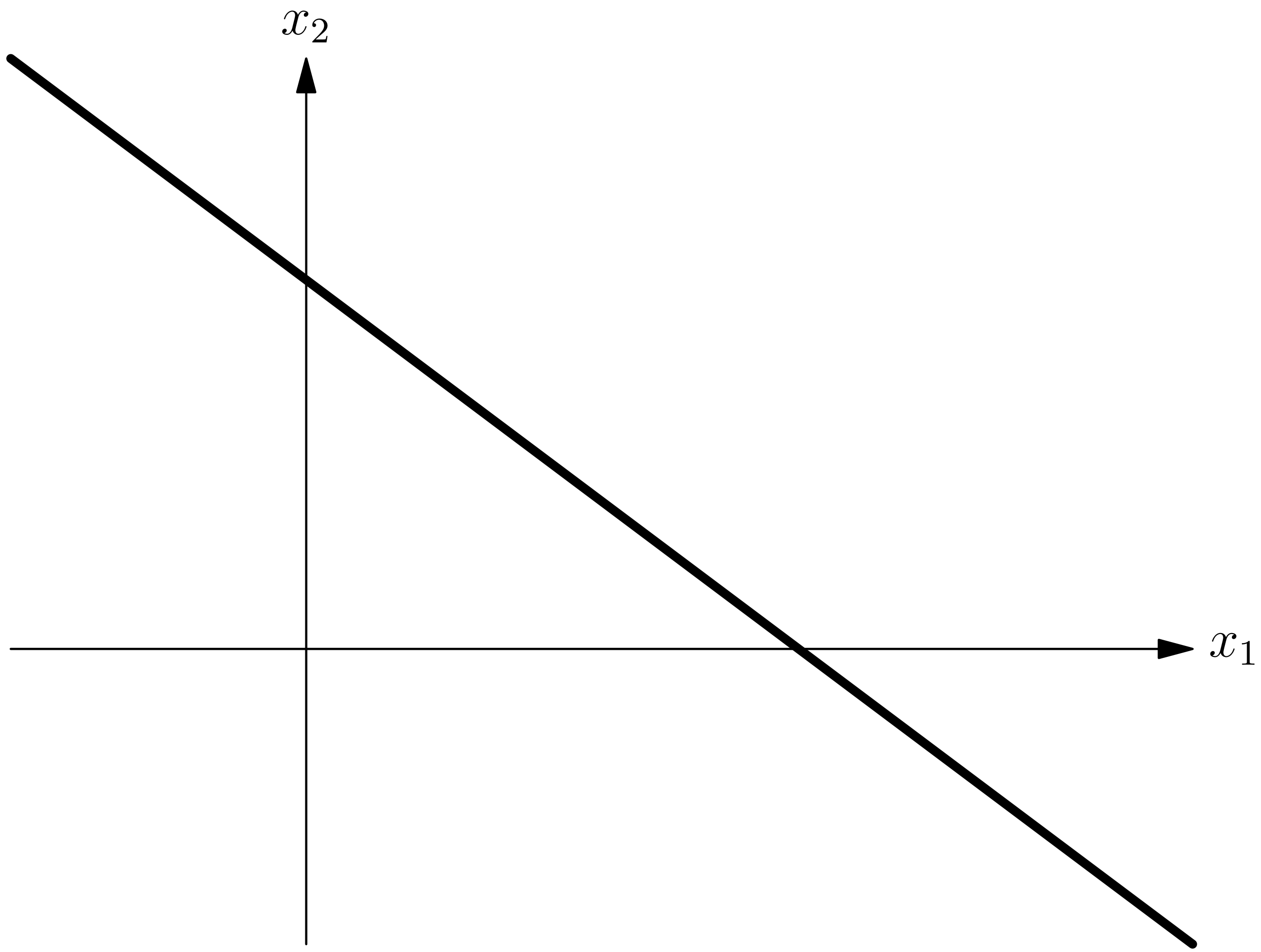

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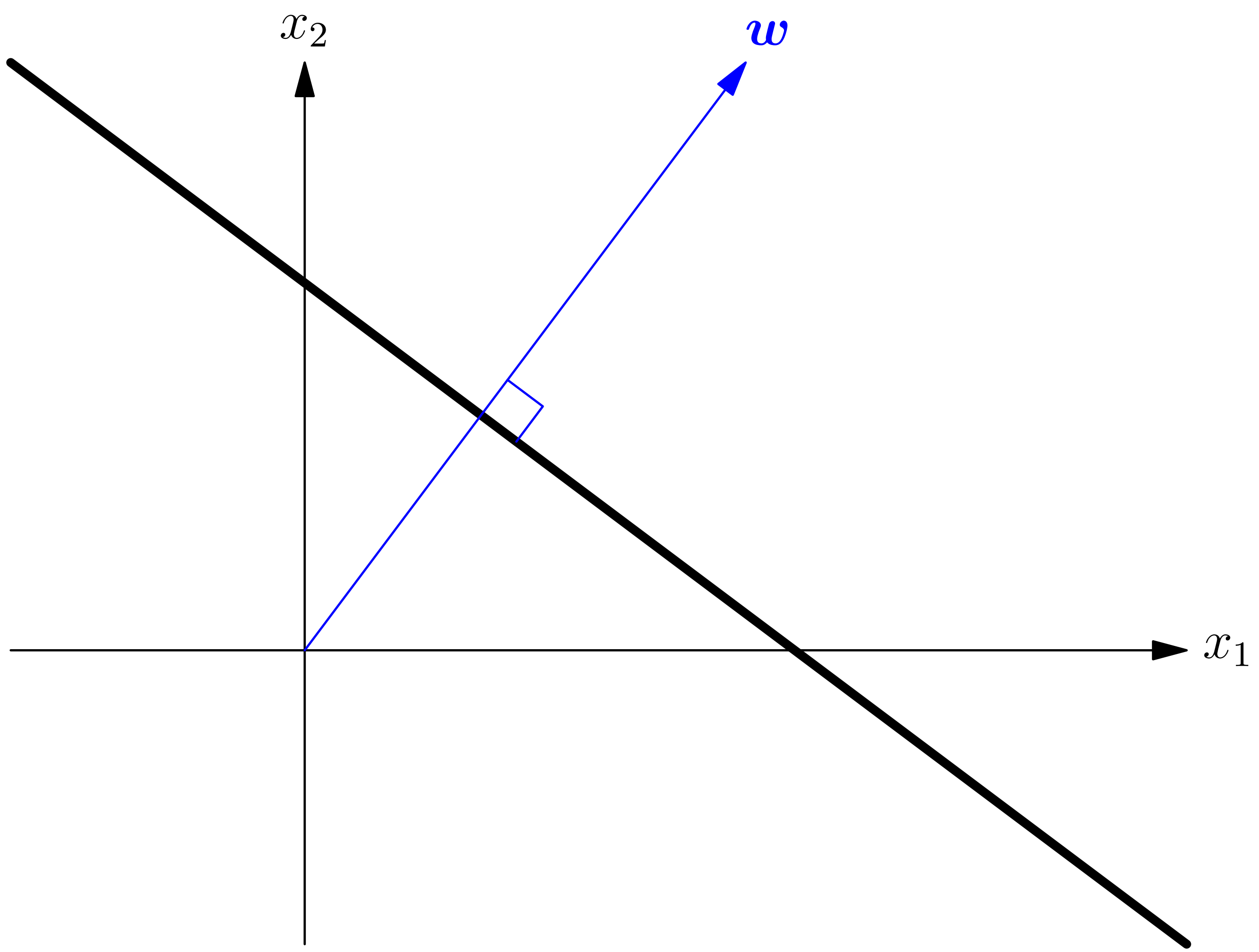

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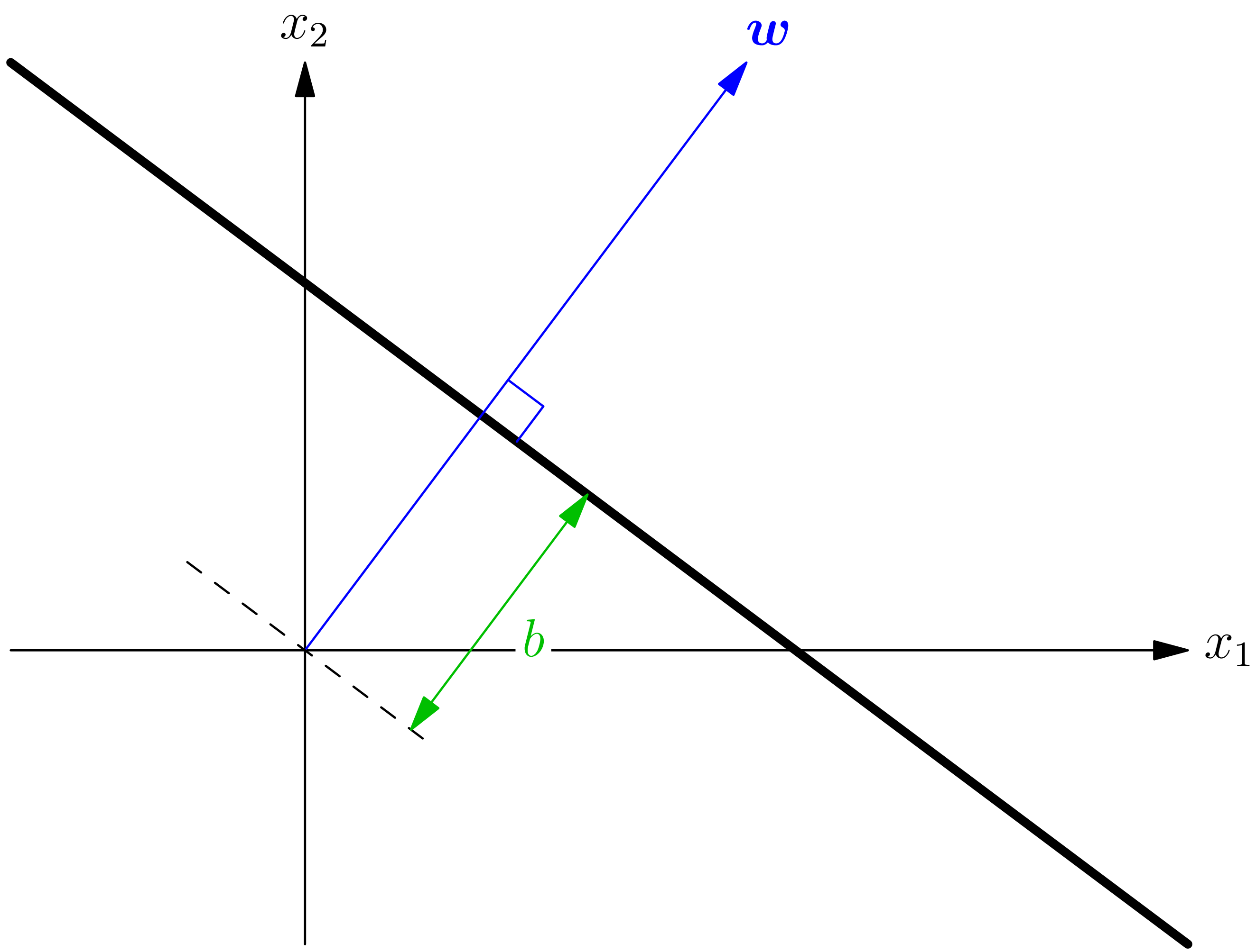

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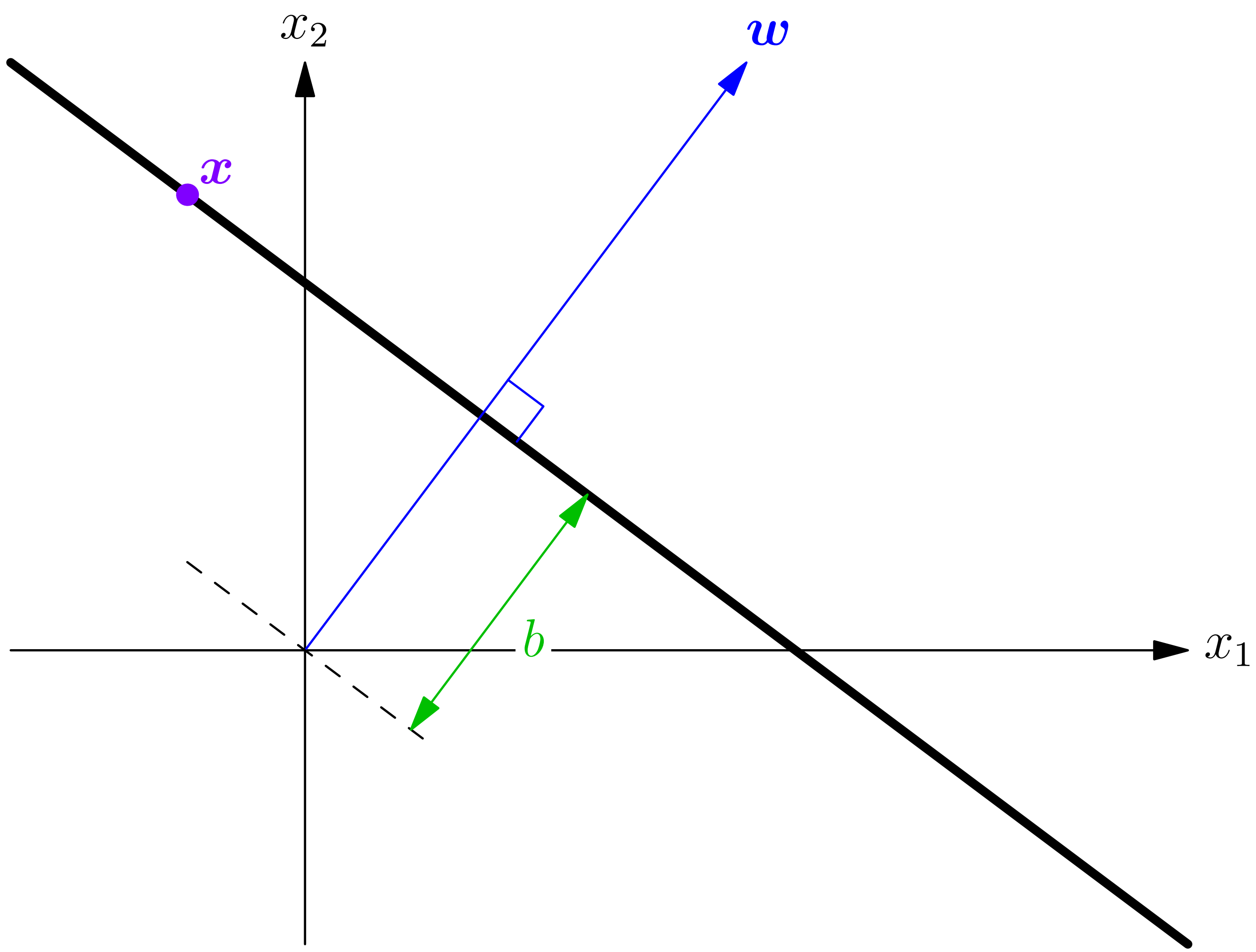

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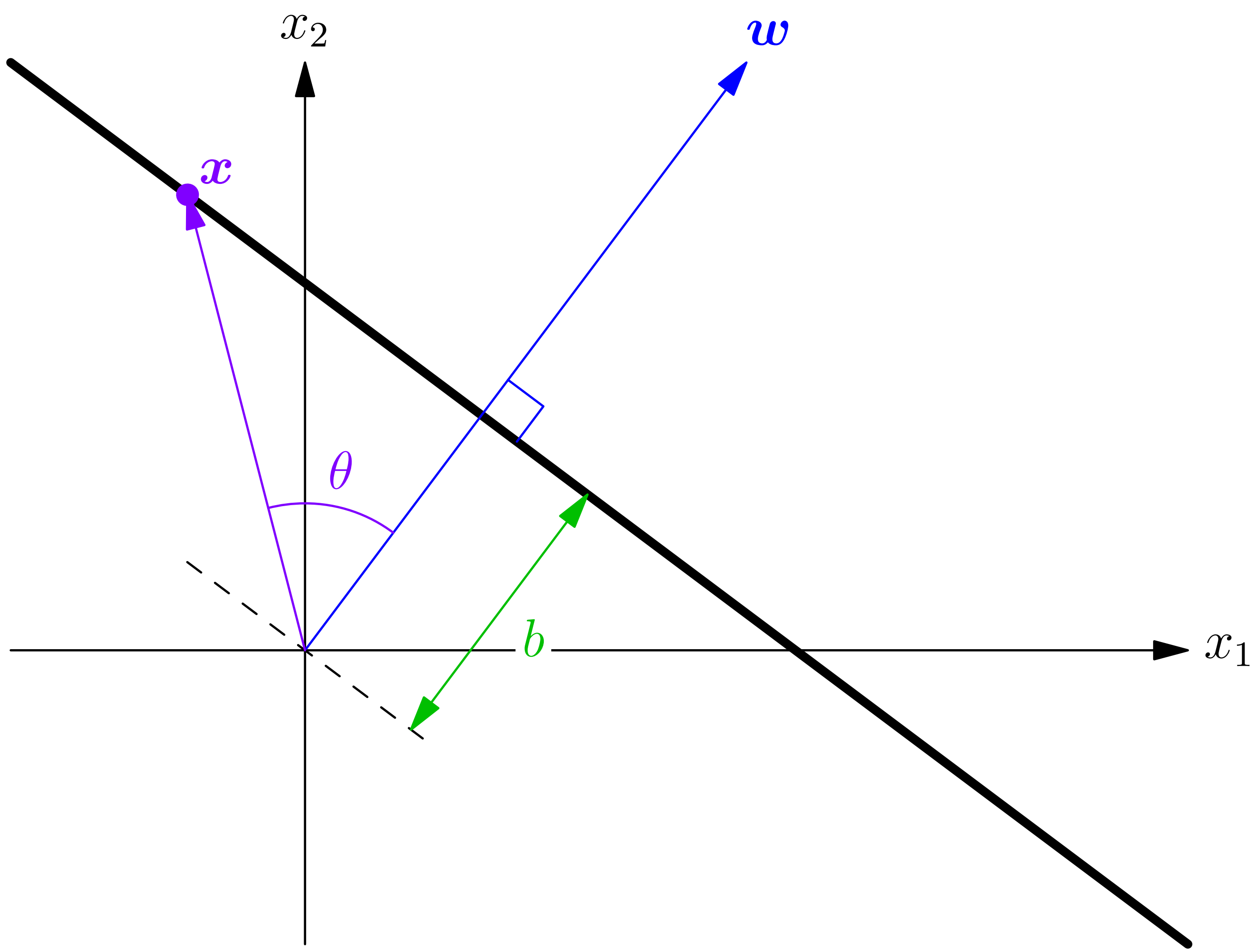

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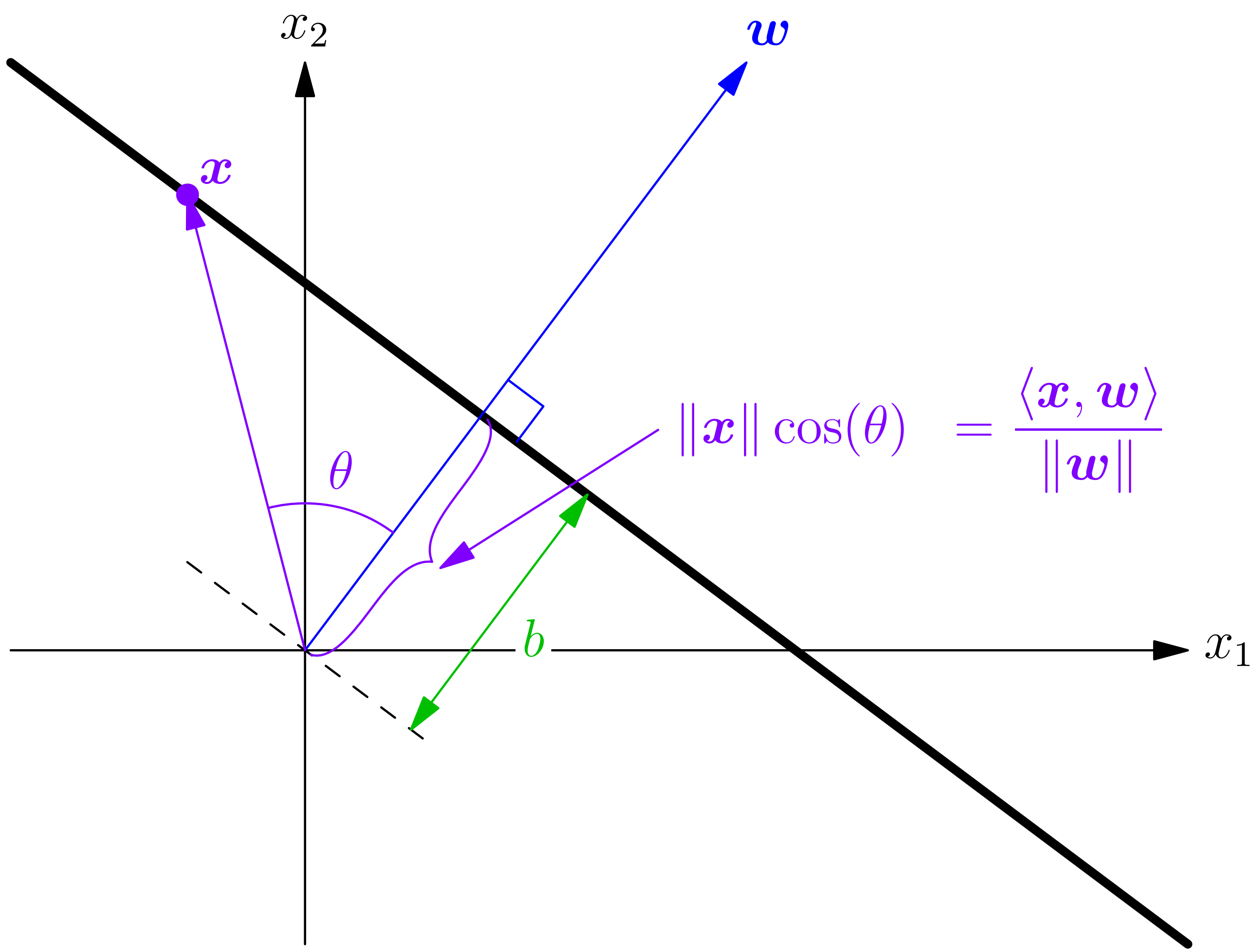

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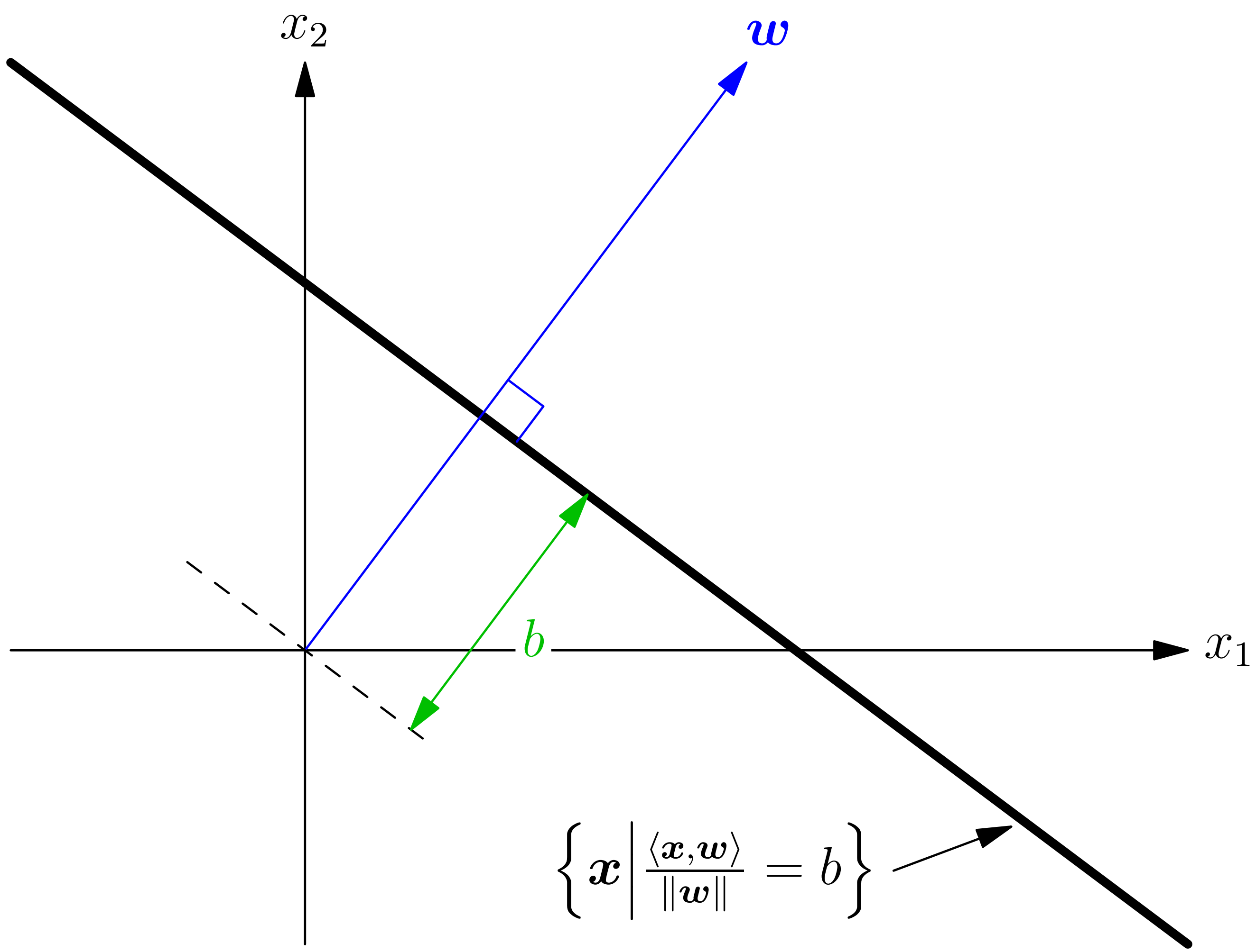

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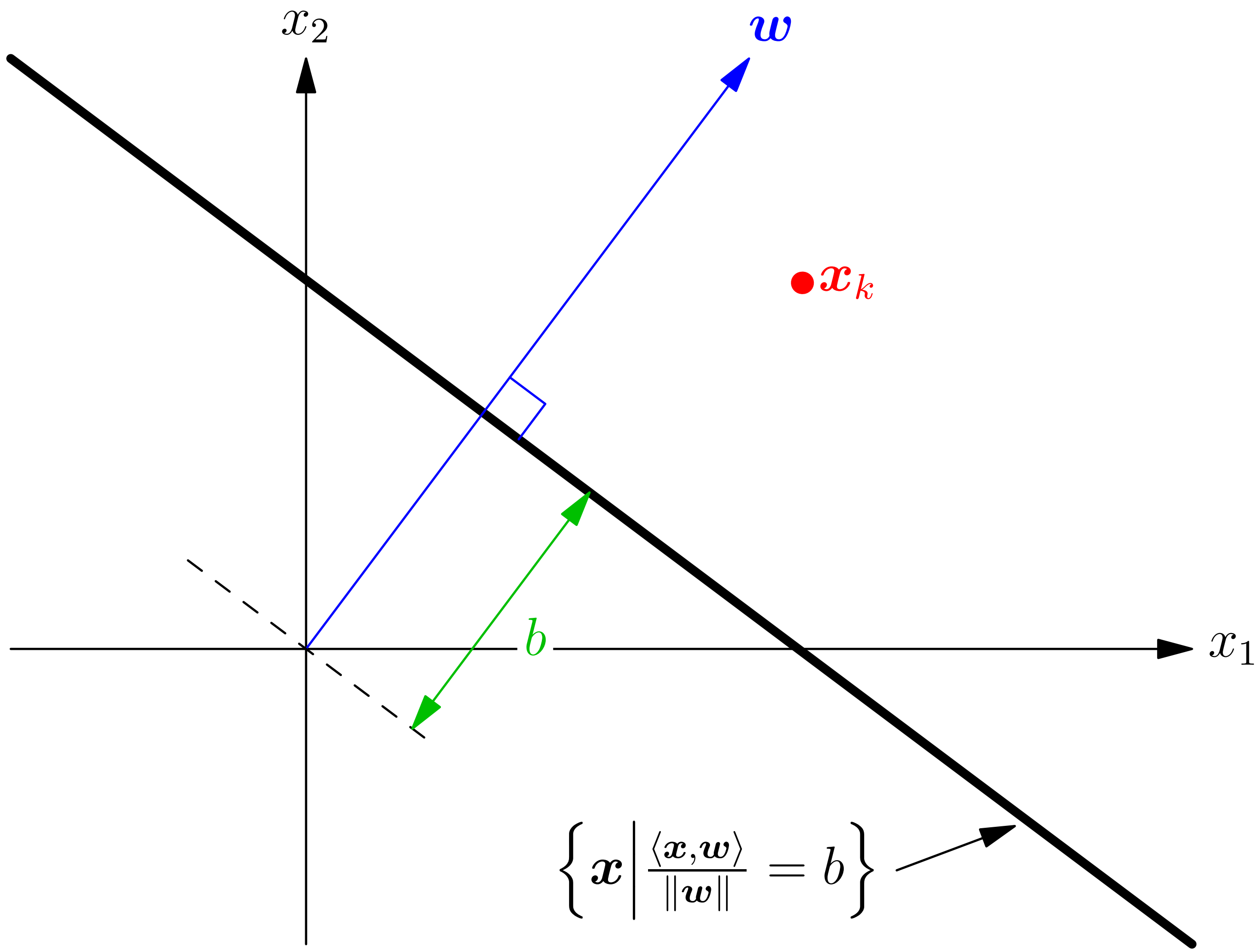

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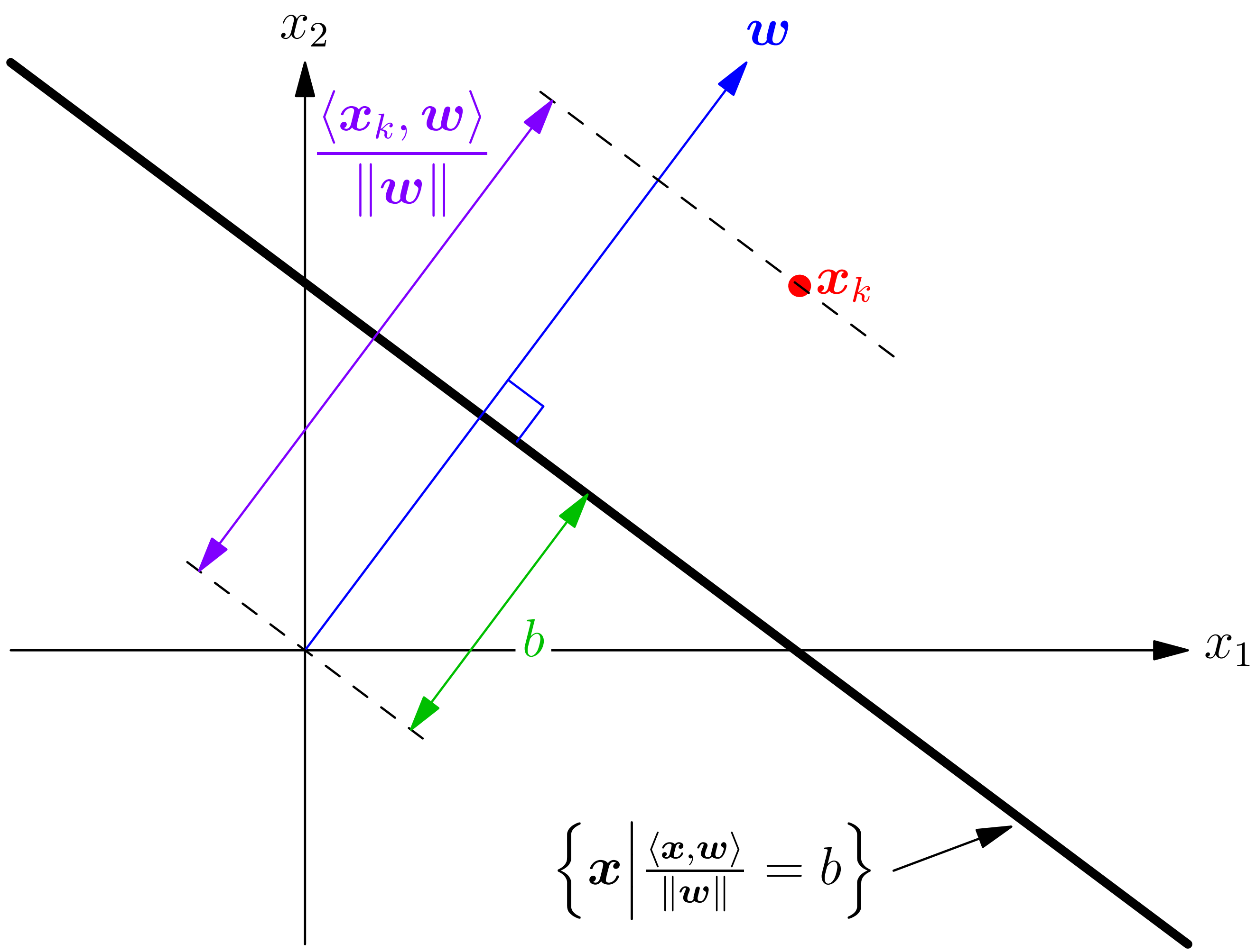

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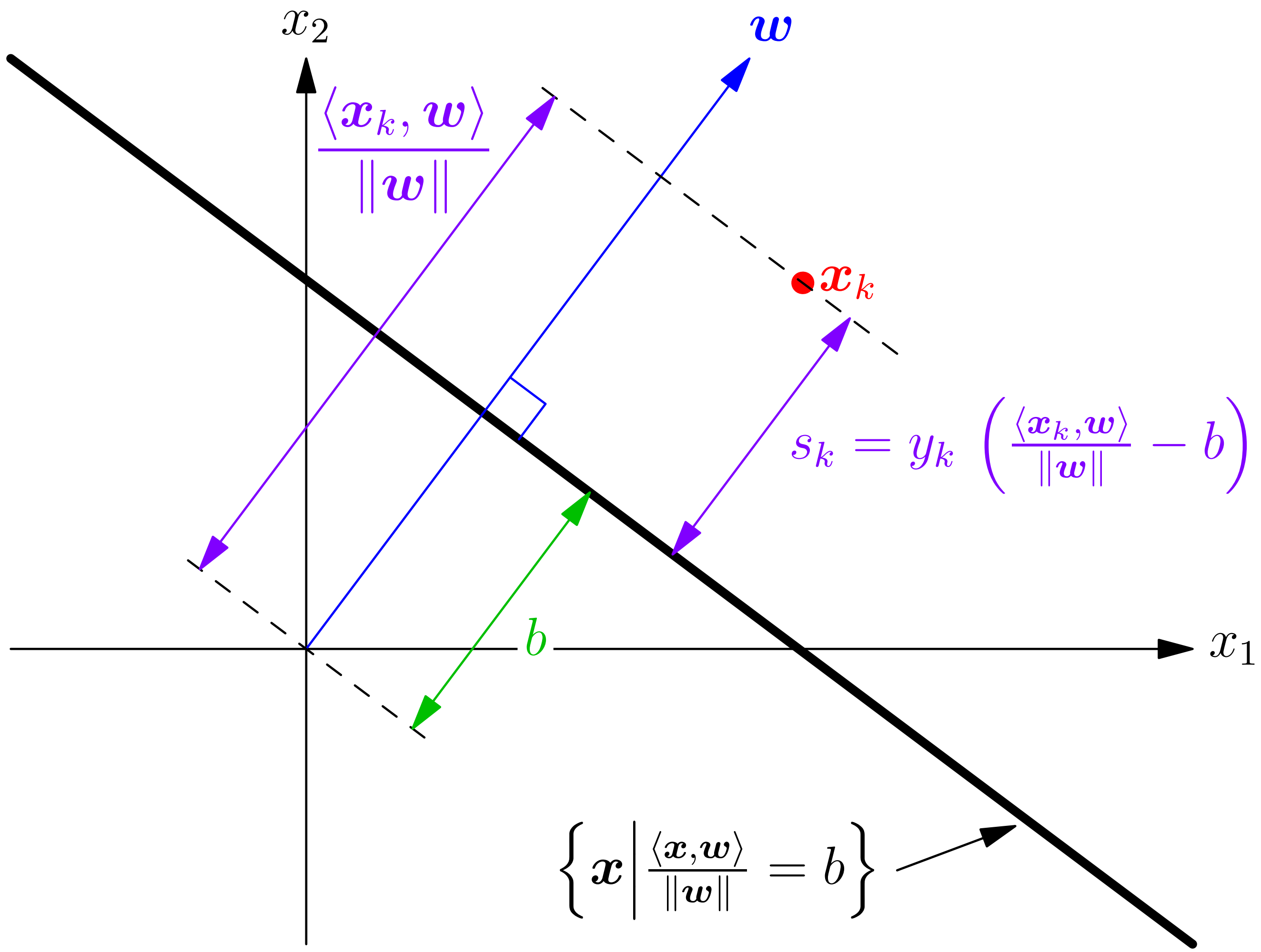

Constrained Optimisation

- Wish to find $\boldsymbol{w}$ and b to maximise Δ subject to constraints

$$y_k \left(\frac{\langle \boldsymbol{w}, \boldsymbol{x}_k \rangle}{\|\boldsymbol{w}\|} - b \right) \geq \Delta \quad \text{for all } k = 1, 2, \ldots, m$$

- If we divide through by Δ

$$y_k \left(\frac{\langle \boldsymbol{w}, \boldsymbol{x}_k \rangle}{\Delta \|\boldsymbol{w}\|} - \frac{b}{\Delta} \right) \geq 1 \quad \text{for all } k = 1, 2, \ldots, m$$

- Define $\hat{\boldsymbol{w}} = \boldsymbol{w} / (\Delta \|\boldsymbol{w}\|)$ and $\hat{b} = b/\Delta$

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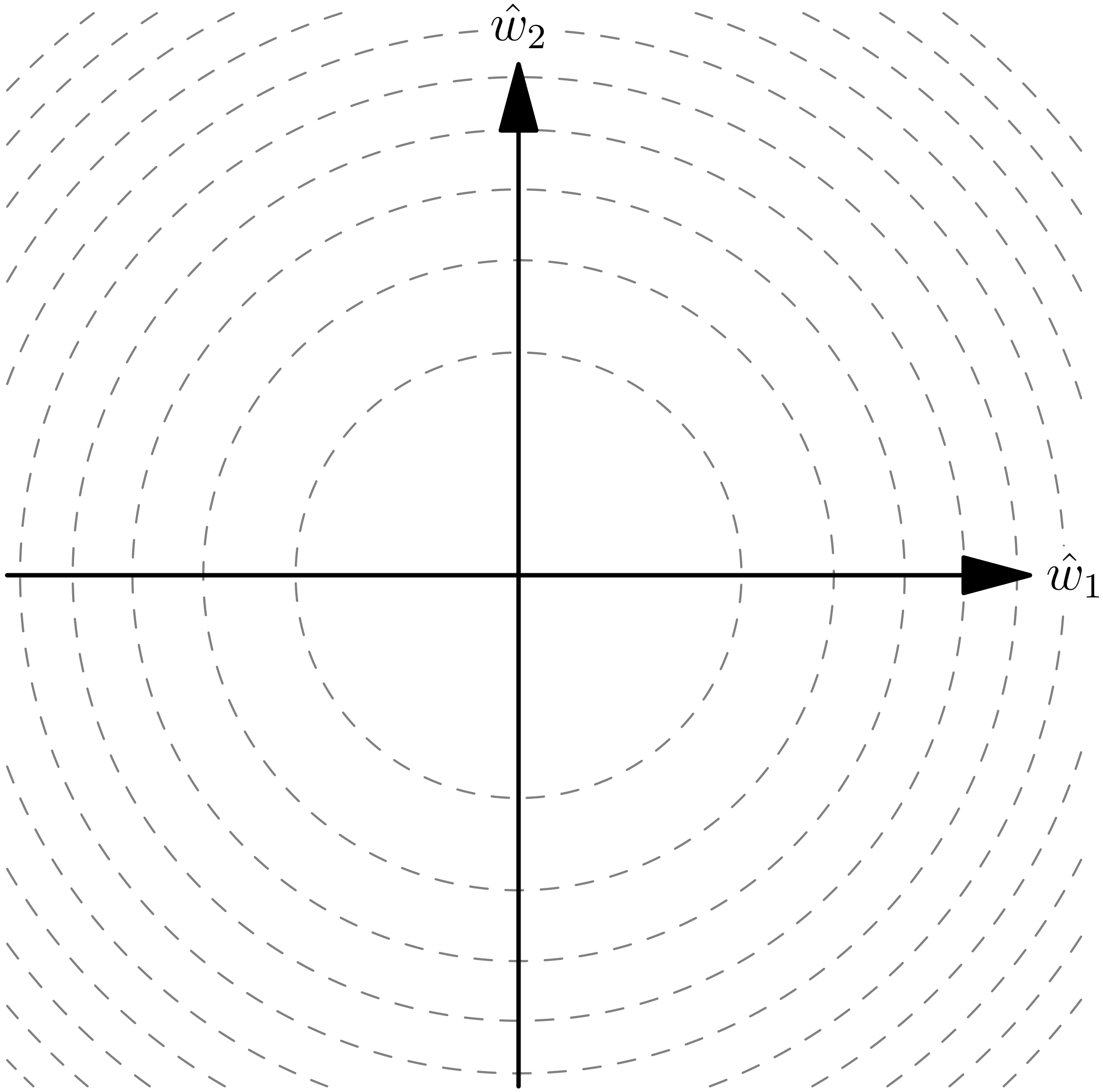

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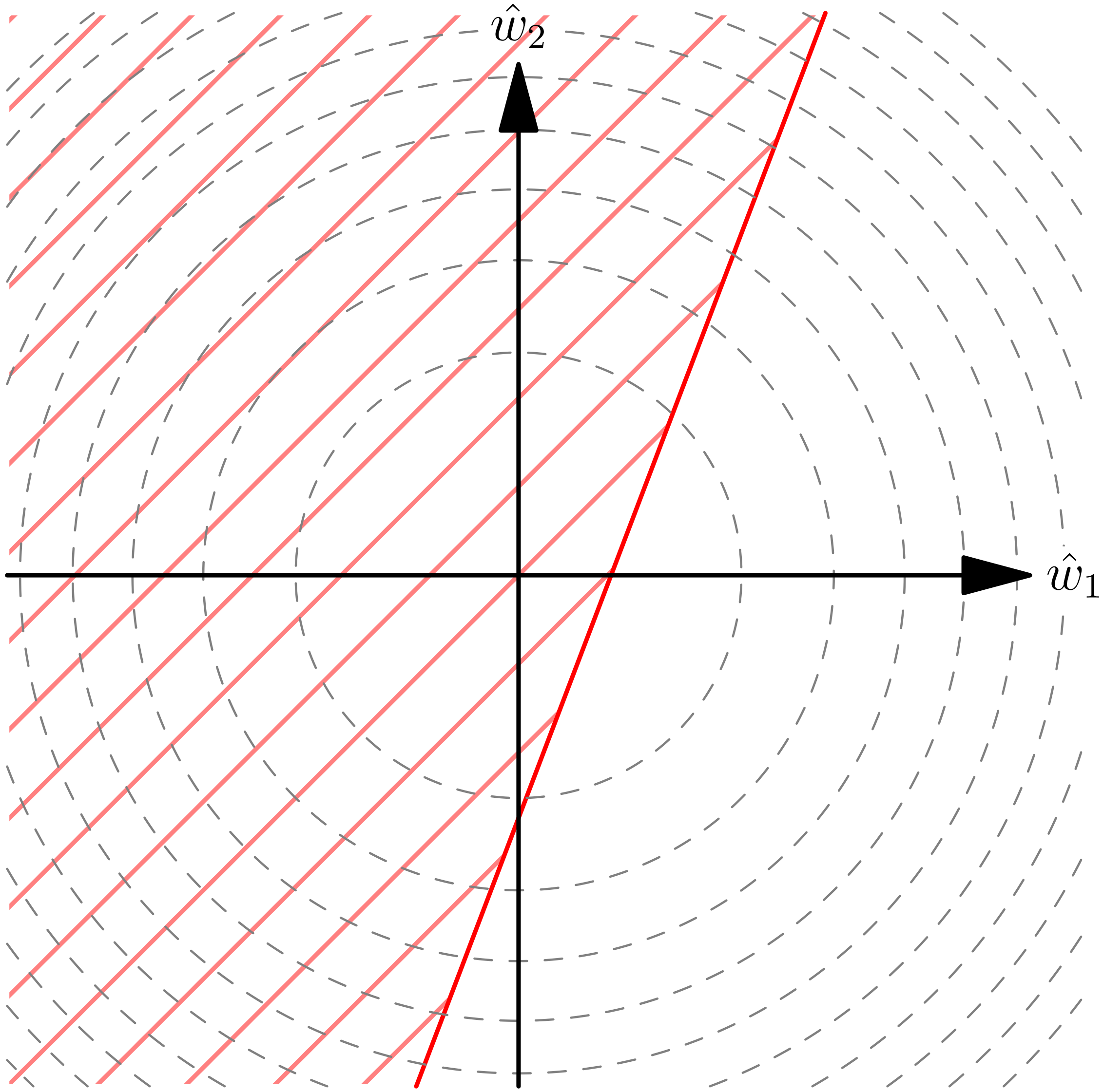

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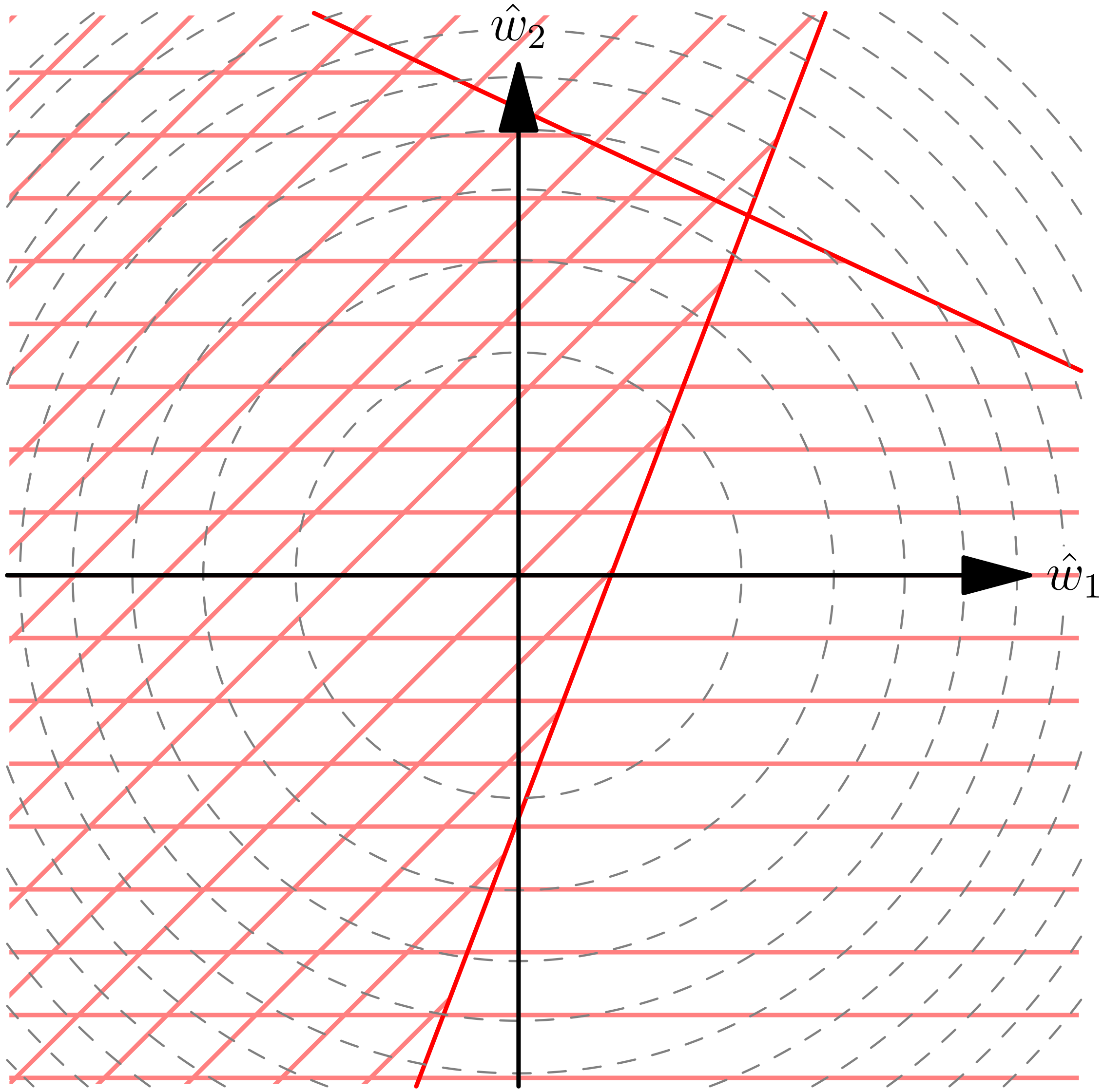

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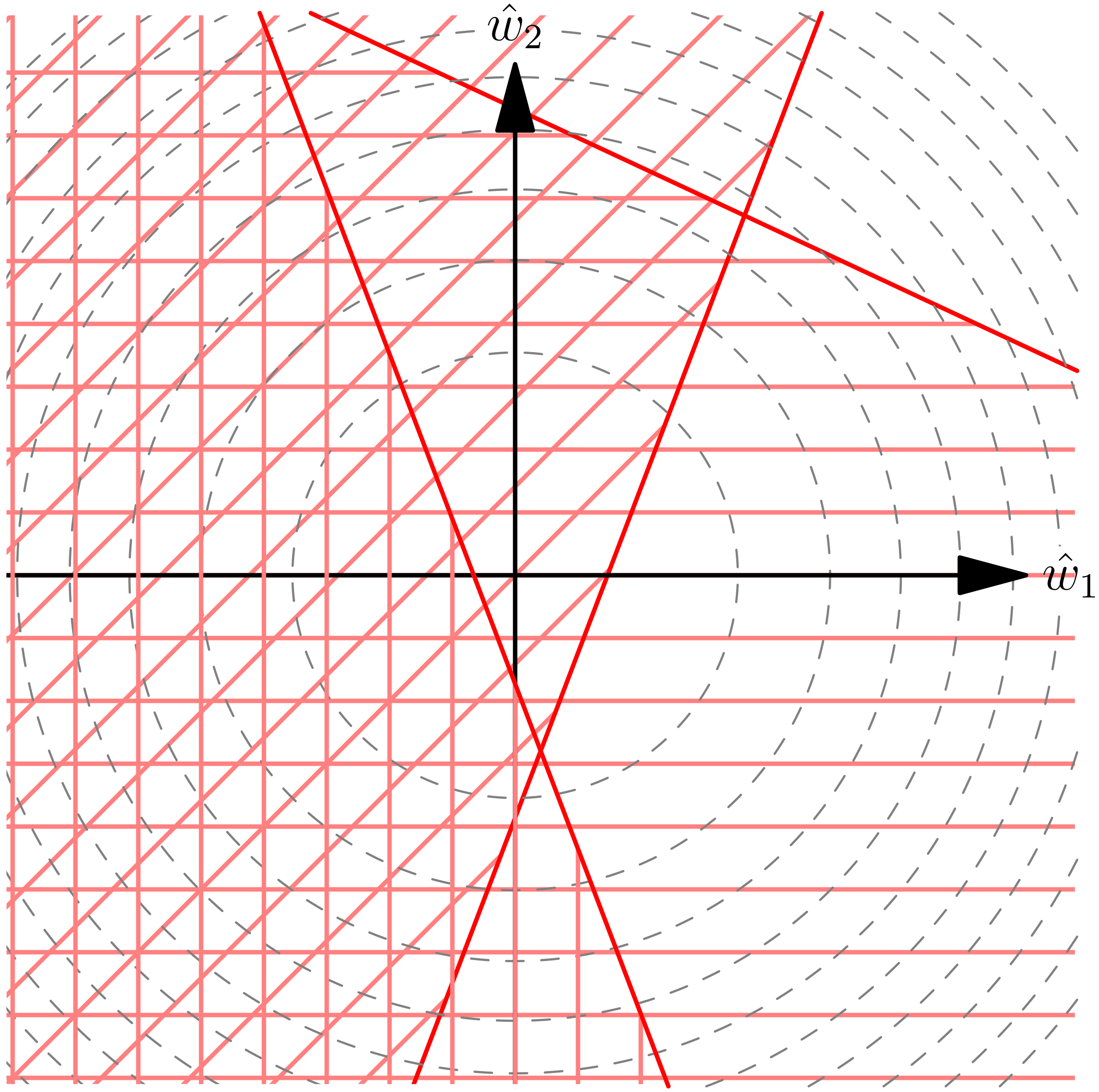

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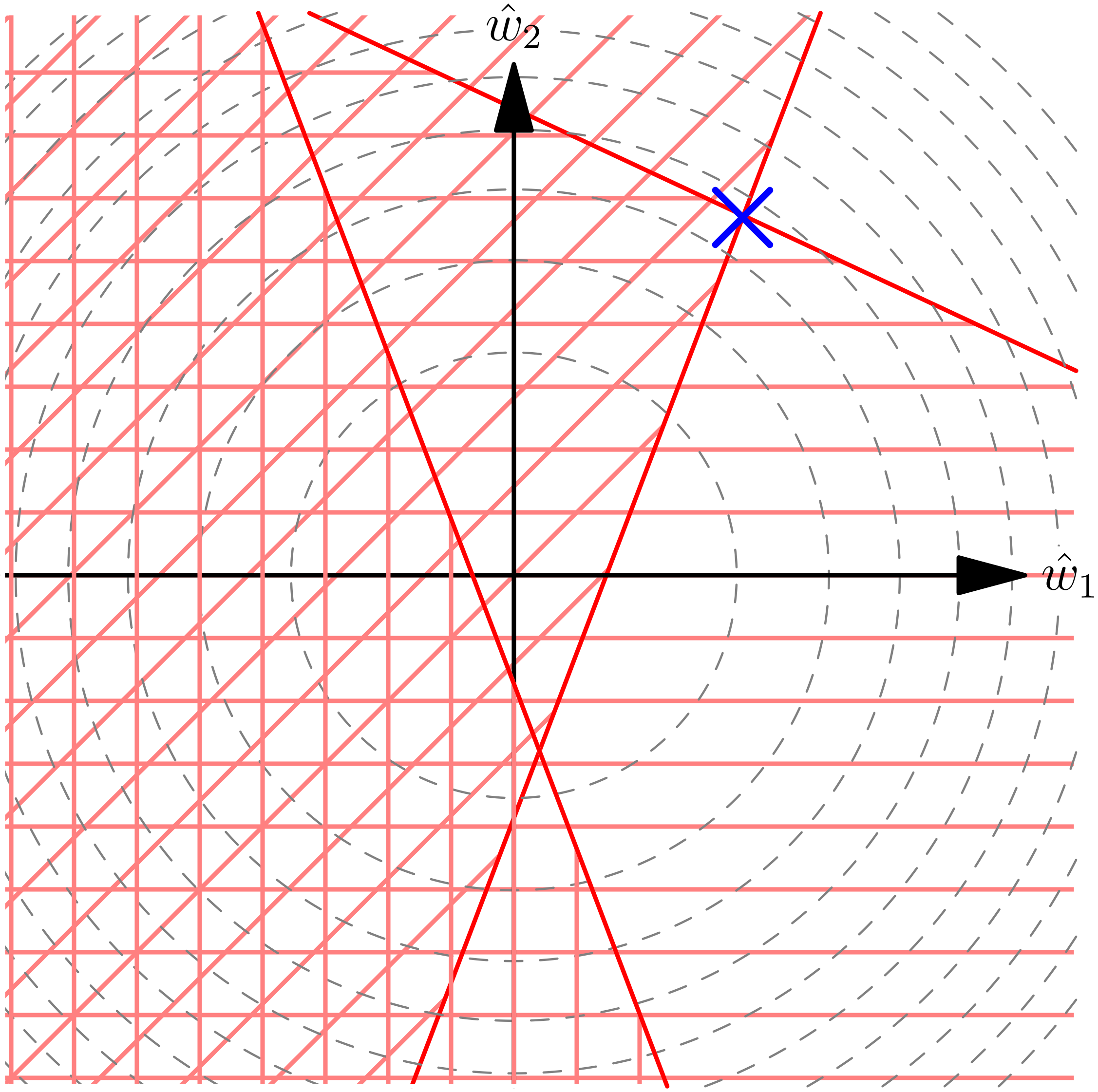

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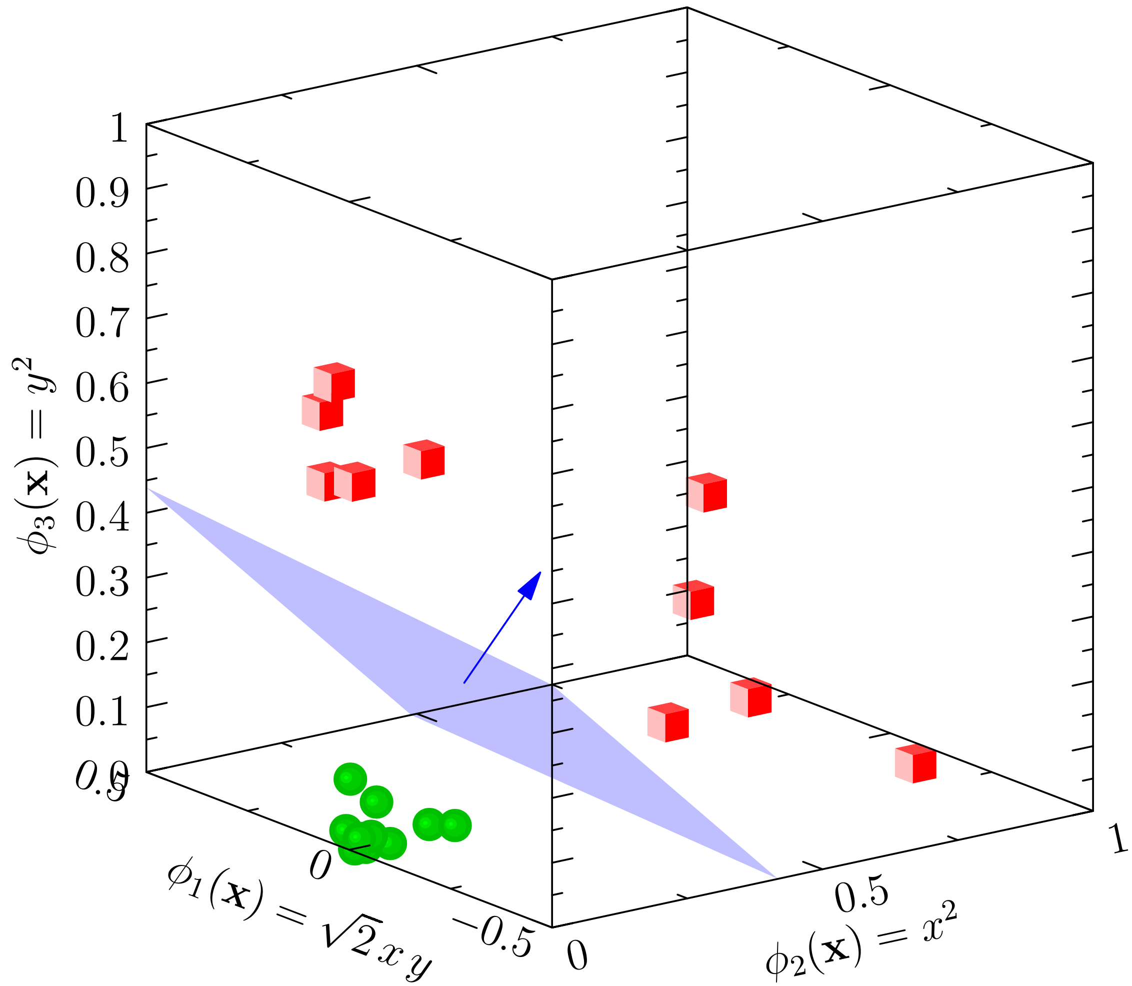
Outline

1. The Big Picture
2. Maximum Margins
3. **Duality**
4. Practice



Extended Feature Space

- We can generalise the SVM if we map all our features vectors to an extended feature space

$$\boldsymbol{x} \to \boldsymbol{\phi}(\boldsymbol{x})$$

- The components of $\boldsymbol{\phi}(\boldsymbol{x})$ will typically be (non-linear) functions of $\boldsymbol{x}$ (e.g. $\phi_1(\boldsymbol{x}) = x_1^2, \phi_2(\boldsymbol{x}) = x_2^2, \phi_3(\boldsymbol{x}) = \sqrt{2}x_1x_2$)
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- But in the extended feature space (involving $\boldsymbol{\phi}(\boldsymbol{x}) = \big(\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \ldots, \phi_r(\boldsymbol{x})\big)$) the time complexity is $O(r^3)$

Lagrangian

- In the extended feature space we can find a separating plane (given by $\boldsymbol{w}$ and b) with maximum margine by solving the problem

$$\min_{\boldsymbol{w},b} \frac{\|\boldsymbol{w}\|^2}{2} \quad \text{subject to } y_k(\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}_k)\rangle - b) \geq 1 \text{ for all } k = 1, 2, \ldots, m$$

- We can write this as a Lagrange problem

$$\min_{\boldsymbol{w},b} \max_{\boldsymbol{\alpha} \geq \boldsymbol{0}} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha})$$

where

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha}) = \frac{\|\boldsymbol{w}\|^2}{2} - \sum_{k=1}^{m} \alpha_k \Big(y_k \left(\langle \boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}_k) \rangle - b \right) - 1 \Big)$$

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Obtaining the Dual Form of the Problem

- Differentiating the Lagrangian with respect to $\boldsymbol{w}$

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Kernel Trick

- We will show in the next lecture that if $K(\boldsymbol{x},\boldsymbol{y})$ is a positive semi-definite function then it can always be written as

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Sequential Minimal Optimisation

- One of the most efficient techniques for training SVMs is *Sequential Minimal Optimisation* or SMO
- This takes two Lagrange multipliers α_i and α_j and adjusts them to maximise the dual objective function
- This is very quick as it can be done in closed form
- Note that because $\sum_{k=1}^{m} y_k \alpha_k = 0$ we have to change at least two variables at the same time
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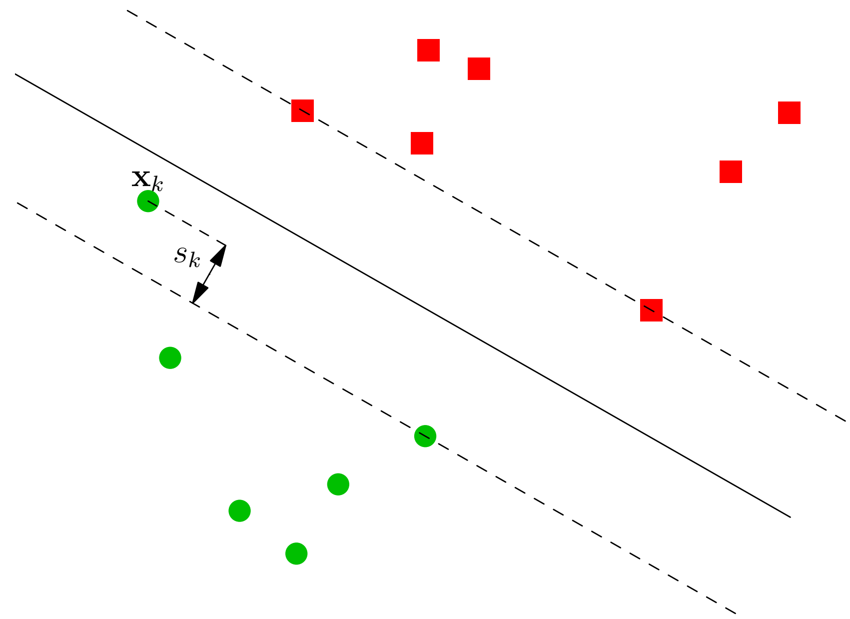
- We can relax the margin constraints by introducing *slack variables*, $s_k \geq 0$



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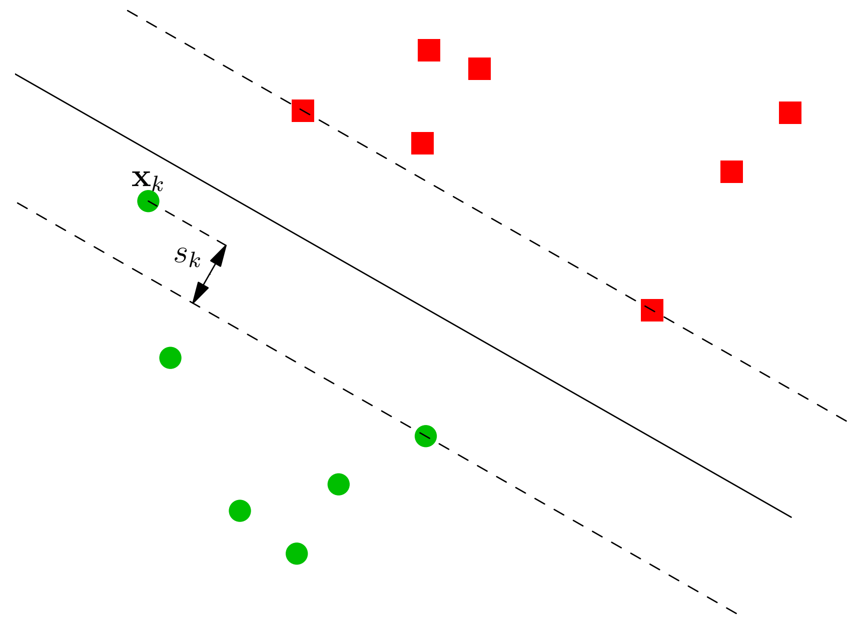

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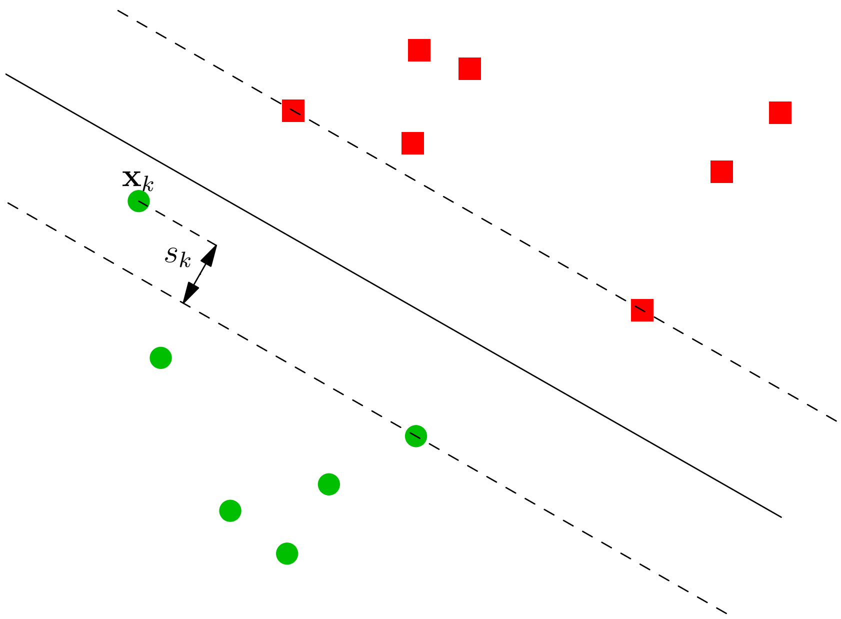

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Dual Problem with Slack Variables

- The Lagrangian with slack variables is

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where β_k are Lagrange multipliers that ensure $s_k \geq 0$ (note that $\beta_k \geq 0$—this is the KKT condition)

- Now minimising with respect to s_i

$$\frac{\partial \mathcal{L}}{\partial s_i} = C - \alpha_i - \beta_i = 0$$

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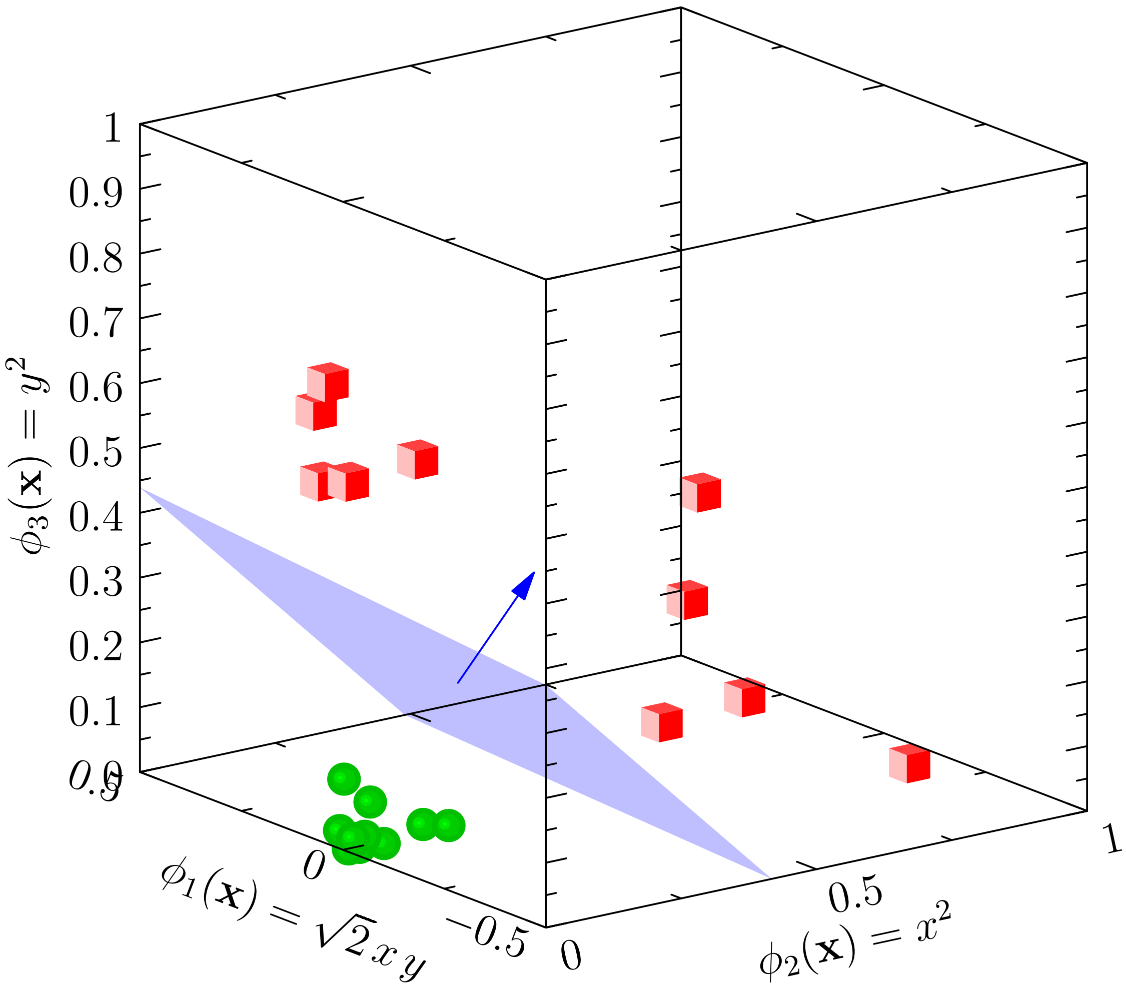
Outline

1. The Big Picture
2. Maximum Margins
3. Duality
4. **Practice**



Getting SVMs to Work Well

- SVMs rely on distances between data points
- These will change relative to each other if we rescale some features but not other—giving different maximum-margin hyper-planes

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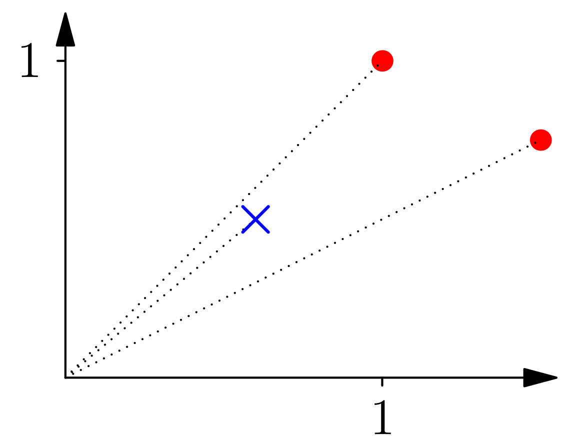

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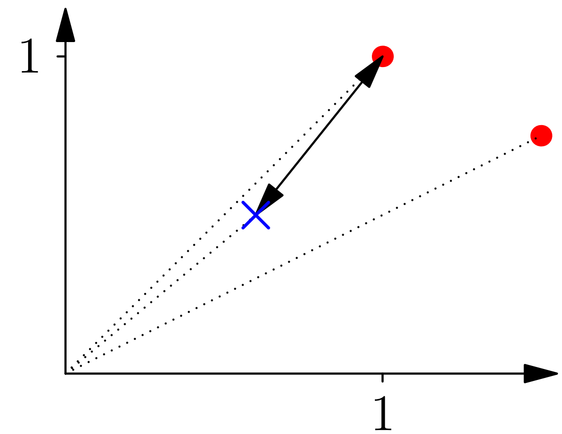

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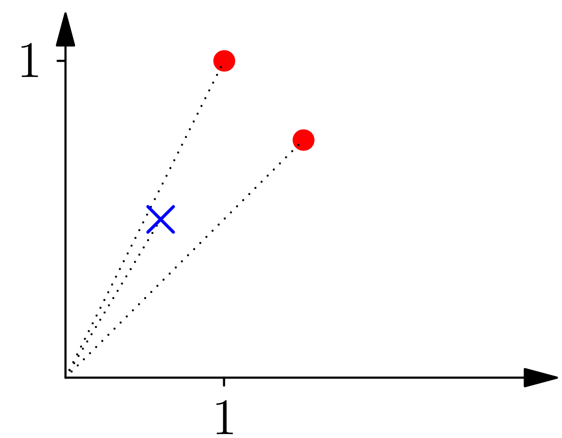

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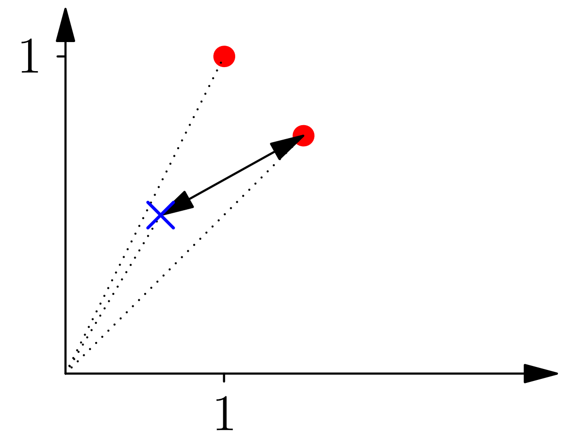

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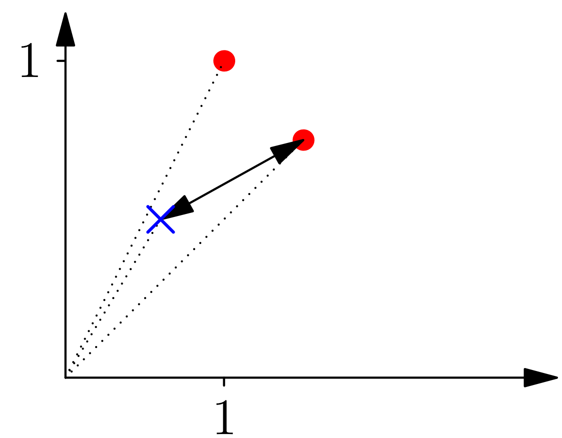

- If we don't know what features are important (most often the case), then it is worth scaling each feature (for example, so their range is between 0 and 1 or their variance is 1)

Optimising C

- Recall that we can introduce soft-margins using slack variables where we minimise $\frac{\|\hat{\boldsymbol{w}}\|^2}{2} + C\sum_{k=1}^{m} s_k$ subject to constraints

- In practice it can make a huge difference to the performance if we change C

- Optimal C values changes by many orders of magnitude e.g. 2^{-5}–2^{15}

- Typically optimised by a grid search (start from 2^{-5} say and double until you reach 2^{15})

- Measure performance on a validation set

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Choosing the Right Kernel Function

- There are kernels design for particular data types (e.g. string kernels for text or biological sequences)
- For numerical data, people tend to look at using no kernel (linear SVM), a radial basis function (Gaussian) kernel or polynomial kernels
- Kernels often come with parameters, e.g. the popular radial basis function kernel

$$K(\boldsymbol{x}, \boldsymbol{y}) = \mathrm{e}^{-\gamma \|\boldsymbol{x}-\boldsymbol{y}\|^2}$$

- Optimal γ values range over 2^{-15}–2^3

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- There are kernels design for particular data types (e.g. string kernels for text or biological sequences)
- For numerical data, people tend to look at using no kernel (linear SVM), a radial basis function (Gaussian) kernel or polynomial kernels
- Kernels often come with parameters, e.g. the popular radial basis function kernel

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Multi-Class Problems

- By construction SVMs separate only two classes
- If we have a multi-class problem we have to use multiple SVMs
- There are two major ways practitioners do this

  One-versus-all: for each class, train a separate classify to determine that class versus all others

  All-pairs: train a classify for all pairs of classes
- In both cases choose the class which the classifier is most certain about
- Beware SVMs don't like imbalanced datasets

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SVM Libraries

- Although SVMs have unique solutions, they require very well written optimisers
- If you have a large data set they can be very slow
- There are good libraries out there: svmlib, svm-lite, (now old), scikit-learn, etc.
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Conclusions

- We've seen how SVMs work
- We've learnt how to use them
- We've seen that we can find the maximum margin hyper-plane by solving a quadratic programming problem (with a unique solution)
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