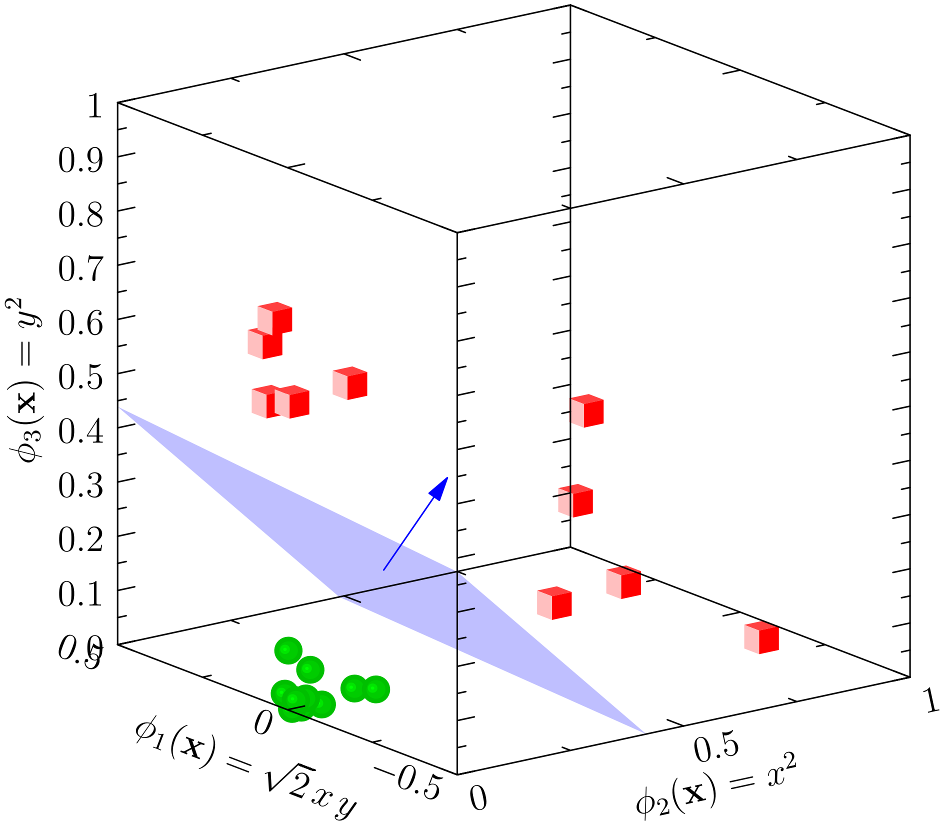
Advanced Machine Learning

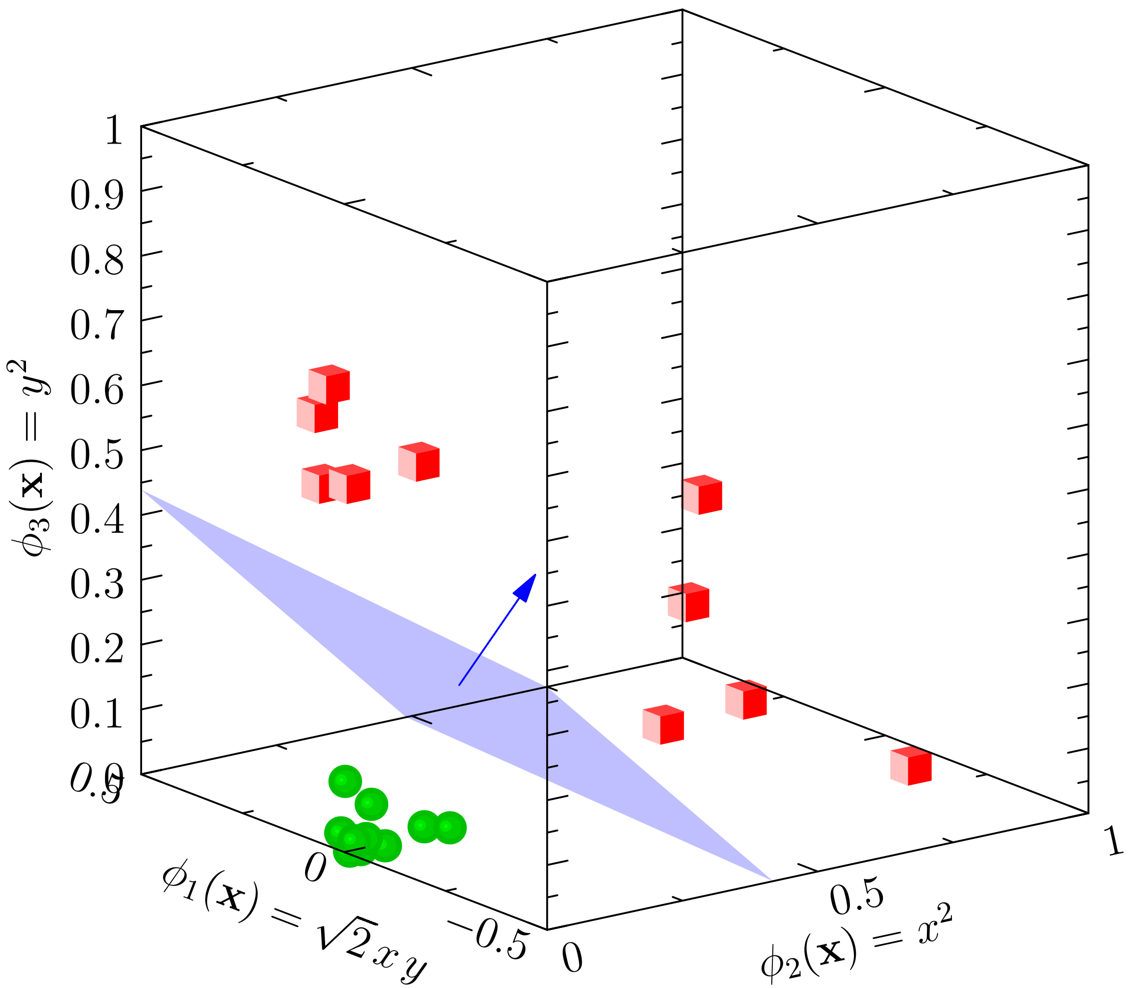
Support Vector Machines



Support Vector Machines, maximum margins

Outline

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



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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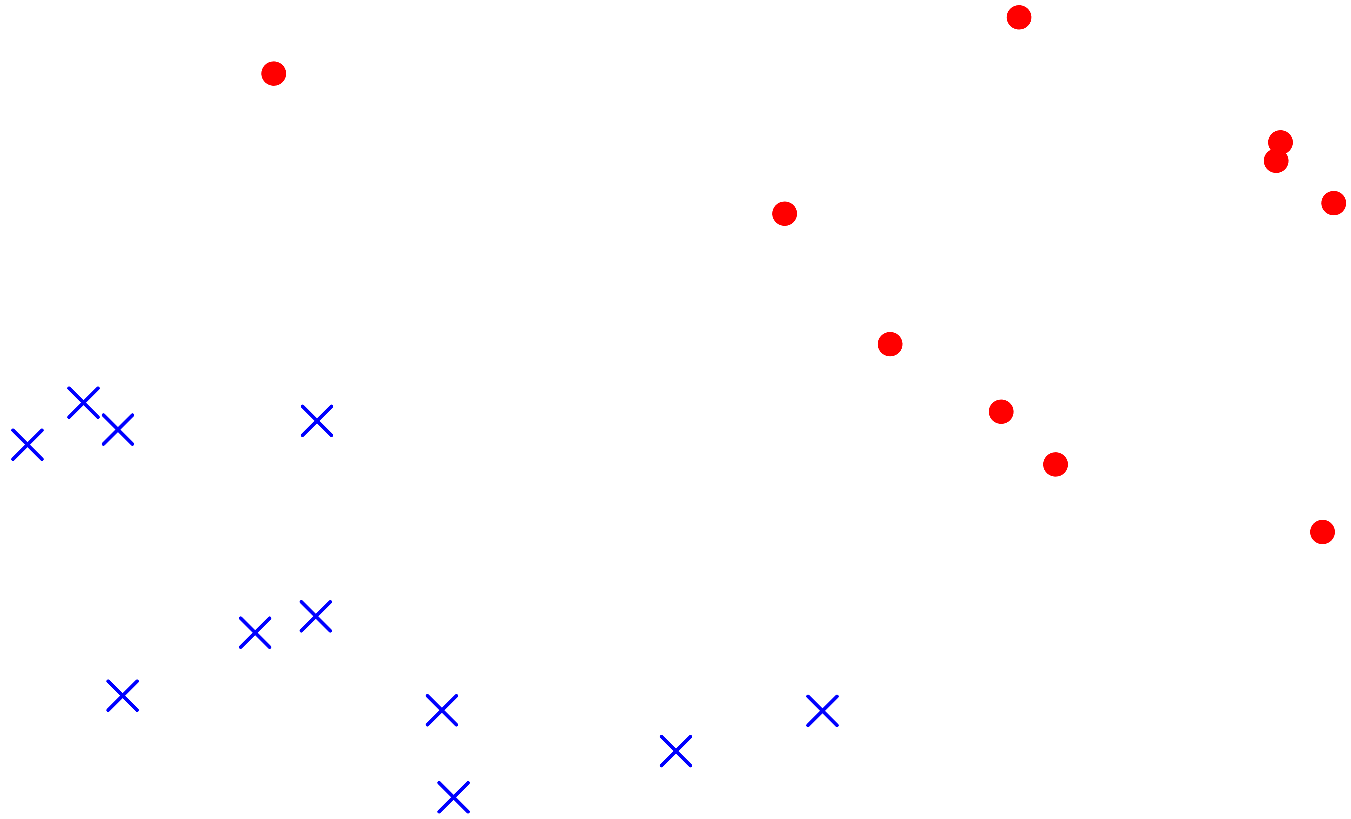
Linear Separation of Data

- SVMs classify linearly separable data



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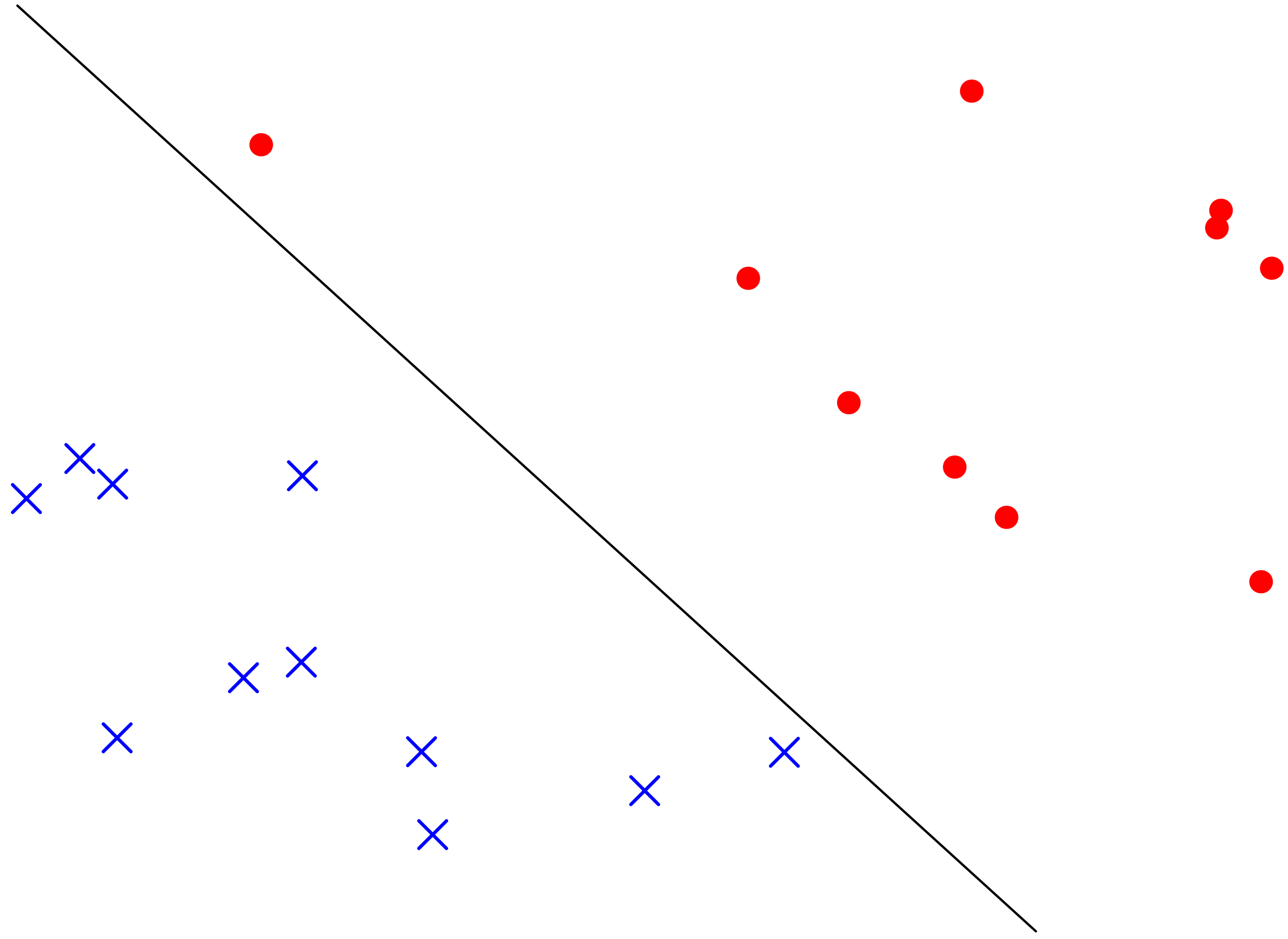

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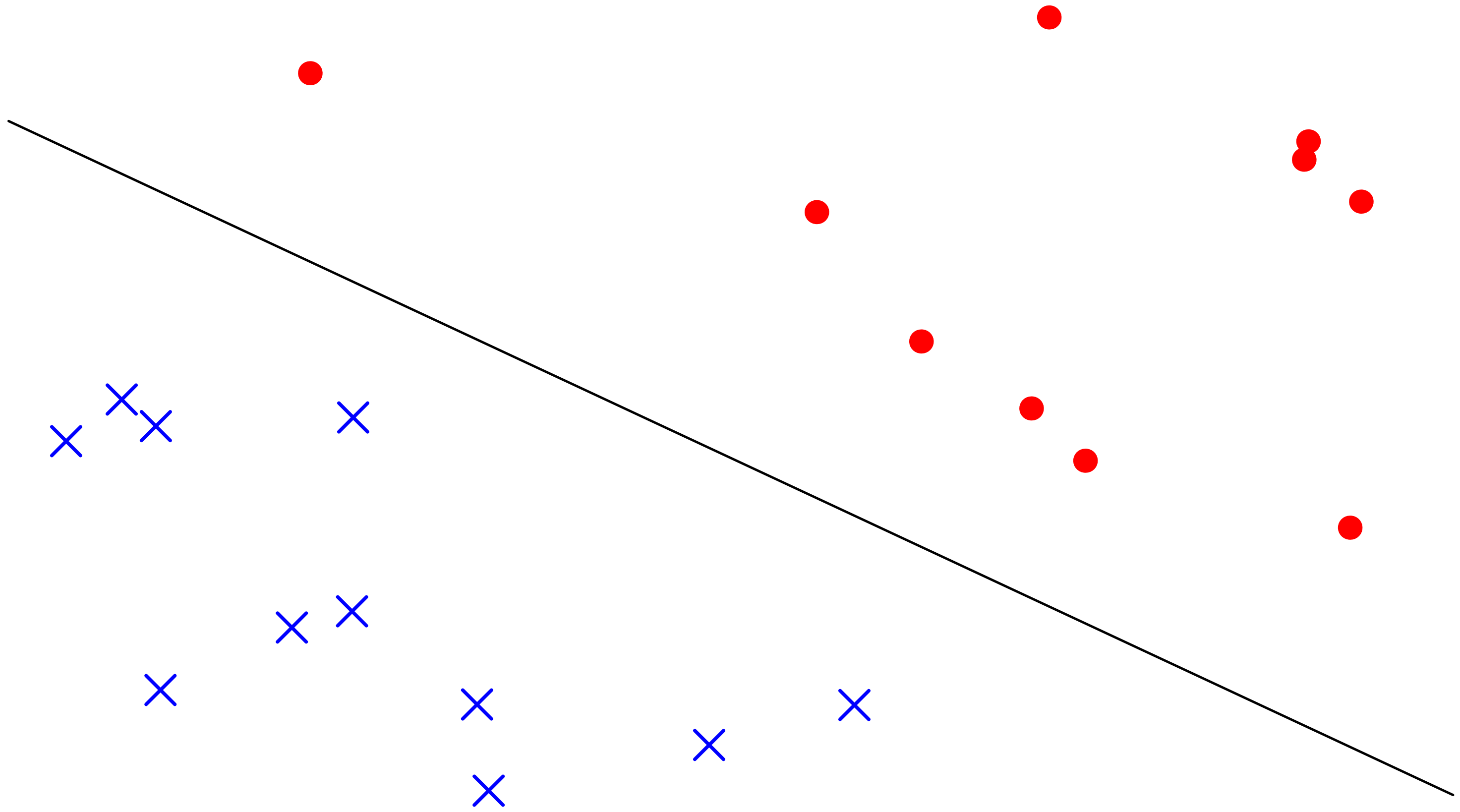

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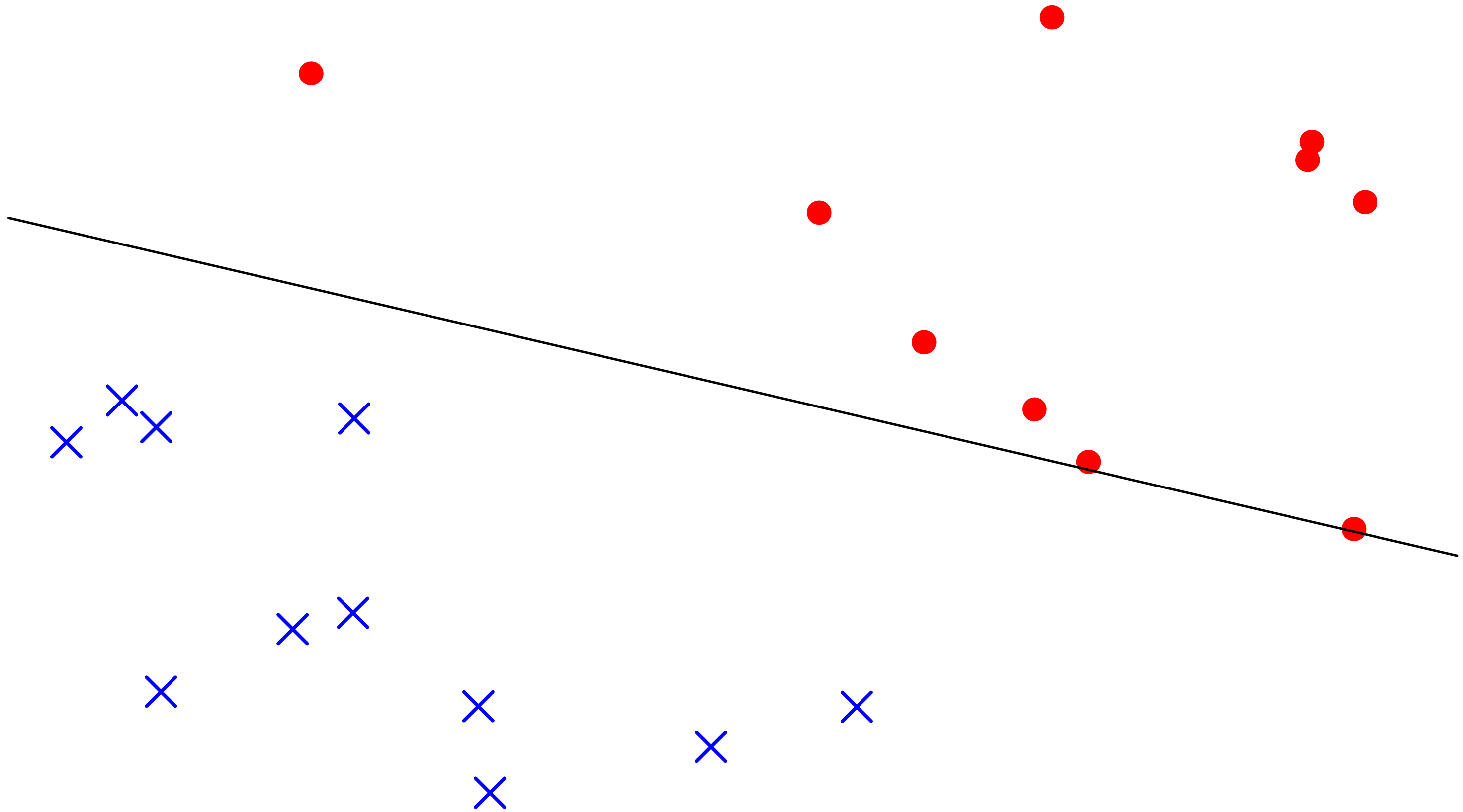

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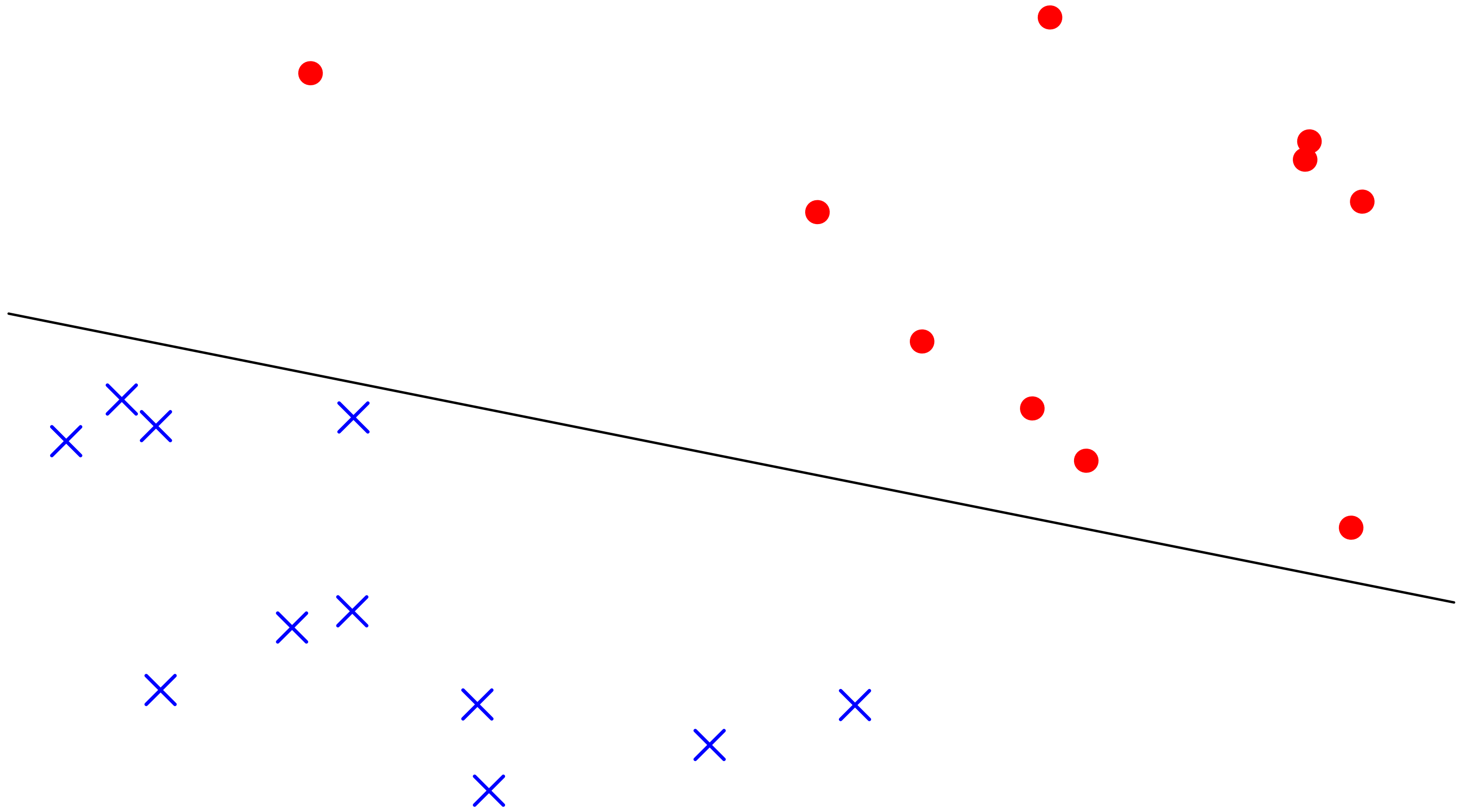

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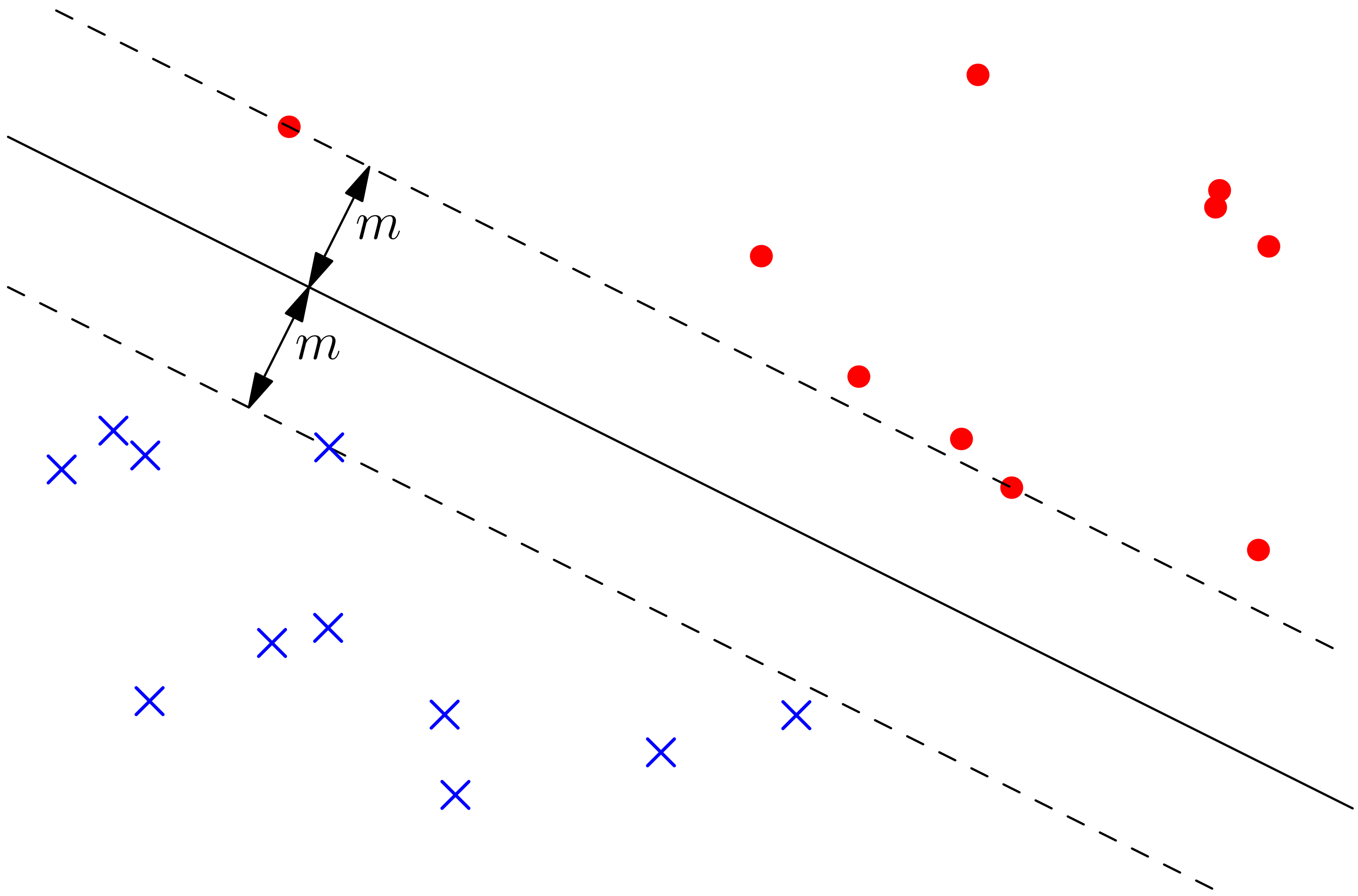

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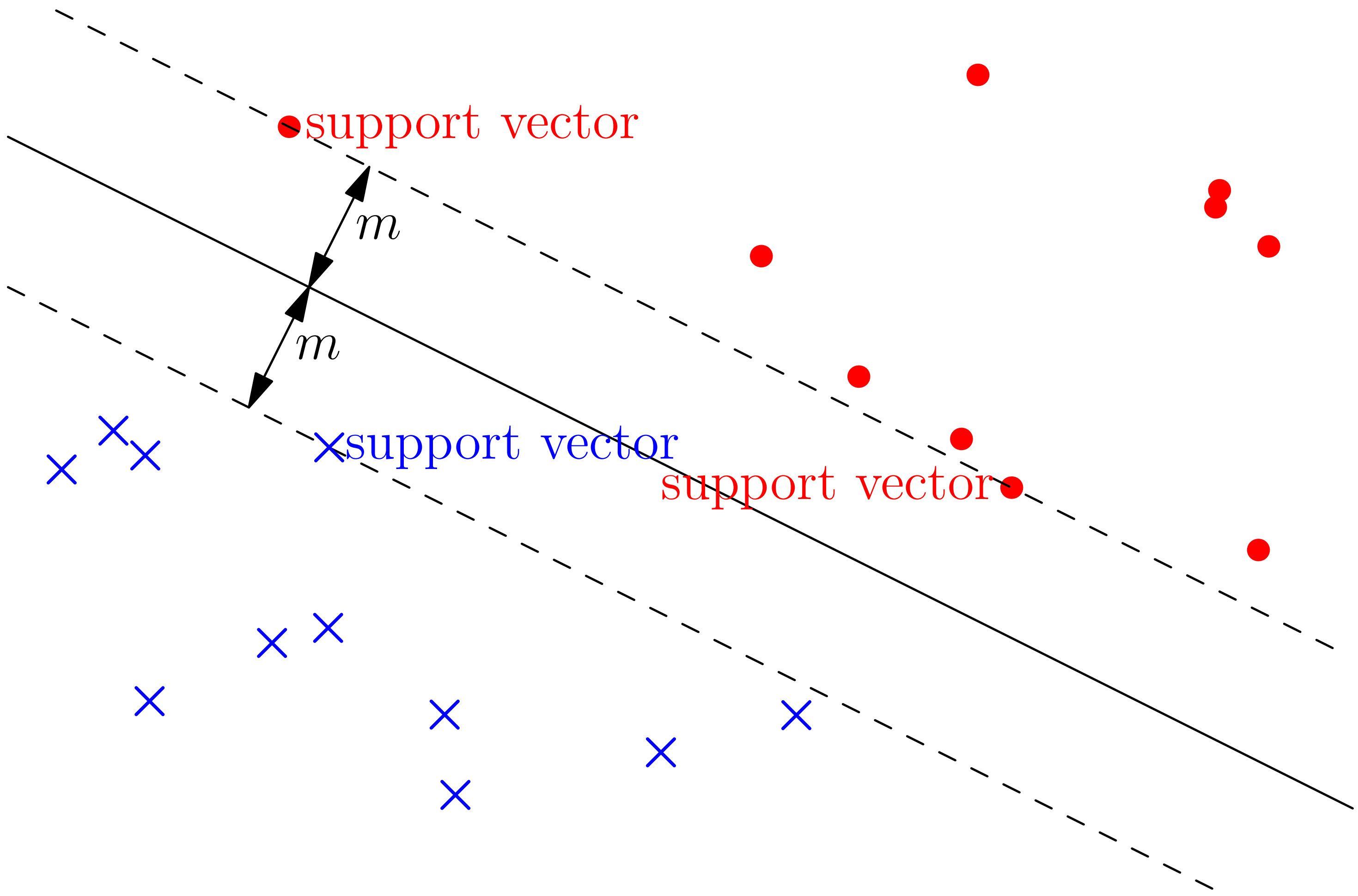

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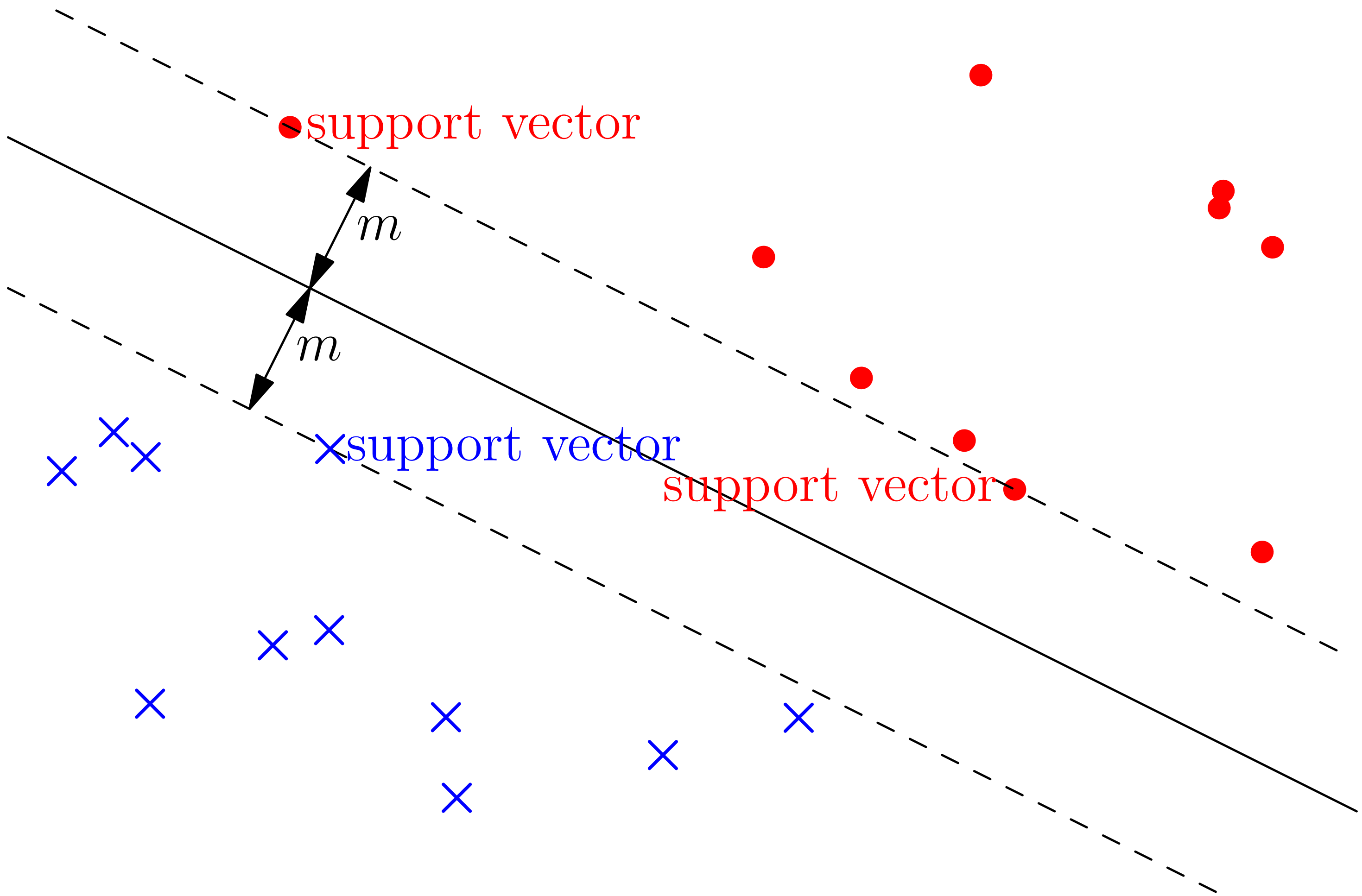

- Finds maximum-margin separating plane

Extended Feature Space

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

$$\boldsymbol{x} = (x_1, x_2, \ldots, x_p) \rightarrow \vec{\phi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \phi_2(\boldsymbol{x}), \ldots, \phi_m(\boldsymbol{x}))$$

$m \gg p$

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

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

$$\vec{\phi}(\boldsymbol{x}_i) \cdot \vec{\phi}(\boldsymbol{x}_j)$$

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$$\vec{\phi}(\boldsymbol{x}_i) \cdot \vec{\phi}(\boldsymbol{x}_j) = \sum_{k=1}^{m} \phi_k(\boldsymbol{x}_i)\, \phi_k(\boldsymbol{x}_j)$$

Kernel Trick

- If we choose a **positive semi-definite** kernel function $K(\boldsymbol{x}, \boldsymbol{y})$ then there exists functions $\phi_k(\boldsymbol{x})$, such that

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \vec{\phi}(\boldsymbol{x}_i) \cdot \vec{\phi}(\boldsymbol{x}_j)$$

  (like an eigenvector decomposition of a matrix)

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Kernel Functions

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

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

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

- 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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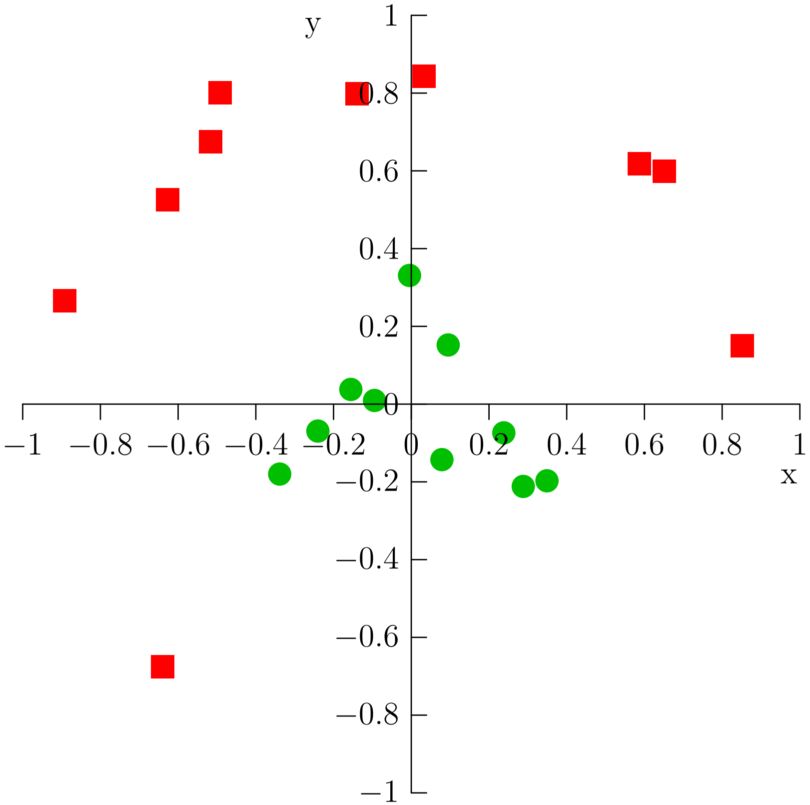

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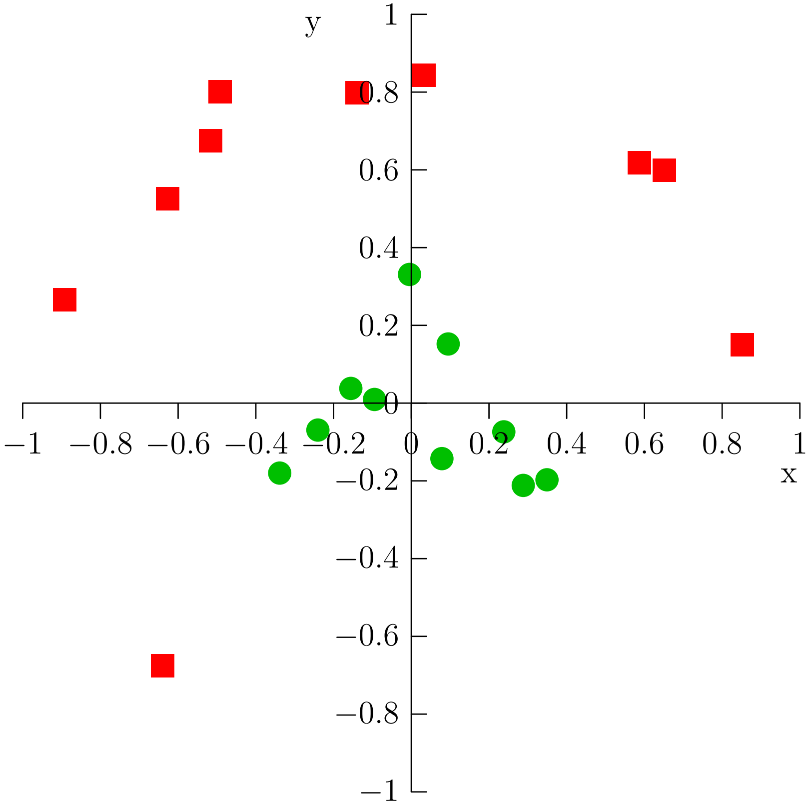

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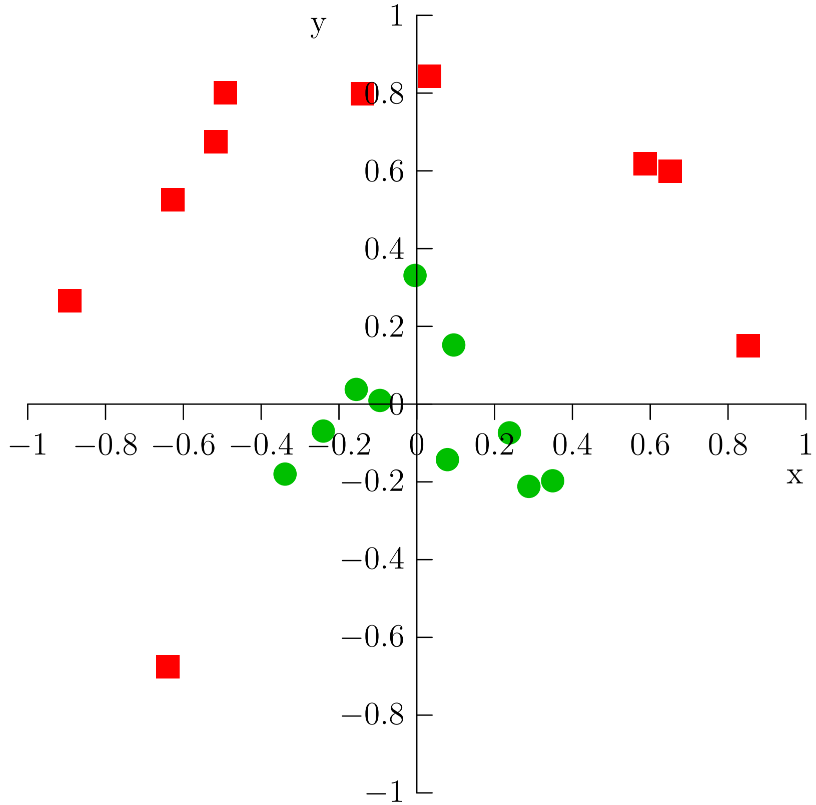

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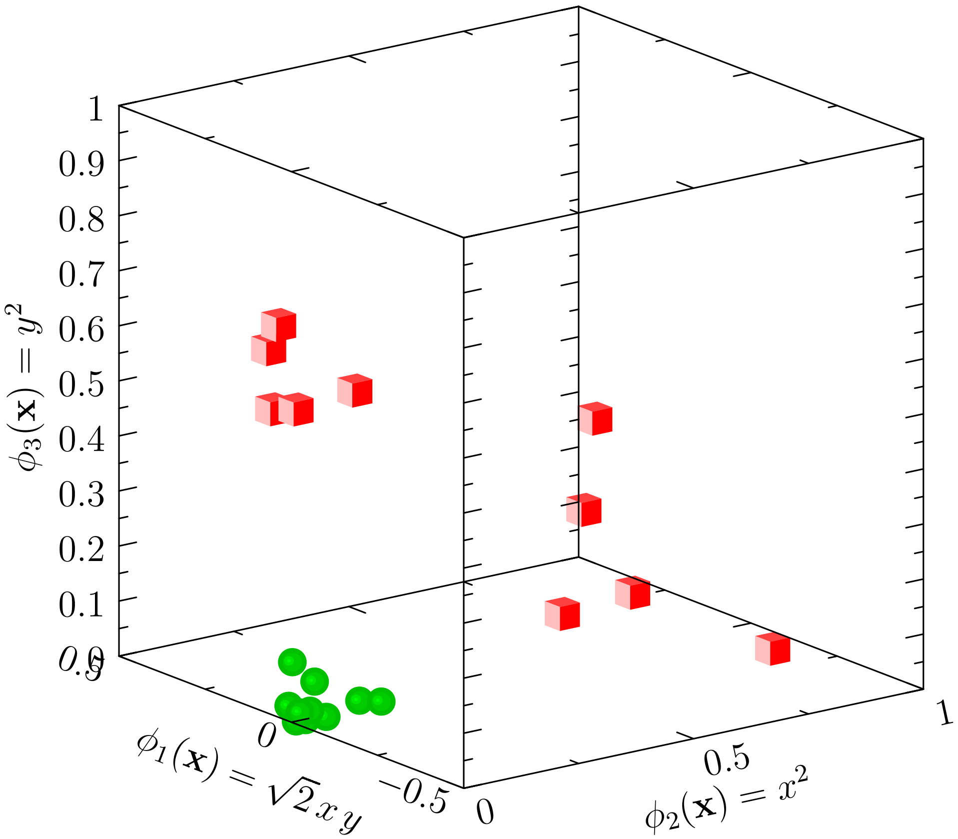

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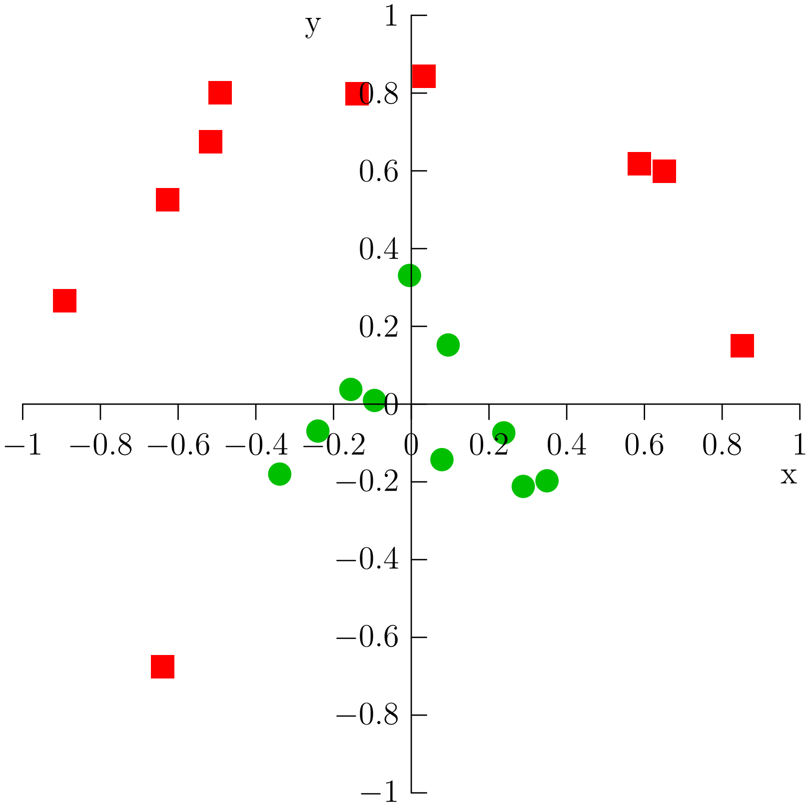

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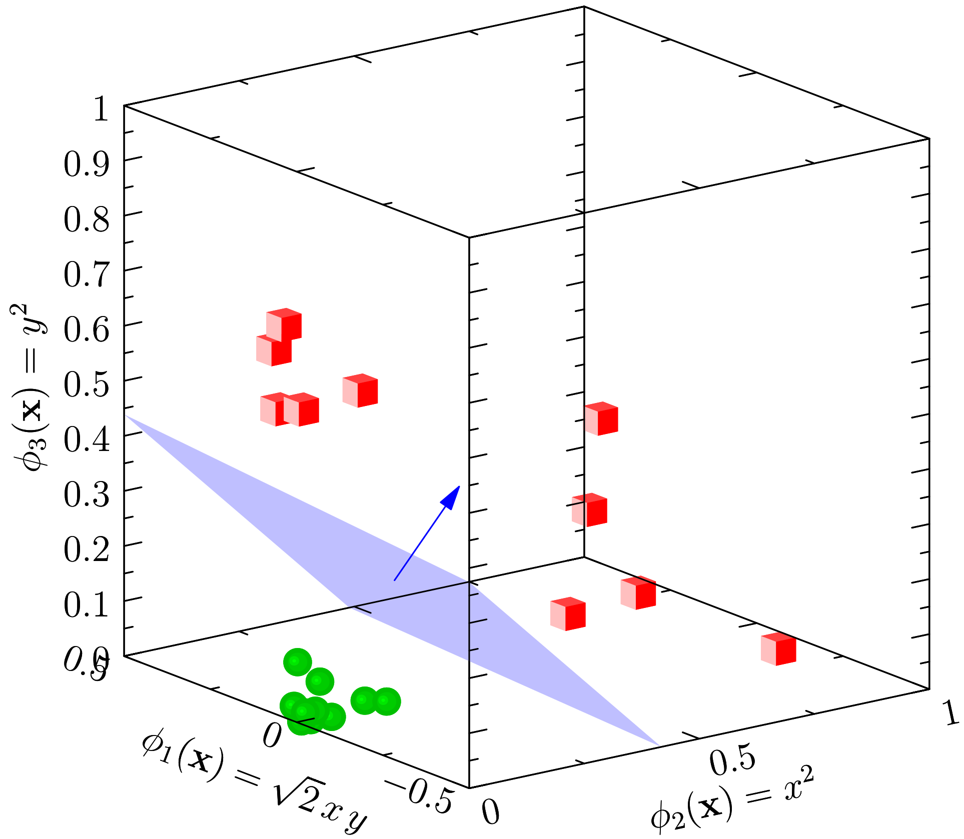

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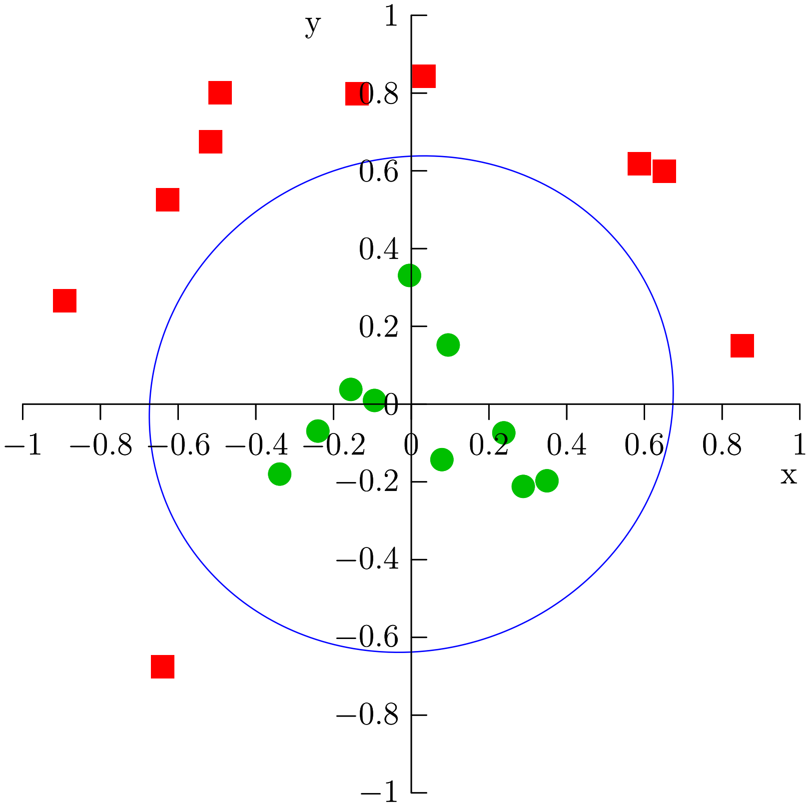

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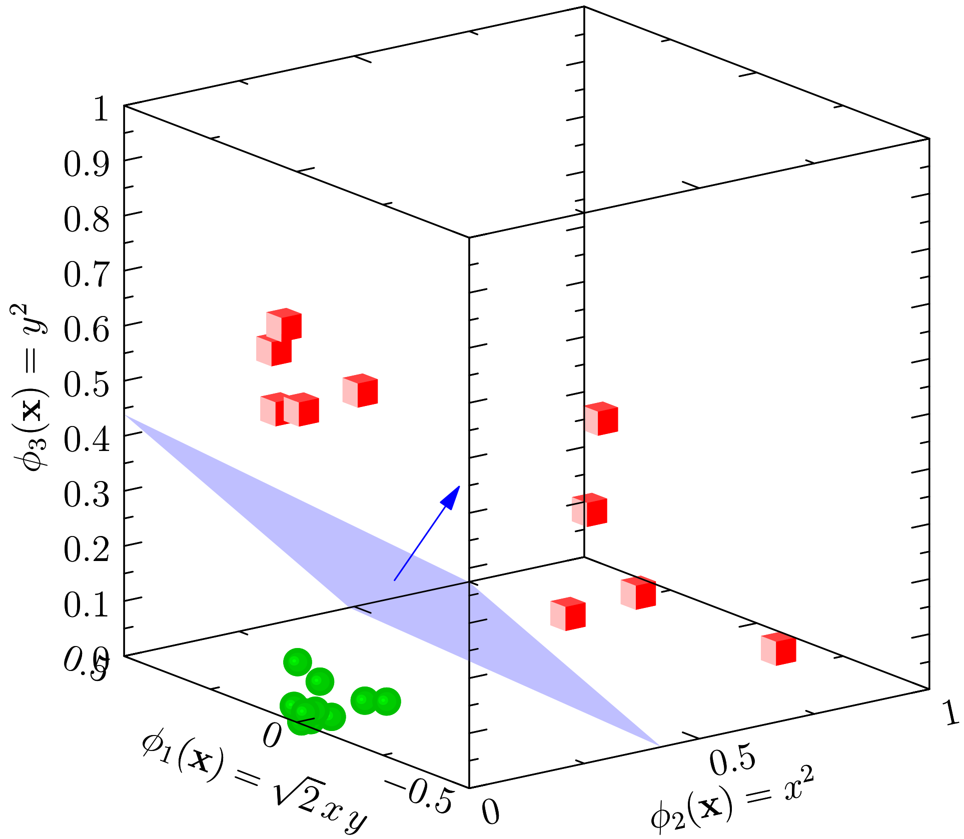

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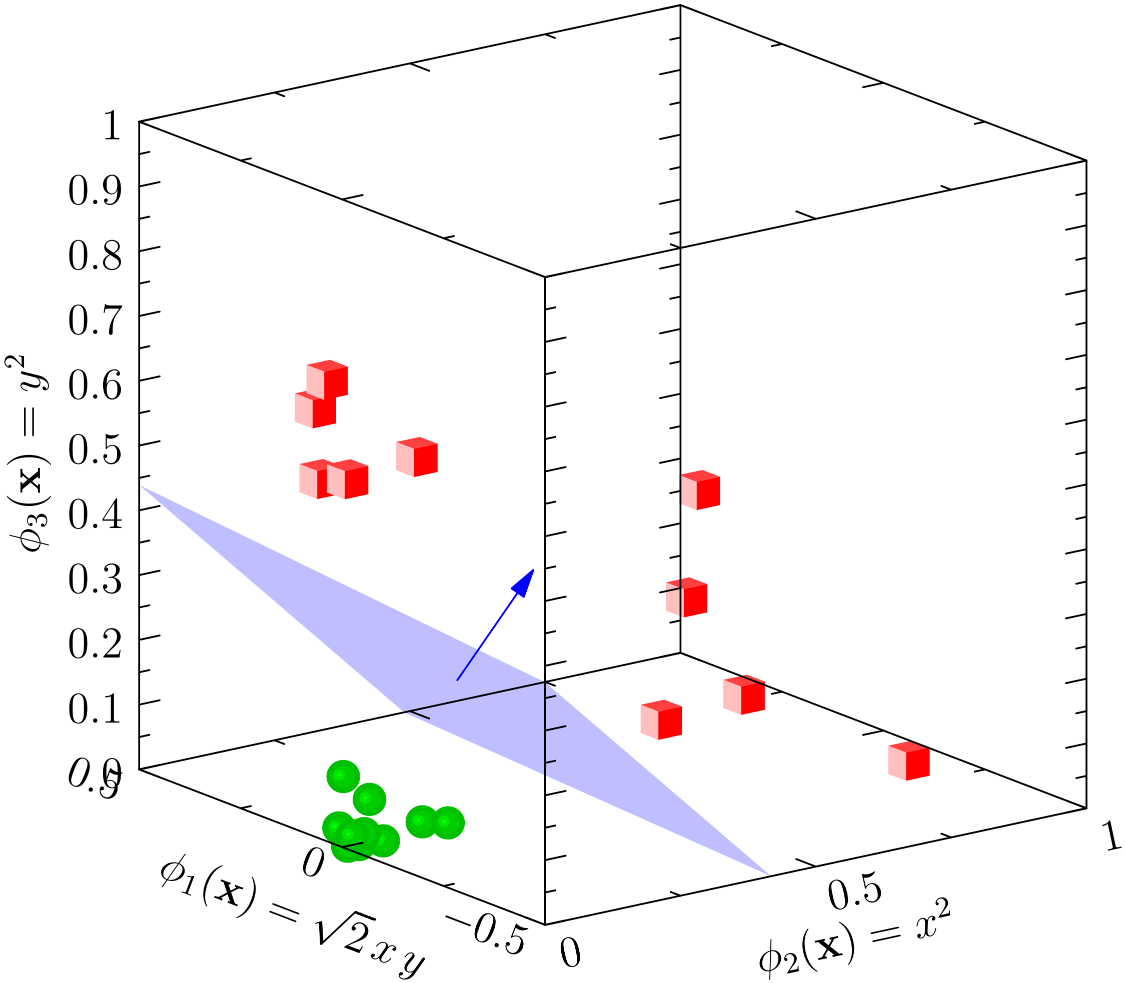

Computing the Maximum-Margin Hyper-plane

- We will derive the formula for the minimum-margin hyper-plane in the next lecture
- This gives us a quadratic programming problem
- Through a neat trick we can represent this problem in a "dual form" where we
- Never need to compute $\boldsymbol{\phi}_i(\boldsymbol{x})$ only need to compute $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$
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- 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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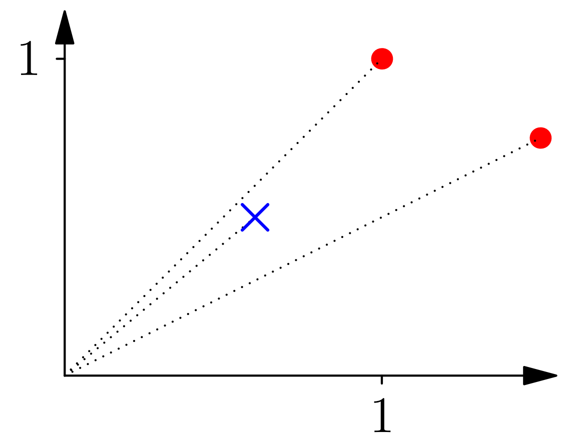

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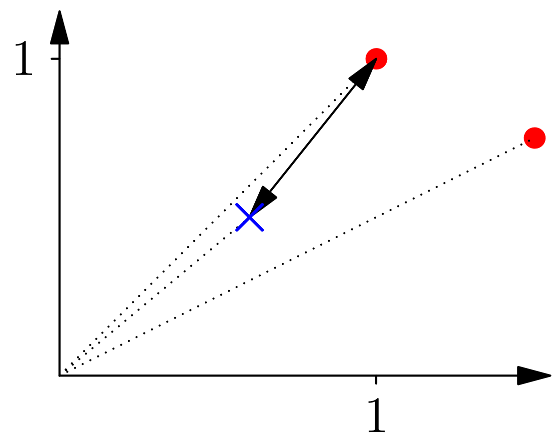

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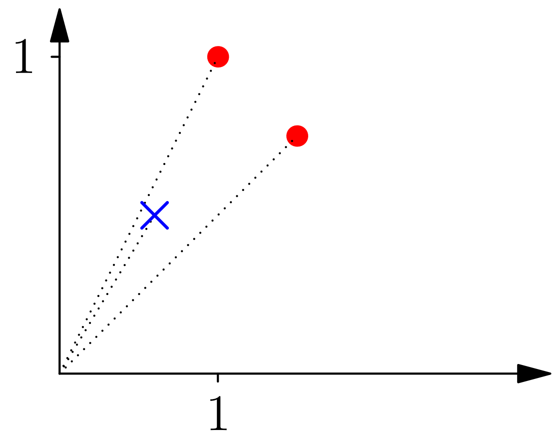

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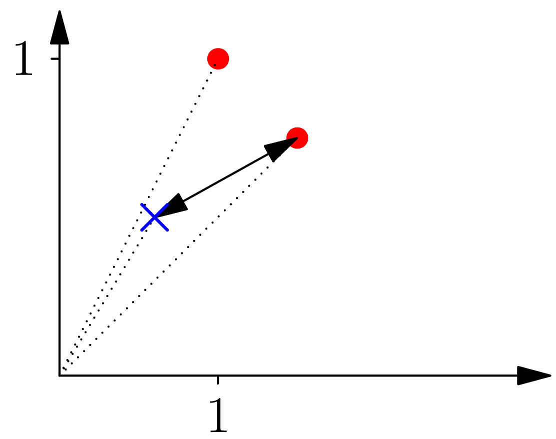

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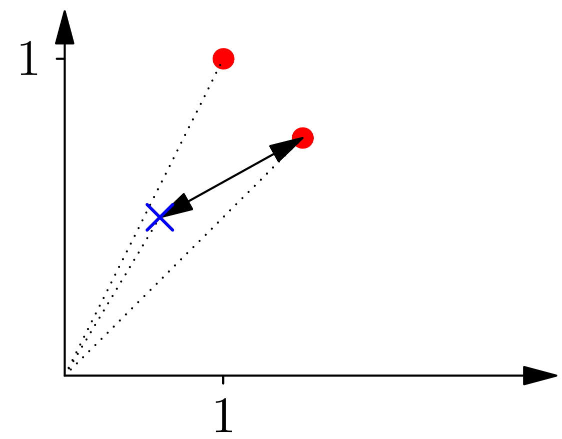
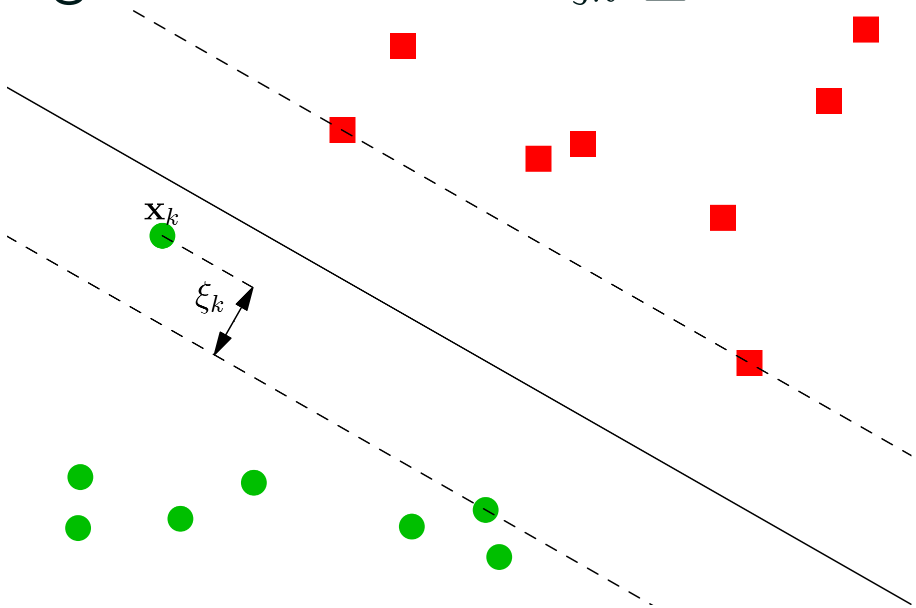


- If we don't know what features are important (most often the case), then it is worth scaling each feature (for example, so their range is between 0 and 1 or their variance is 1)

Soft Margins

- Sometimes the margin constraint is too severe
- Relax constraints by introducing *slack variables*, $\xi_k \geq 0$



$$y_k(\boldsymbol{x}_k^{\mathsf{T}}\boldsymbol{w} - b) \geq 1 - \xi_k$$

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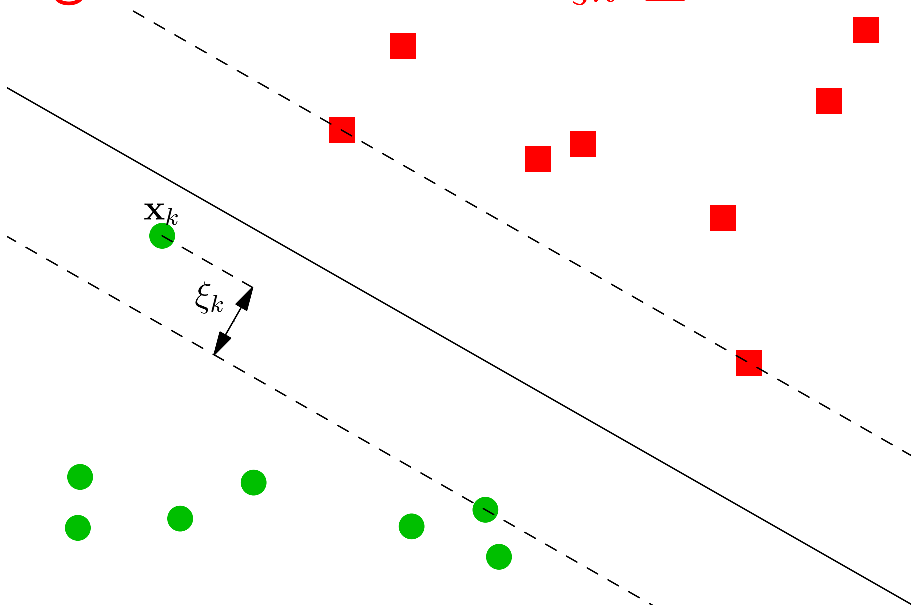

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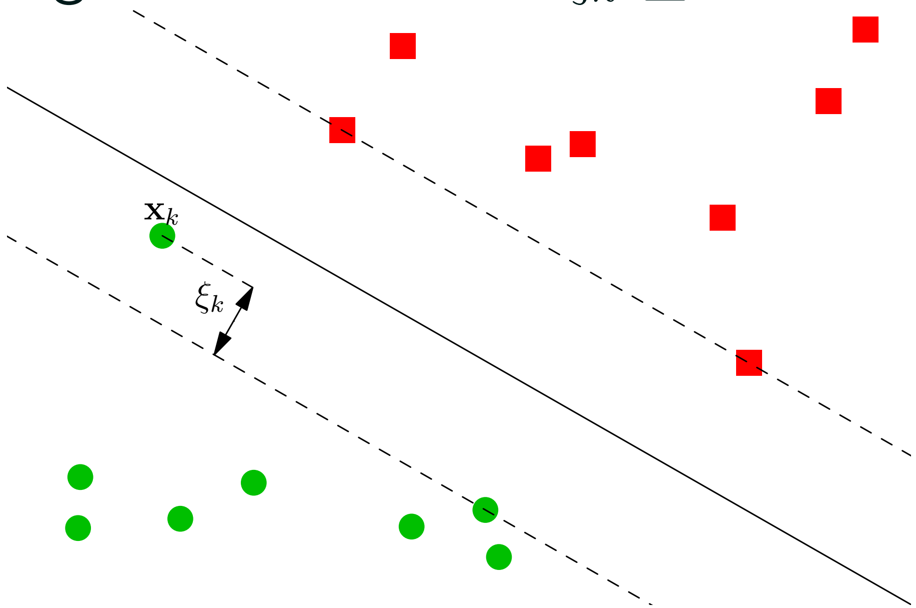

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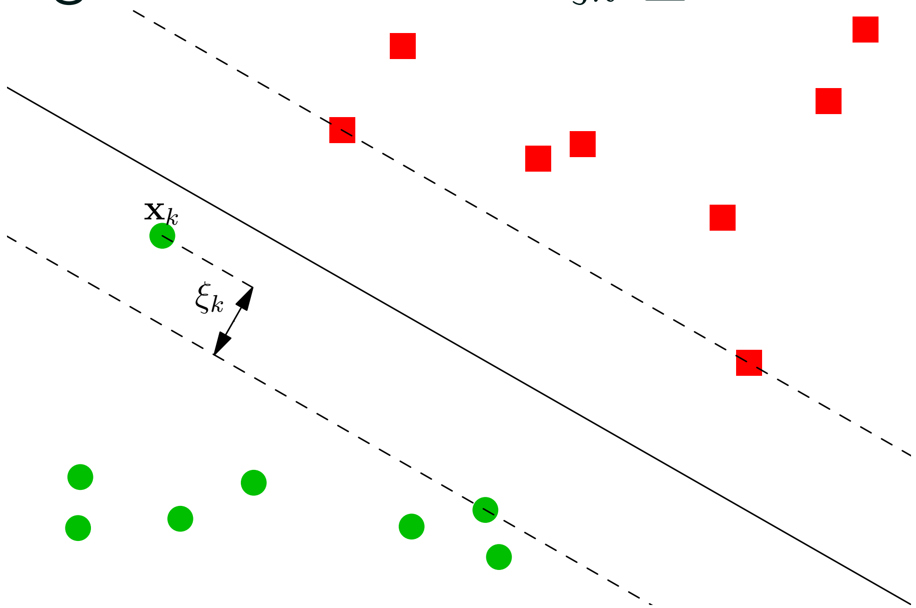

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Choosing the Right Kernel Function

- 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
- Kernel's often come with parameters, e.g. the popular radial basis function kernel

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

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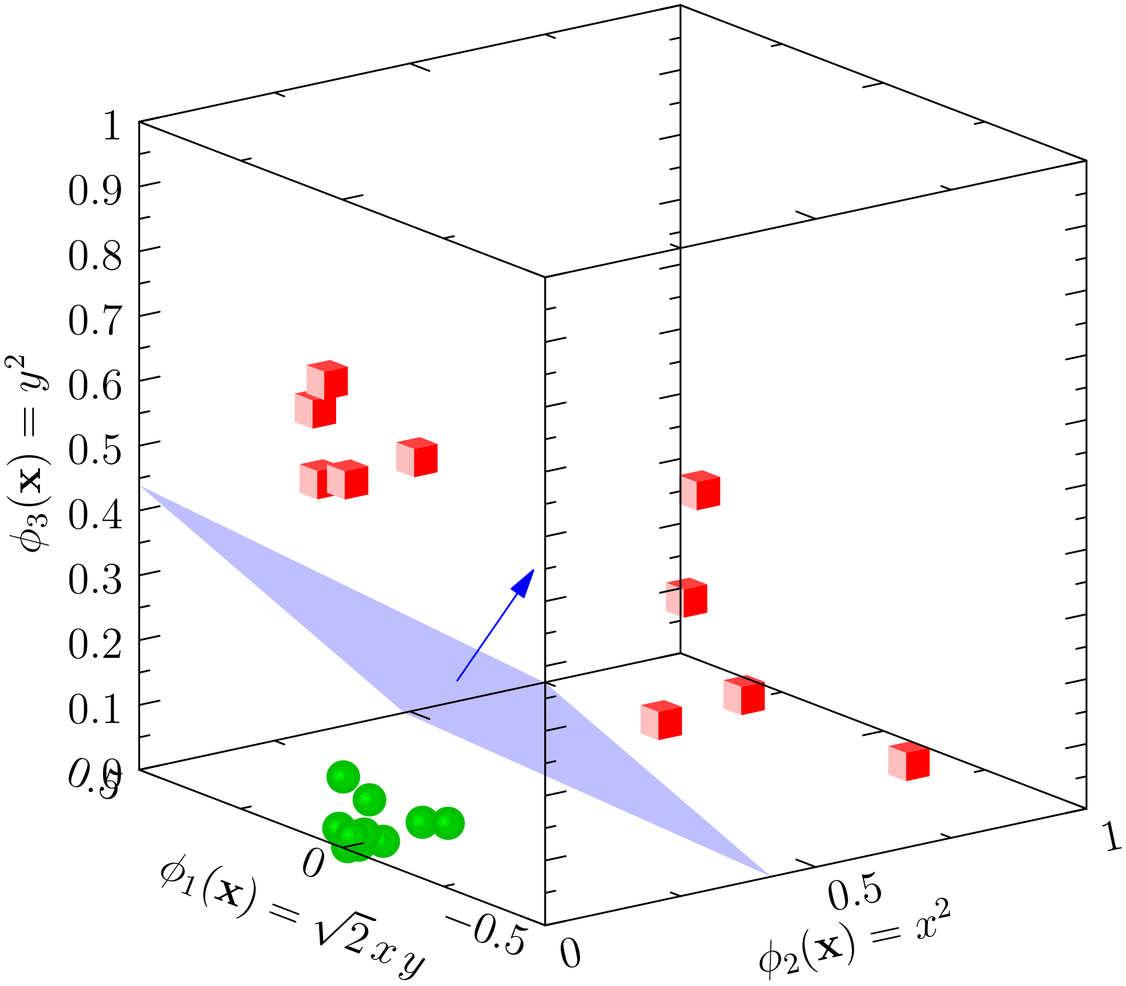
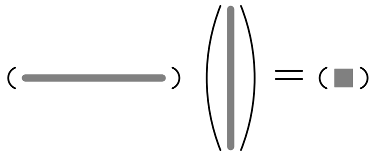
Outline

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



Dot Product

- Recall the dot product



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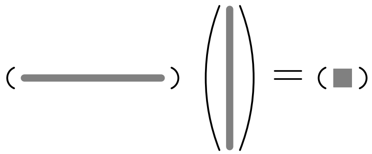

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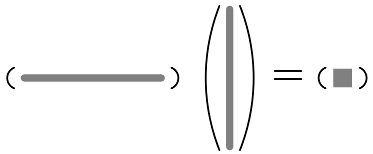

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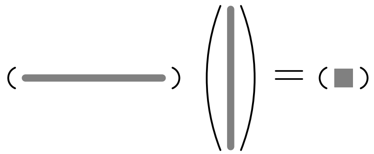

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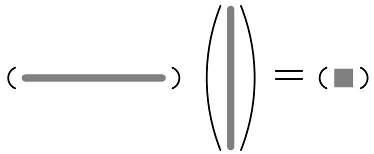

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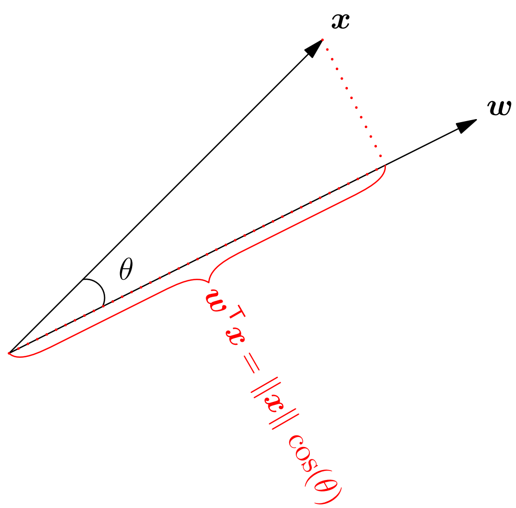

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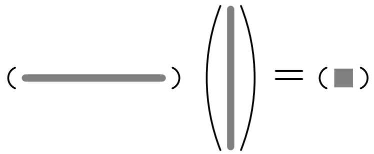

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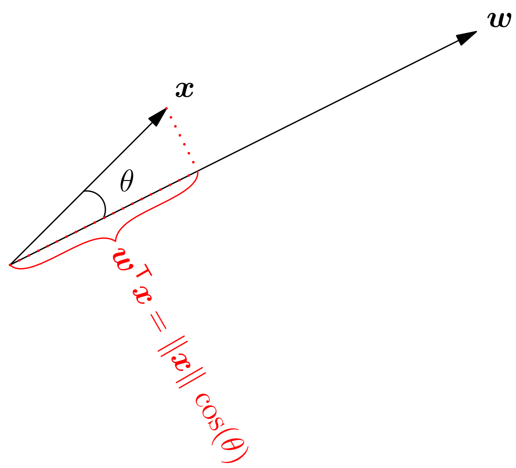

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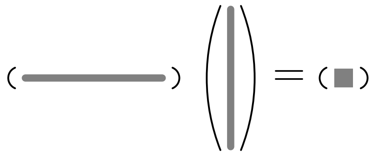

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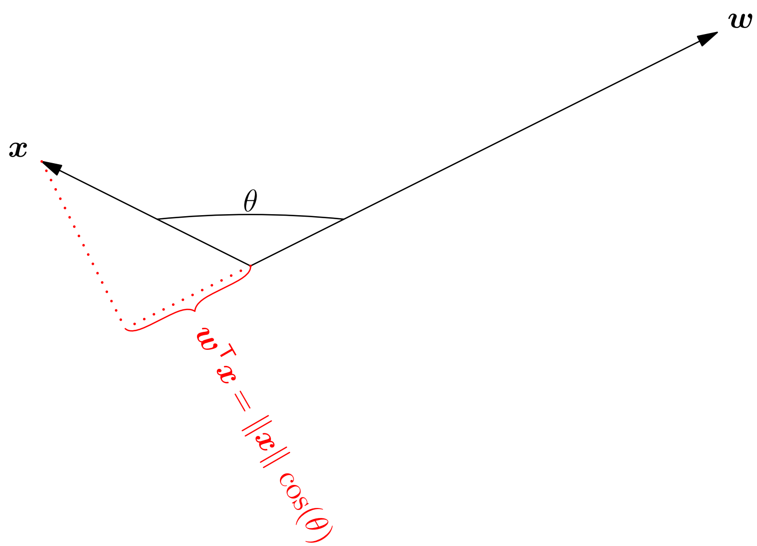

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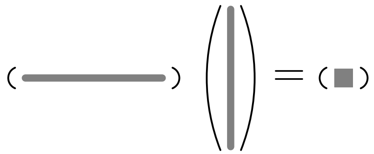

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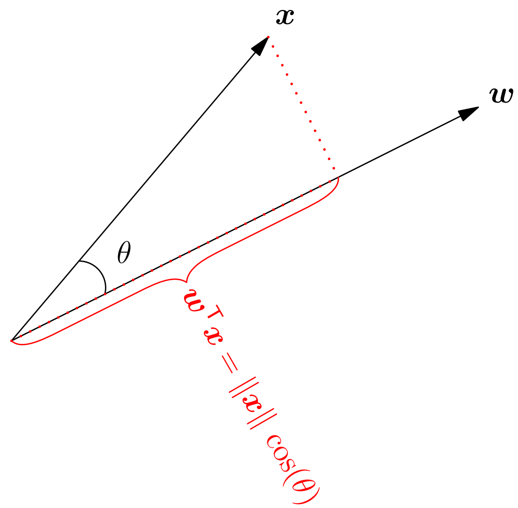

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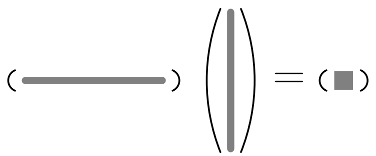

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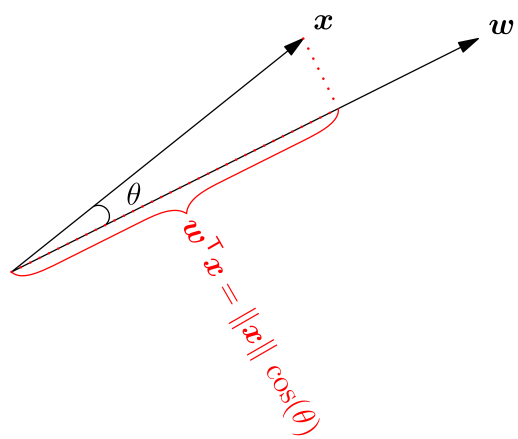

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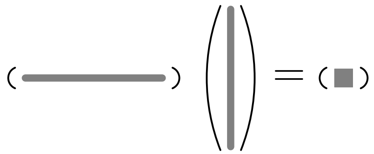

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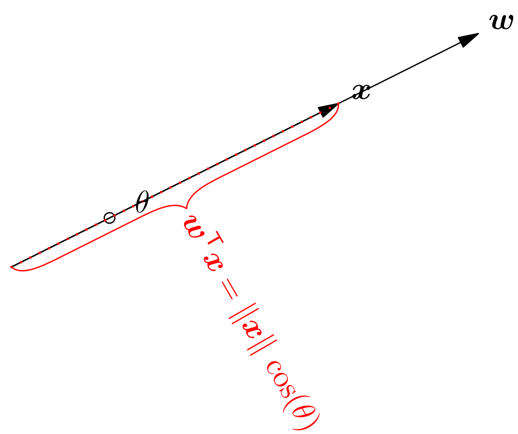

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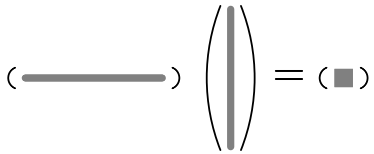

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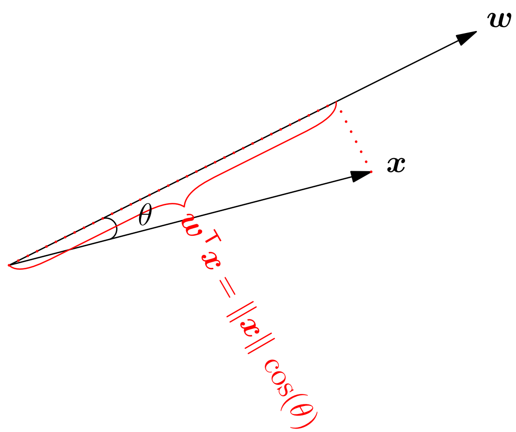

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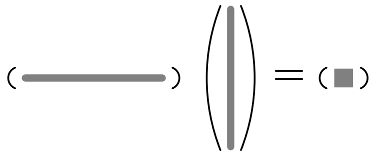

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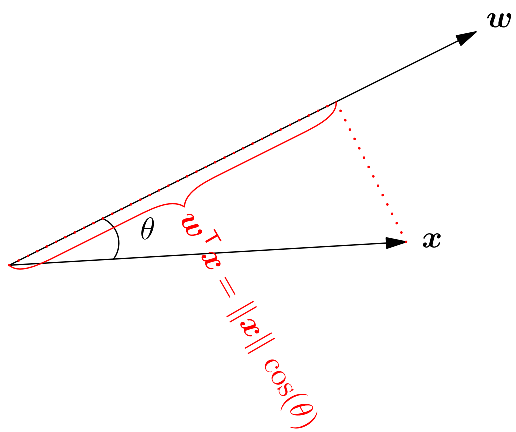

Maximise Margin

- Consider a linearly separable set of data
  - ⋆ $\mathcal{D} = \{(\boldsymbol{x}_k, y_k)\}_{k=1}^{P}$
  - ⋆ $y_k \in \{-1, 1\}$

- 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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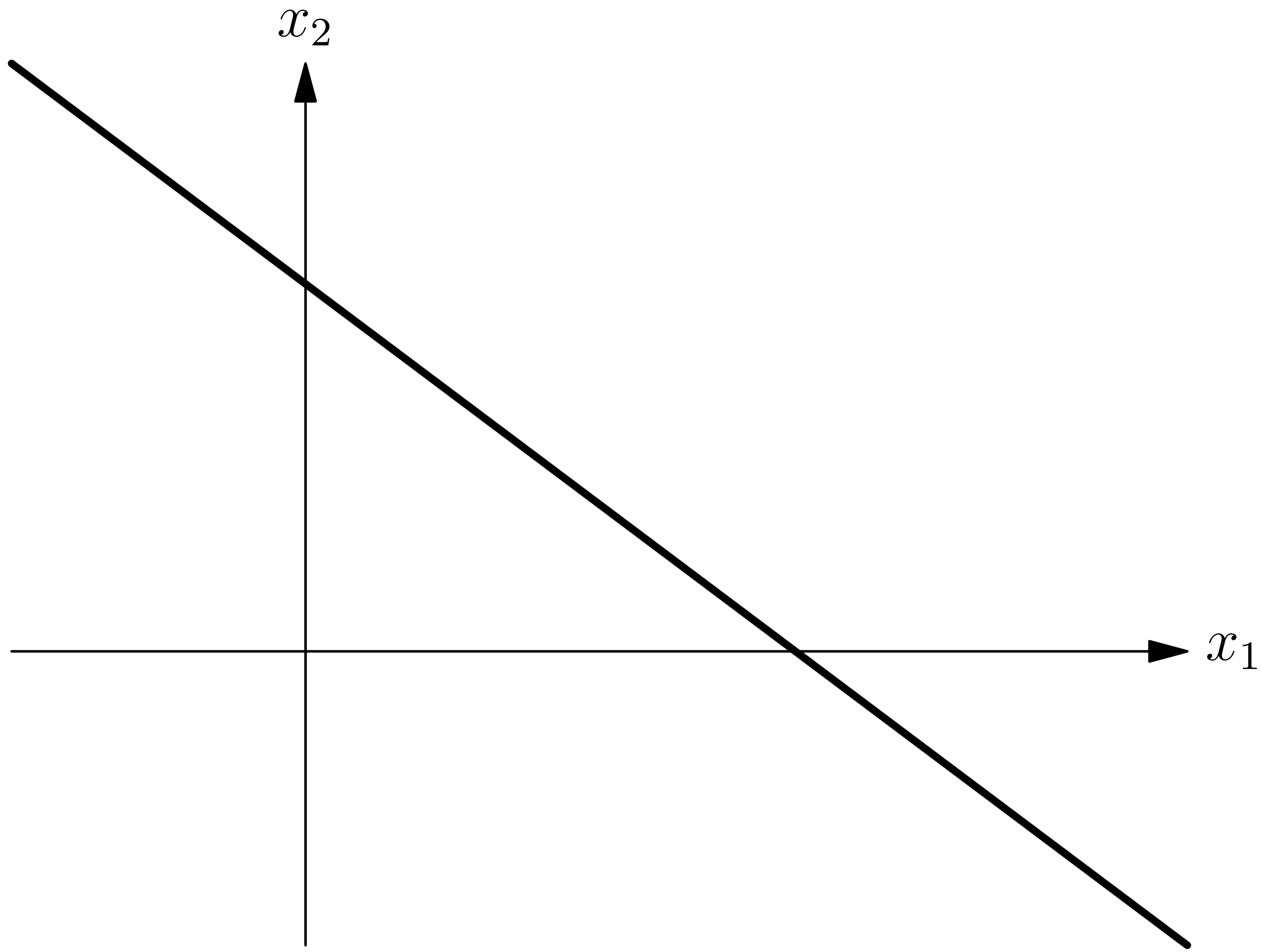

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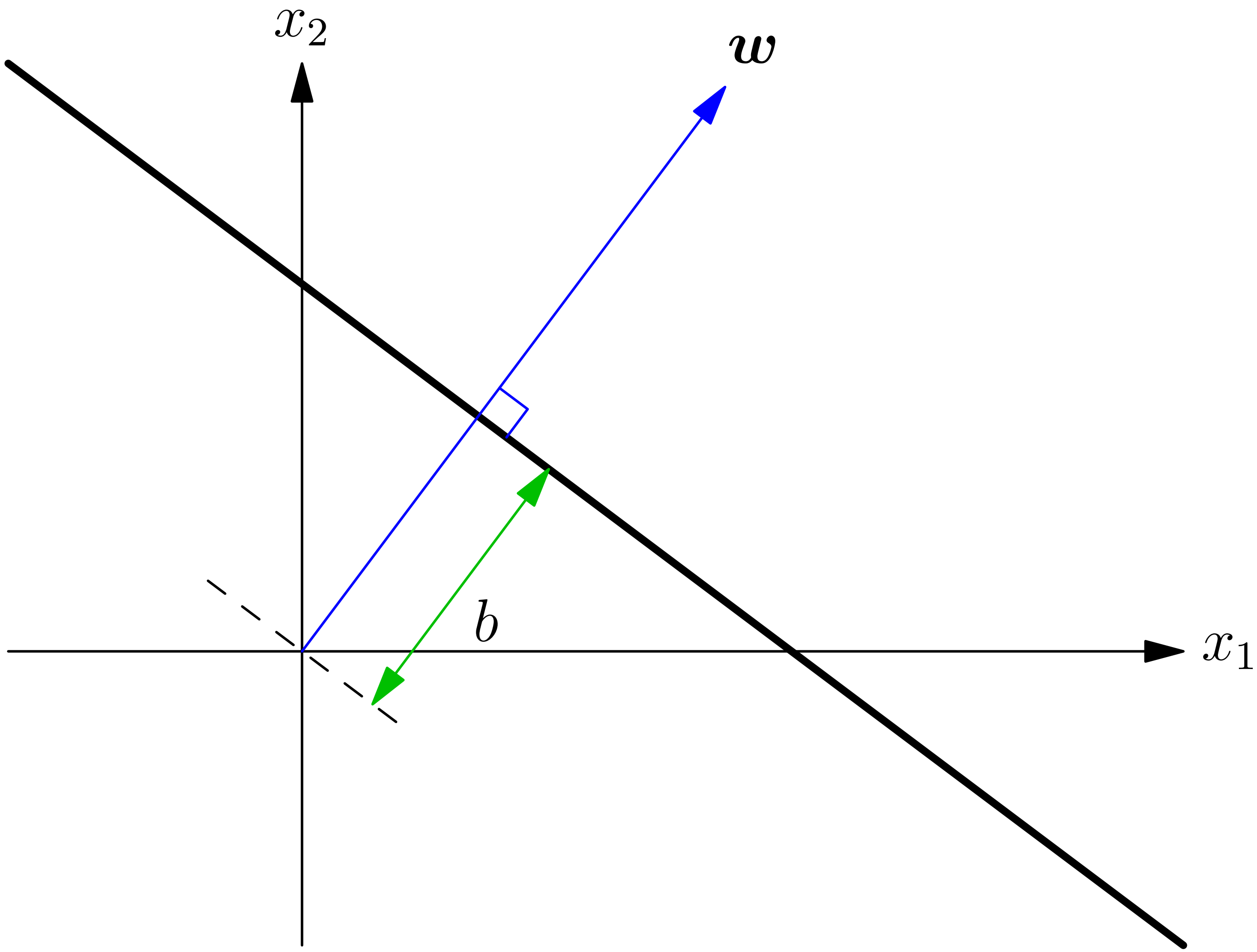

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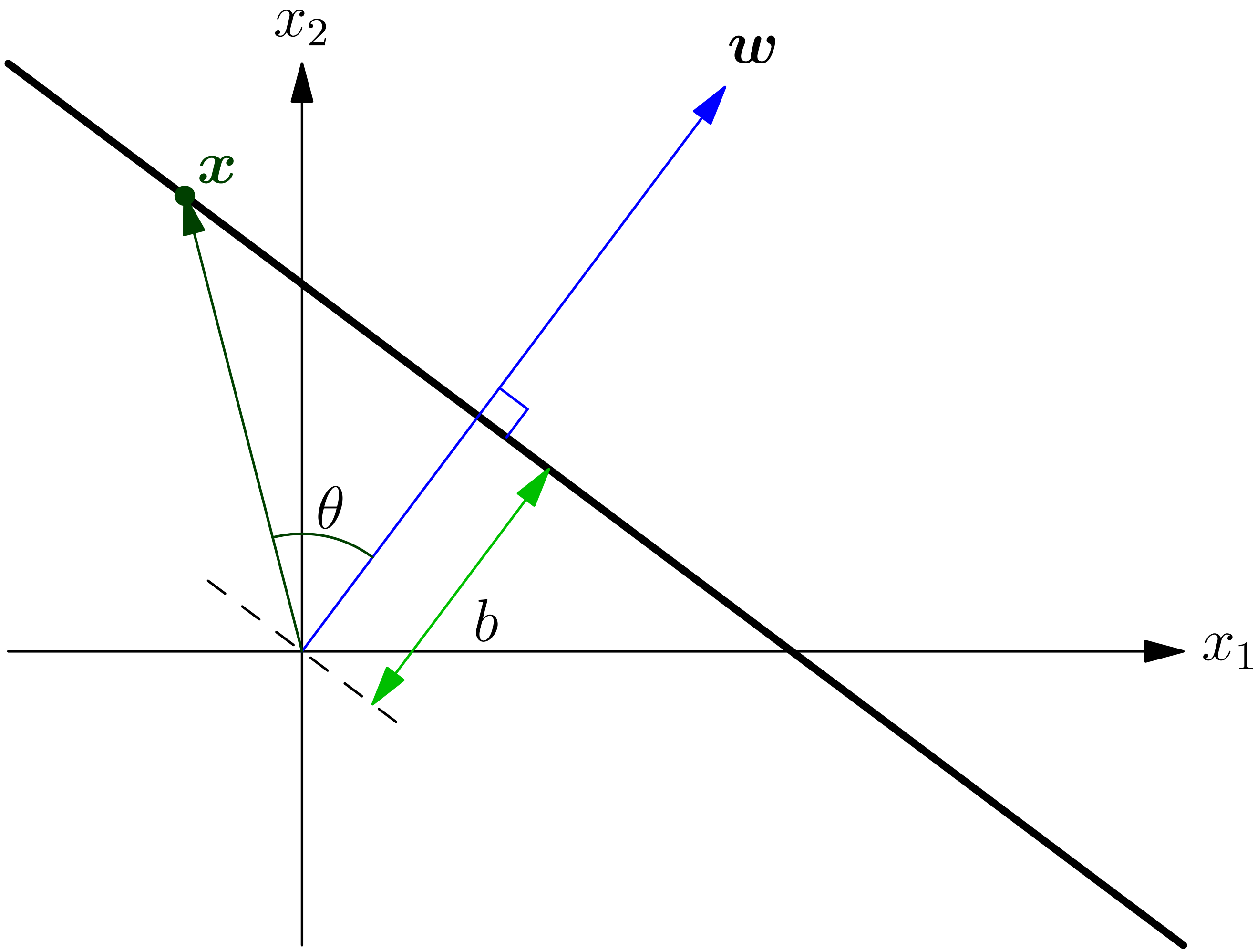

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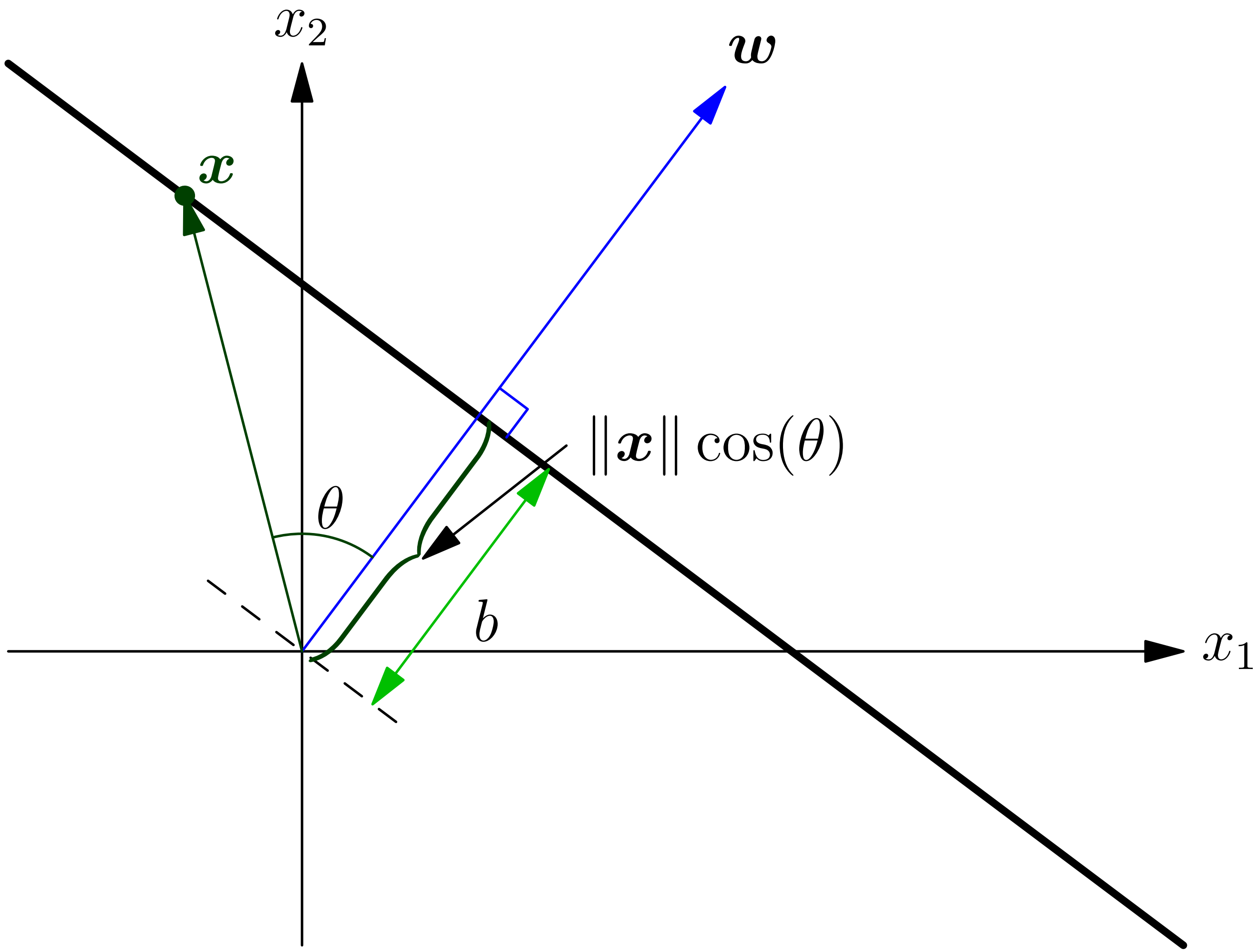

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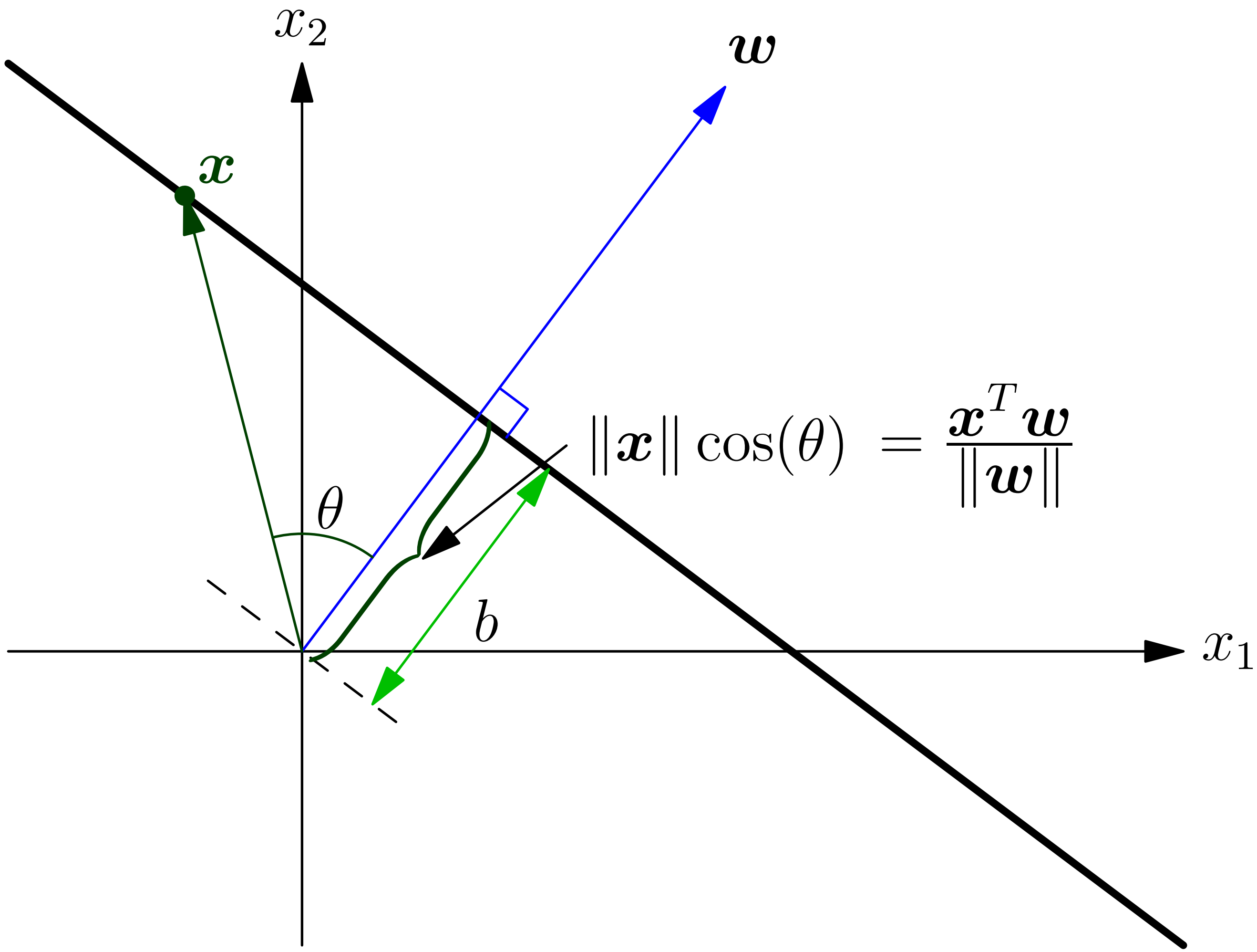

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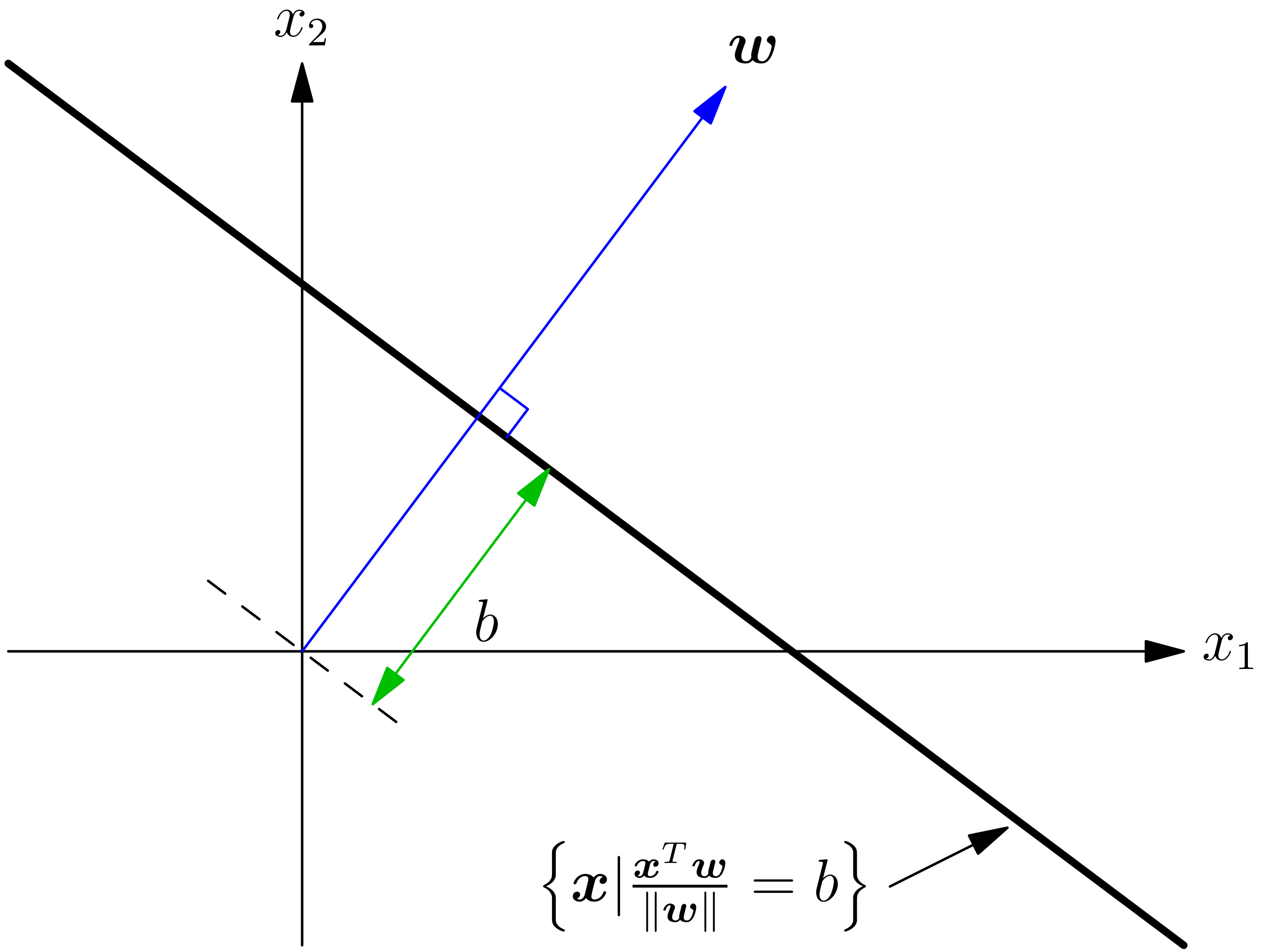

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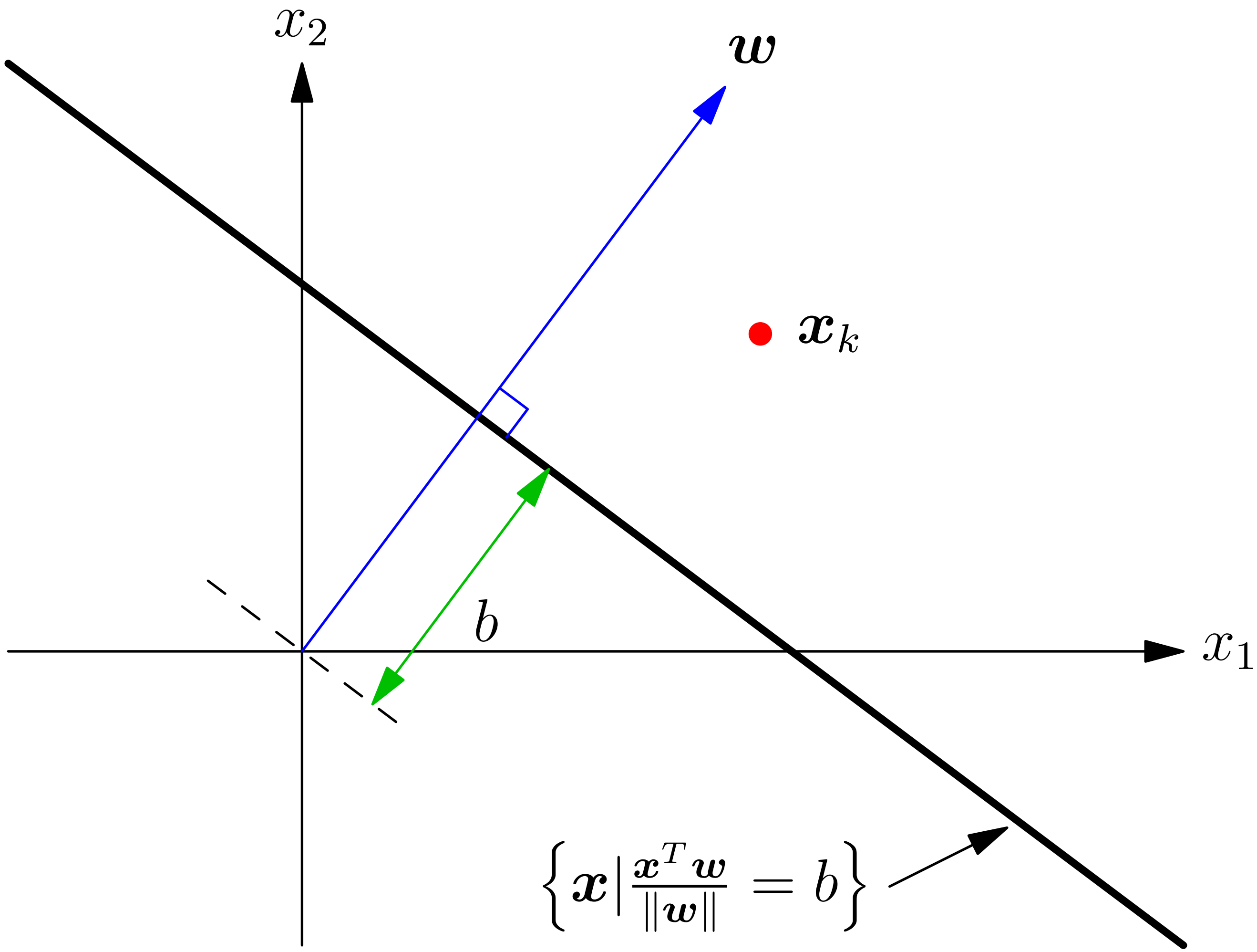

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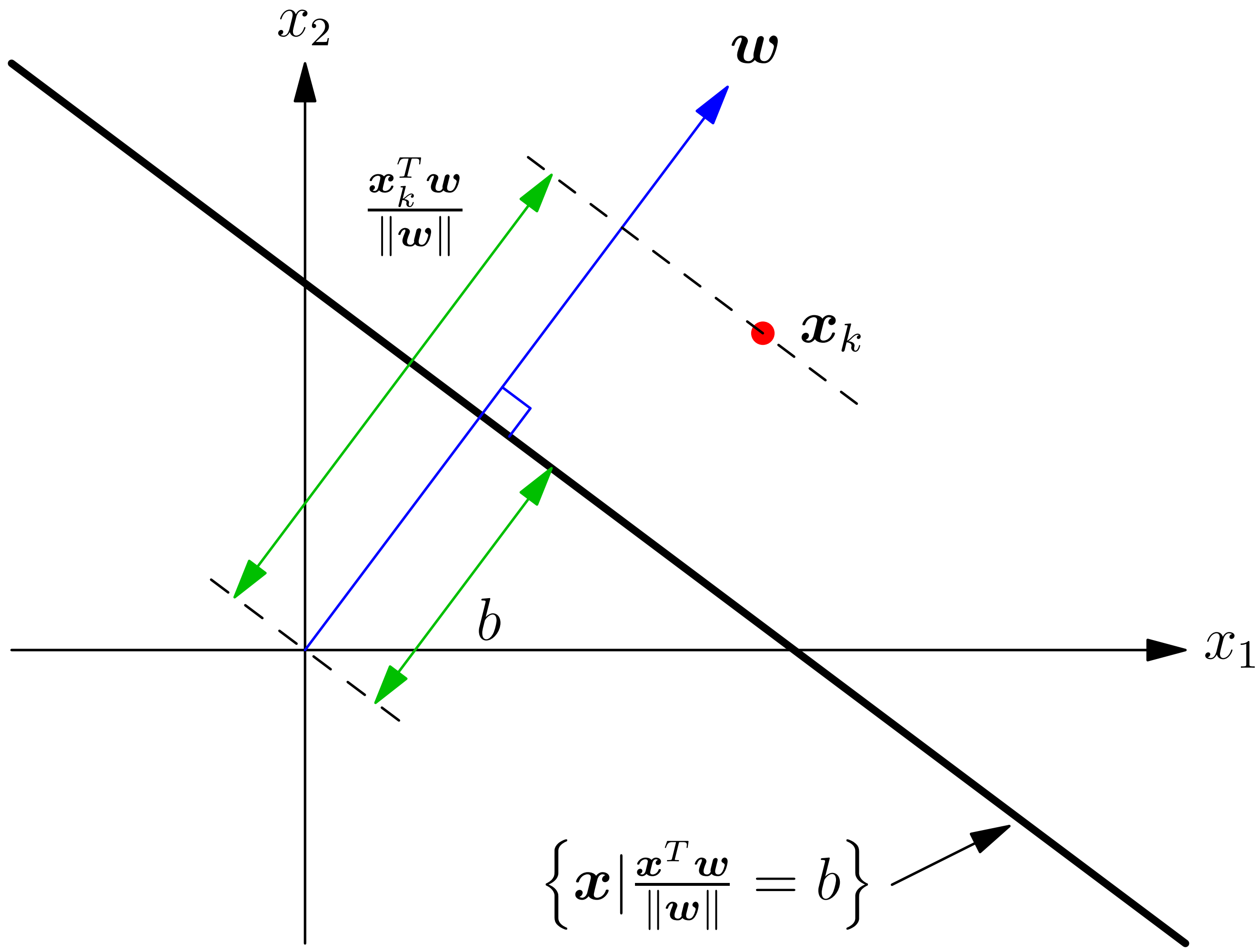

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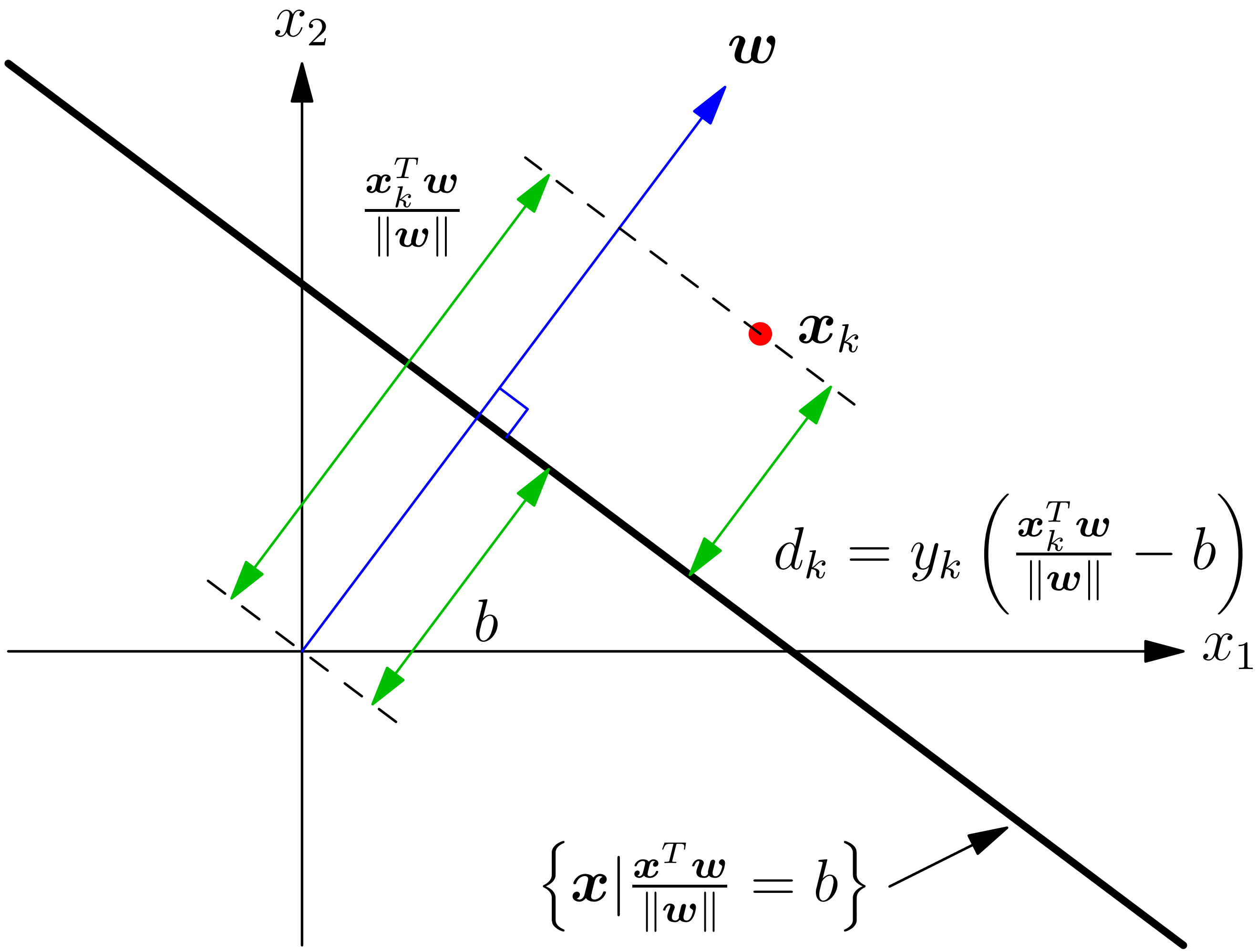

Constrained Optimisation

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

- If we divide through by m

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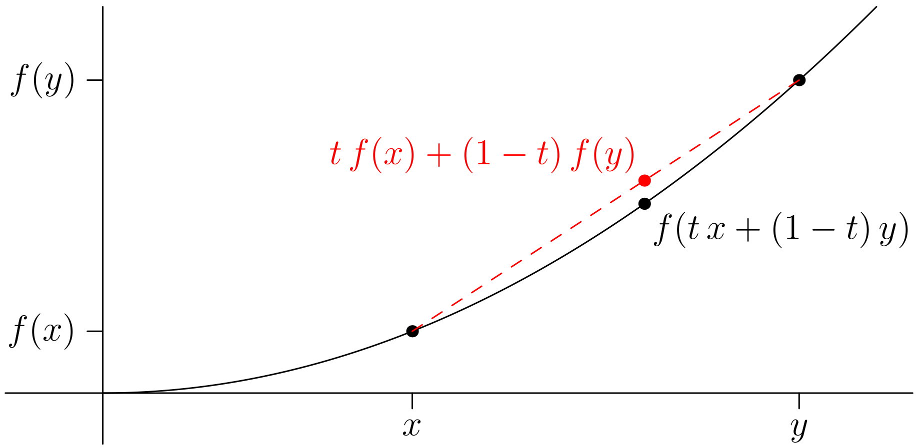
Convexity

- The quadratic function $f(x) = x^2$ is an example of a *convex* function satisfying

$$f(tx + (1-t)y) \leq t f(x) + (1-t) f(y) \quad \text{for } 0 \leq t \leq 1$$



- This extends to high dimensions
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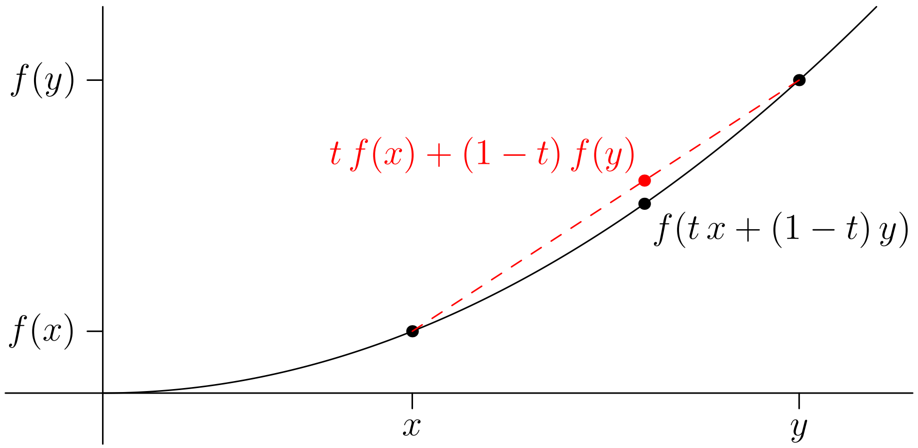

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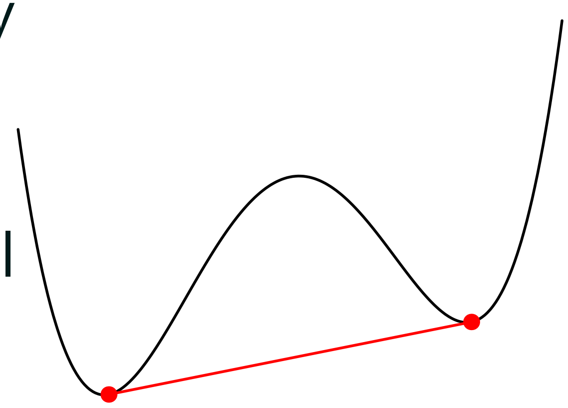
Unique Minimum

- Convex function have a unique minimum

- The existence of a local minimum would break convexity
  - The line connecting a local minimum to a global minimum would be strictly decreasing
  - Thus there are points next to the local minimum with lower values
  - This is a contradiction



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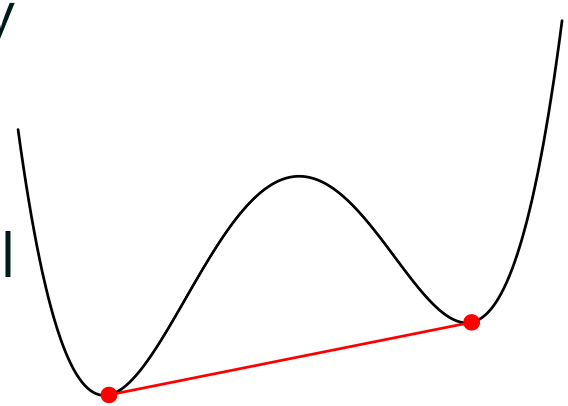

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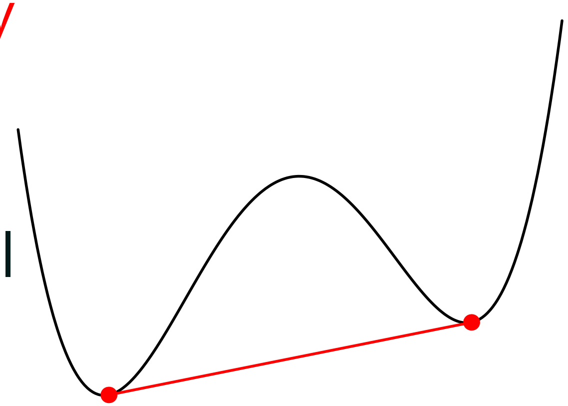

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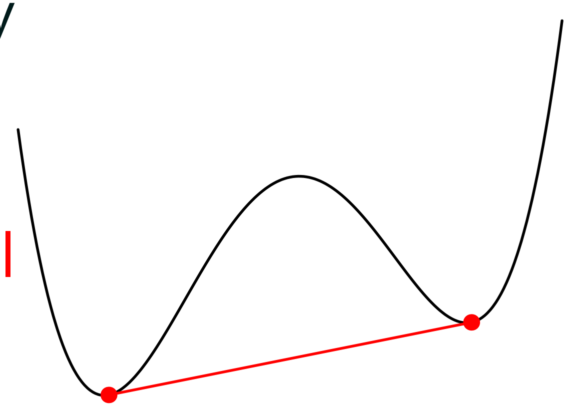

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    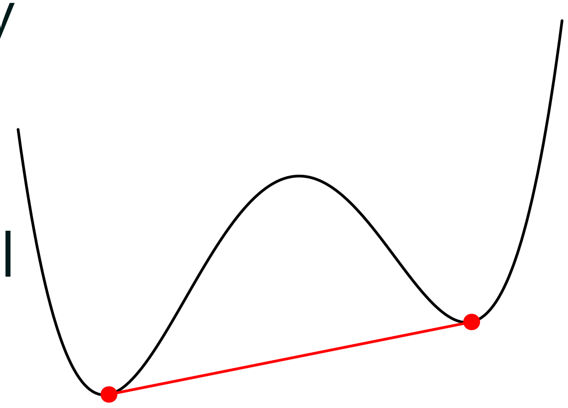

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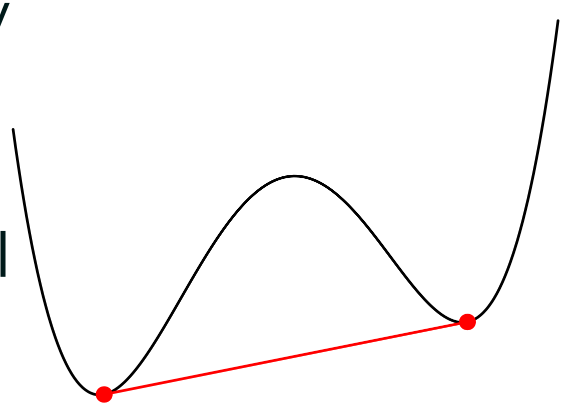

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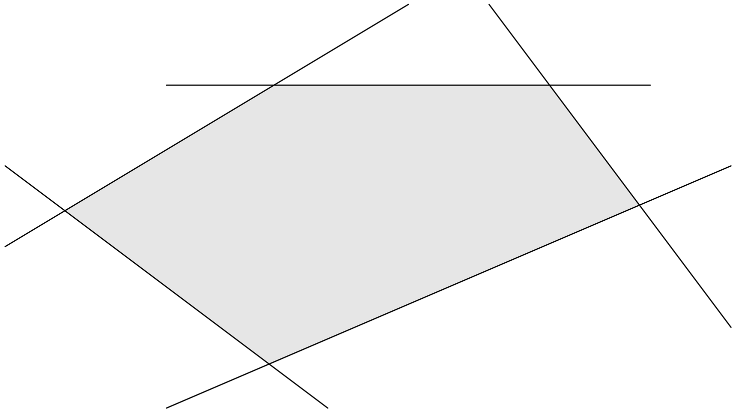

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- Convex function constrained to lie in a convex region will also have unique minima as minima can't hide in corners unlike concave regions

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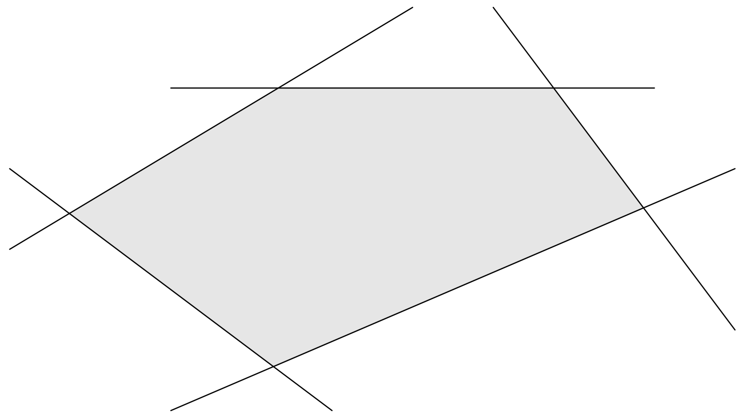

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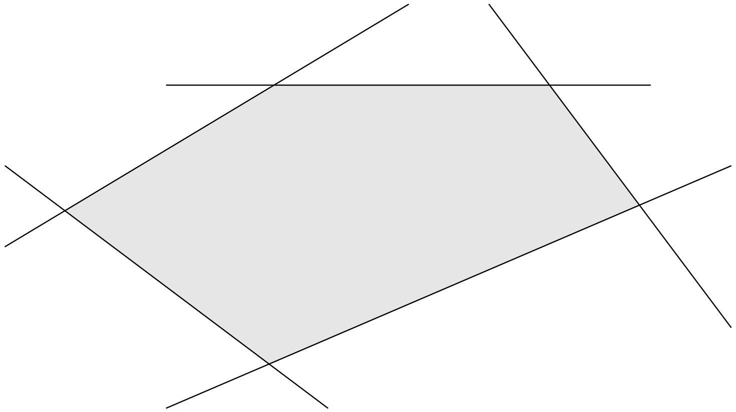

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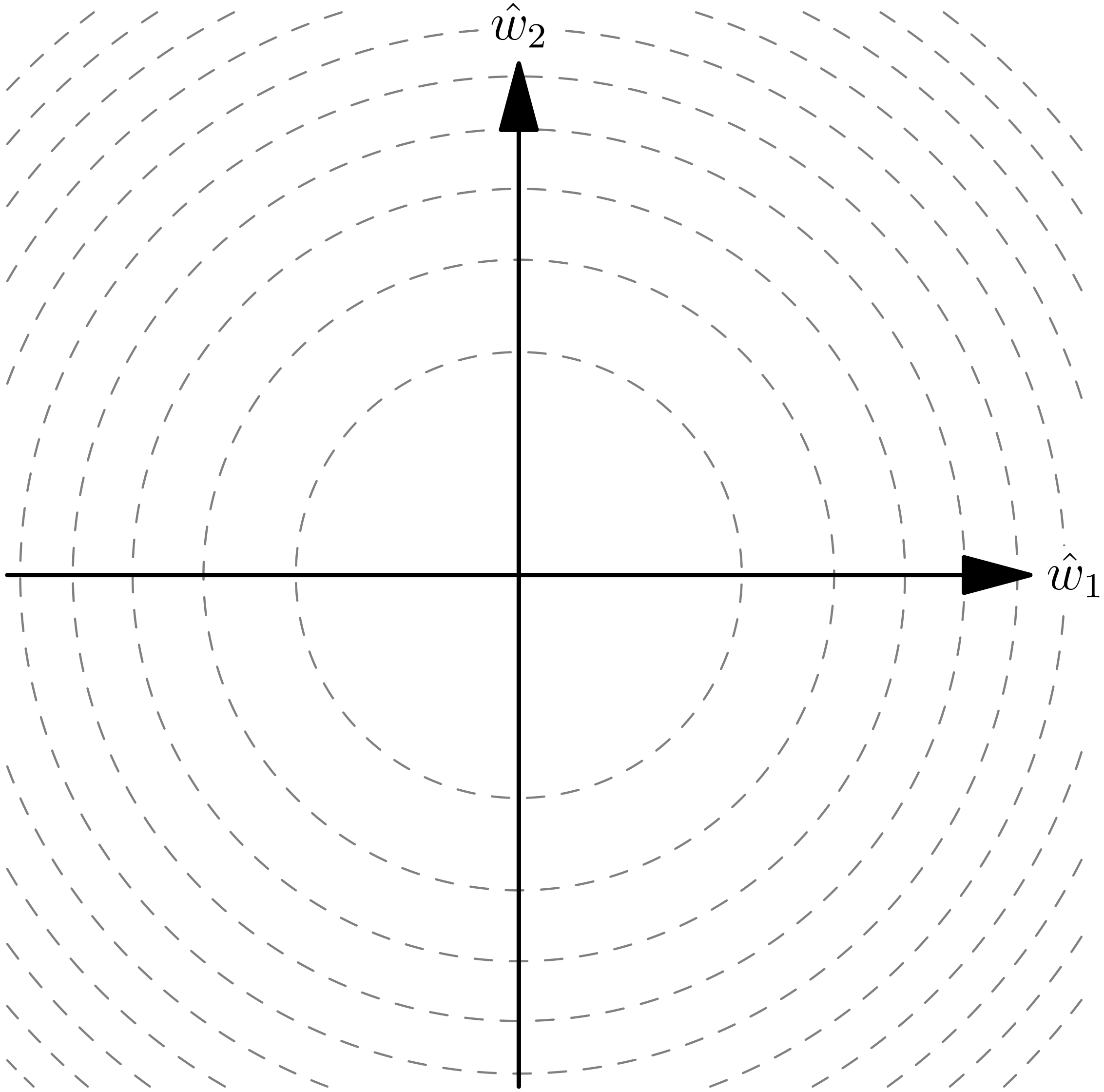
Quadratic Programming in SVMs



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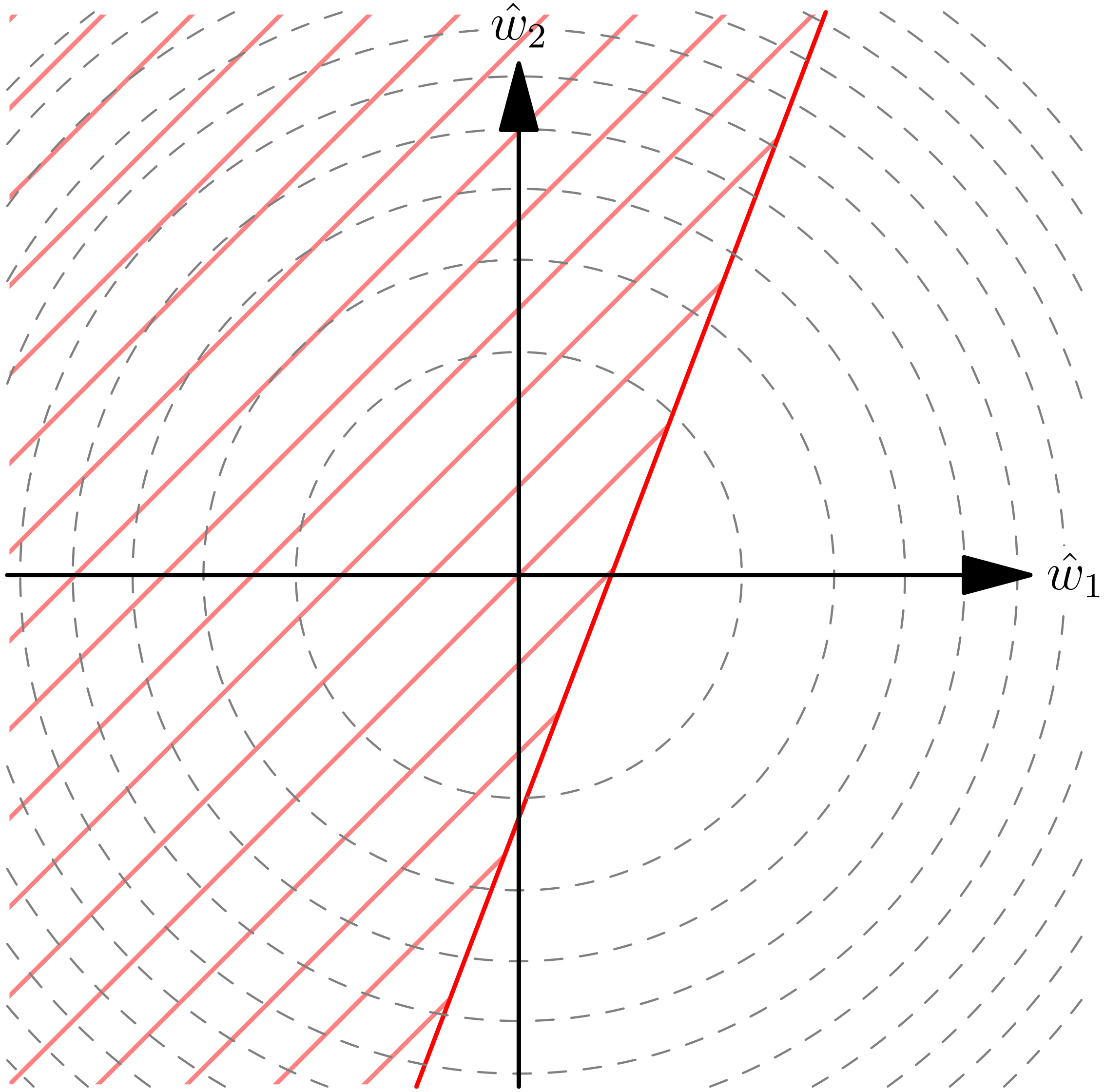

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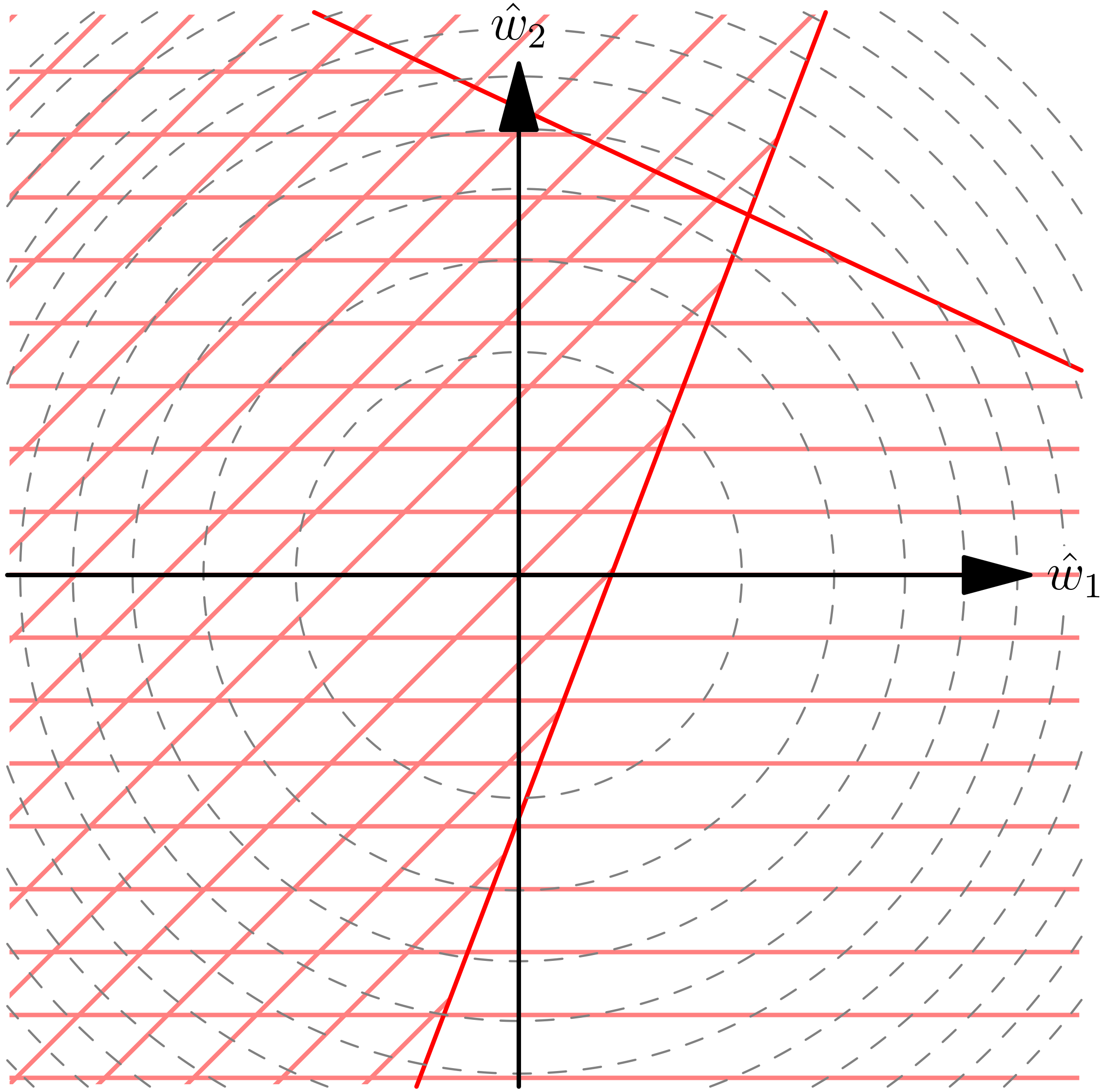

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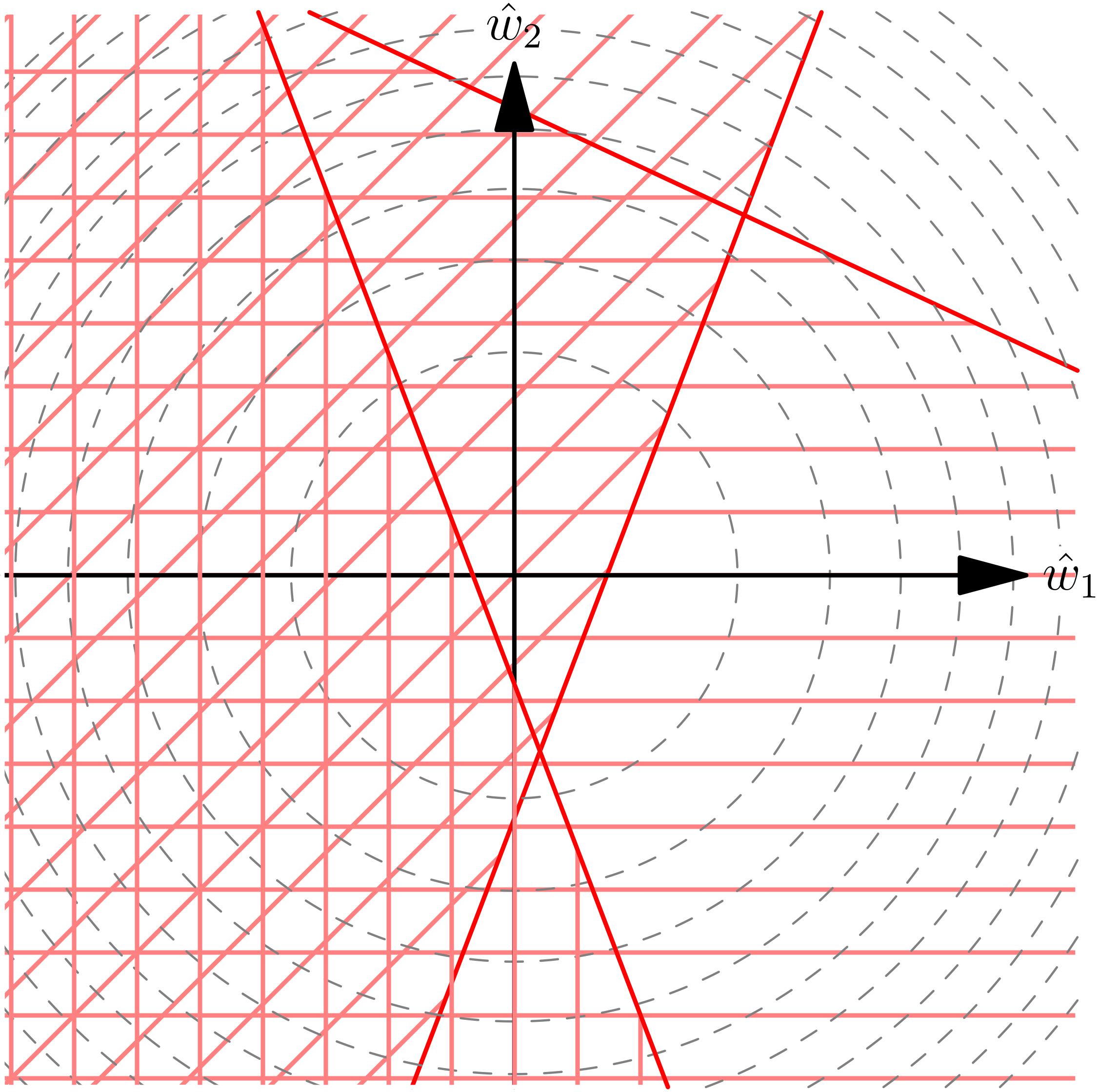

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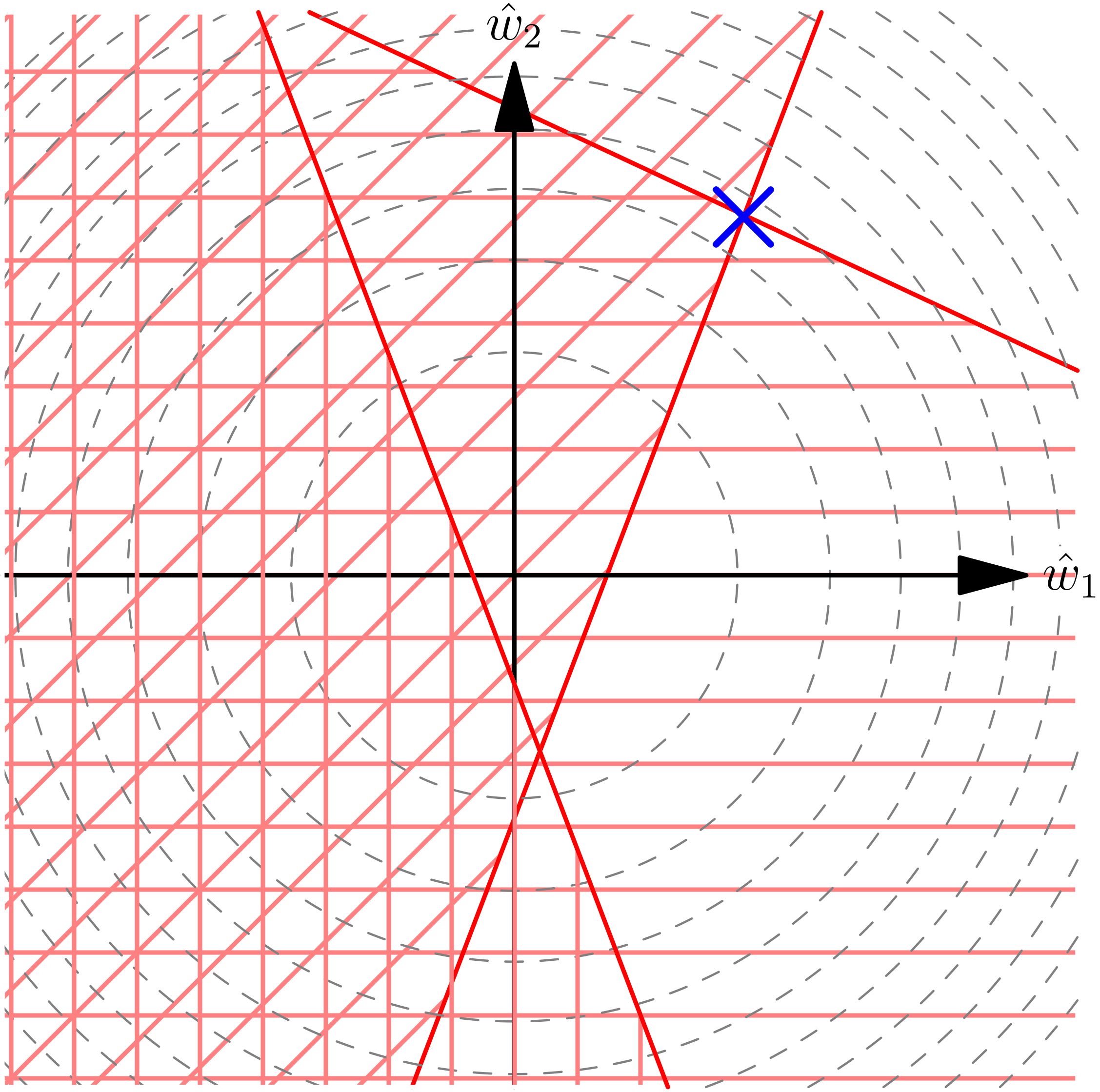

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- We have a quadratic programming problem for the weights $\hat{\boldsymbol{w}} = (\hat{w}_1, \hat{w}_2, \ldots, \hat{w}_n)$ and bias b and P constraints
- This is a classic but fiddly optimisation problems
- It can be solved in $O(n^3)$ time (it involves inverting matrices)
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Soft Margins

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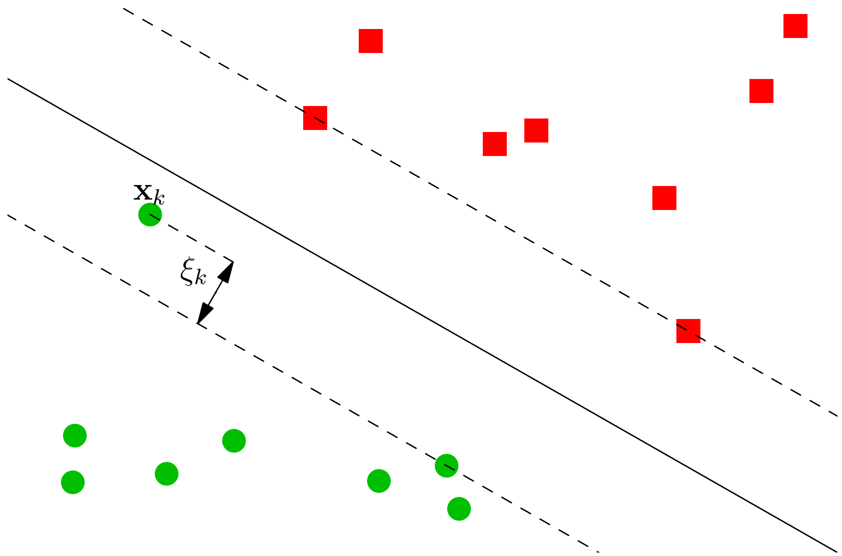
$$y_k(\hat{\boldsymbol{w}}^\mathsf{T}\boldsymbol{x}_k - \hat{b}) \geq 1 - \xi_k$$



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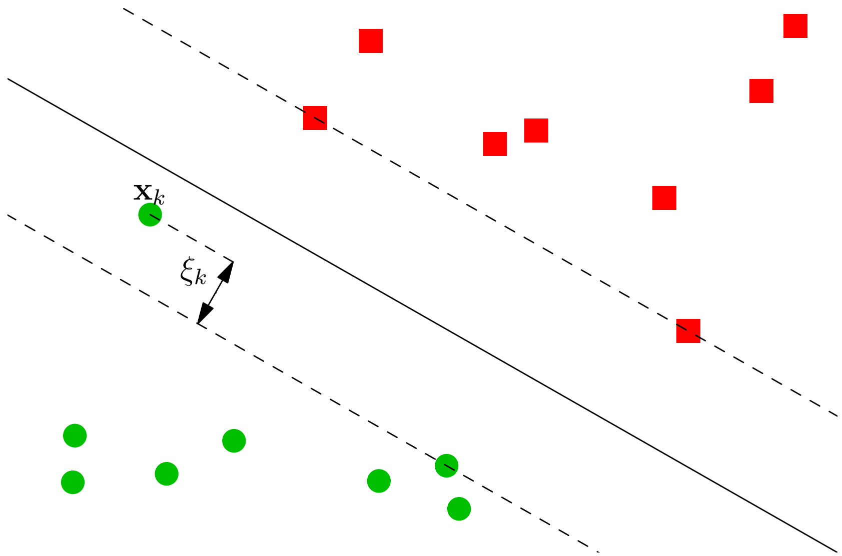

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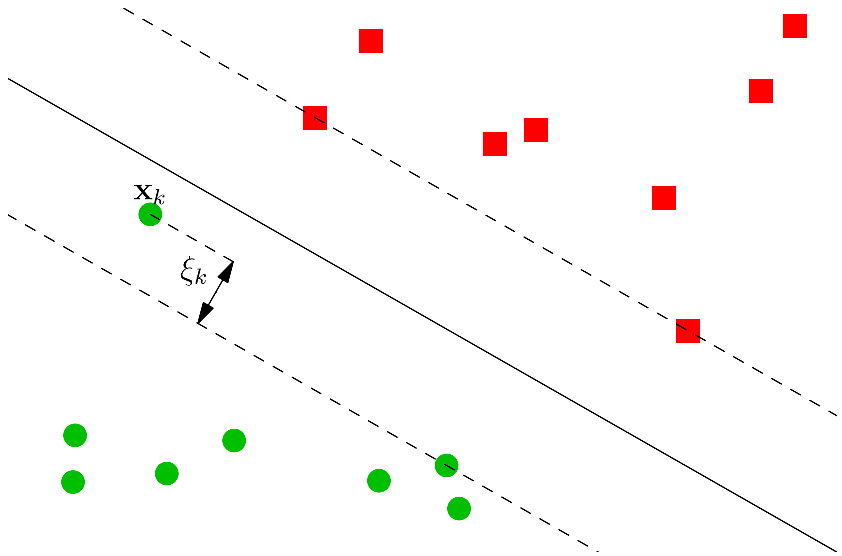

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