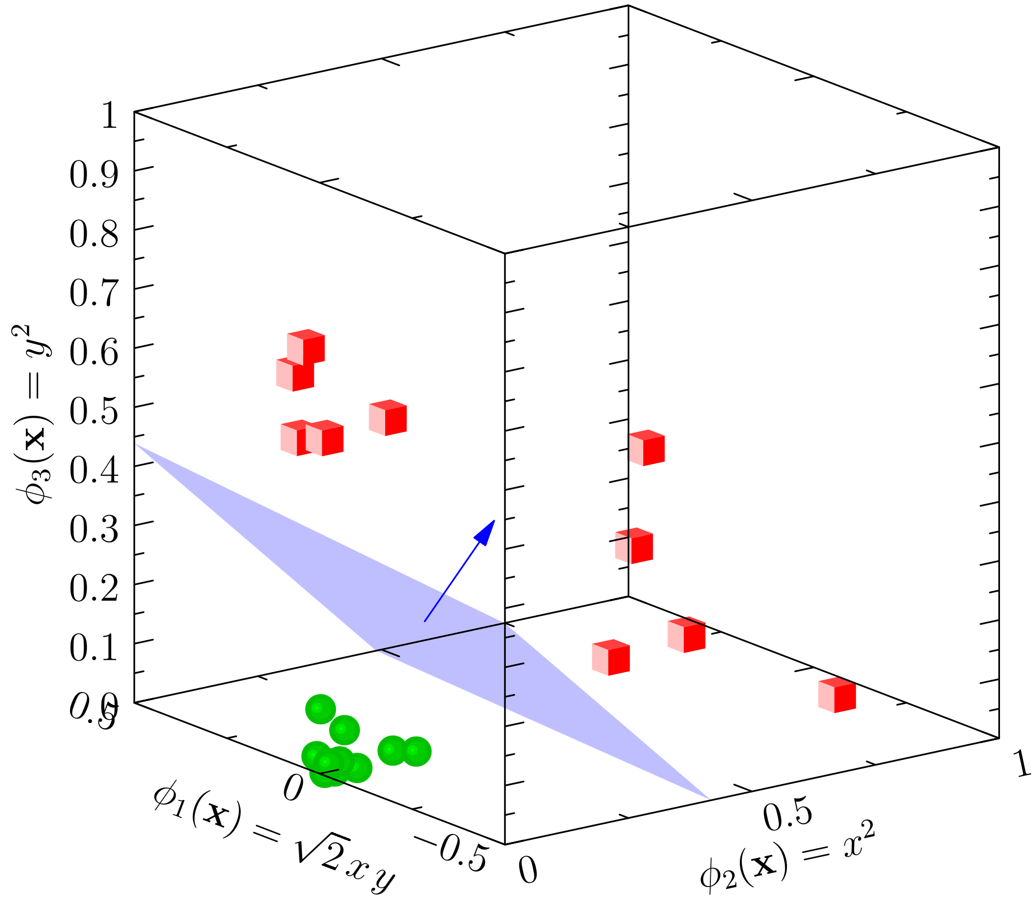
Advanced Machine Learning

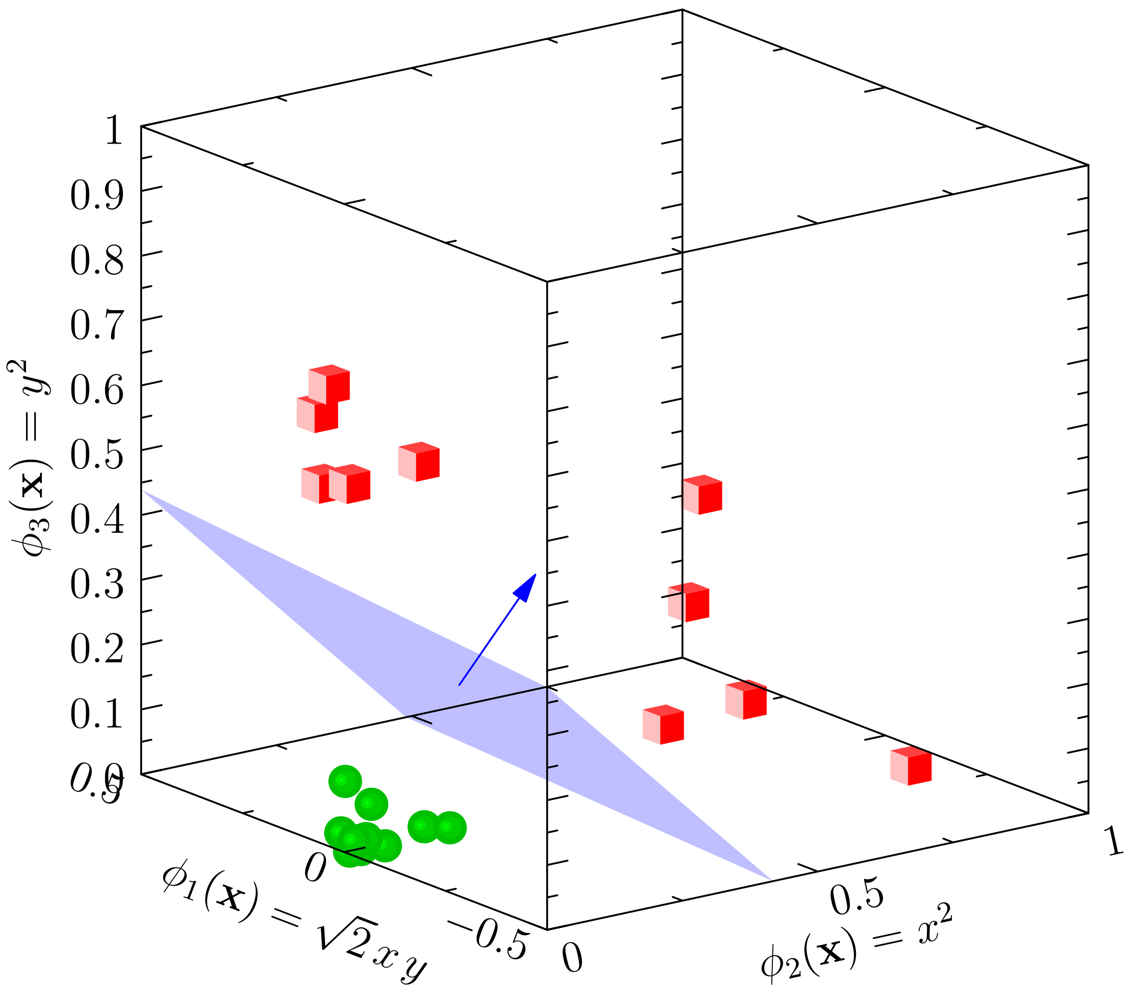
Dual Algorithm



Constrained Optimisation, Lagrangians, Dual Algorithm

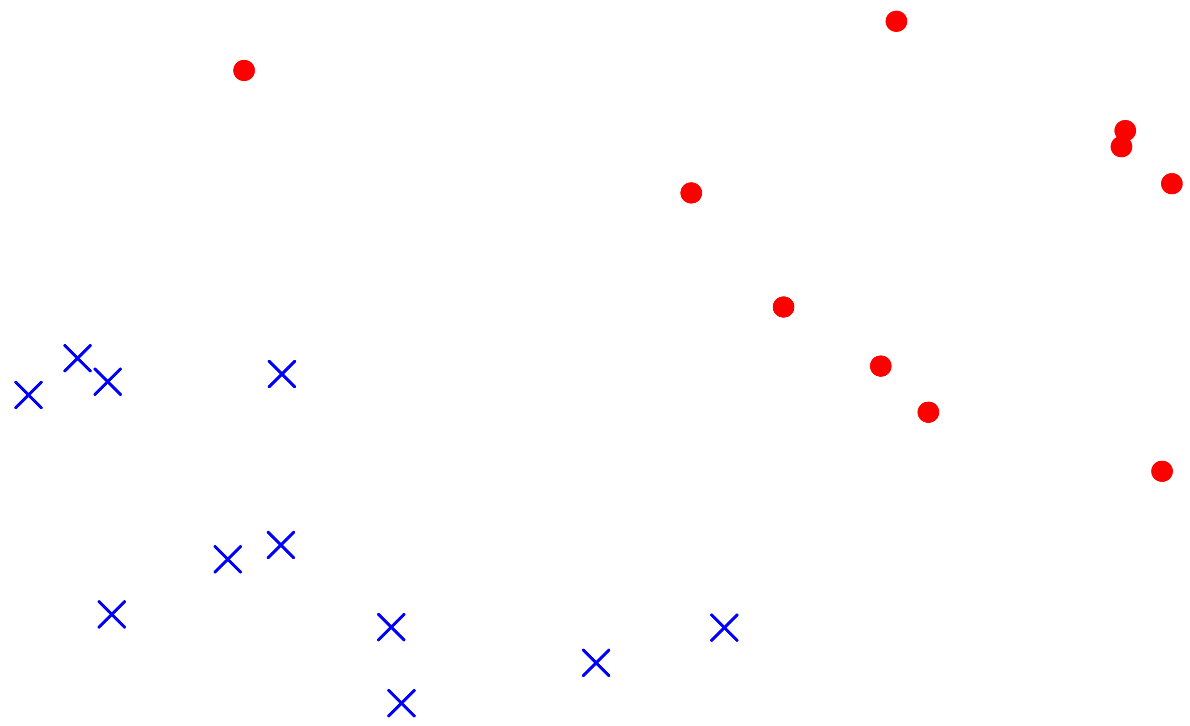
Outline

1. **Recap**
2. Constrained Optimisation
3. Duality



Linear SVM

- SVMs finds hyperplane which separates two sets of linearly separable data with maximum margin



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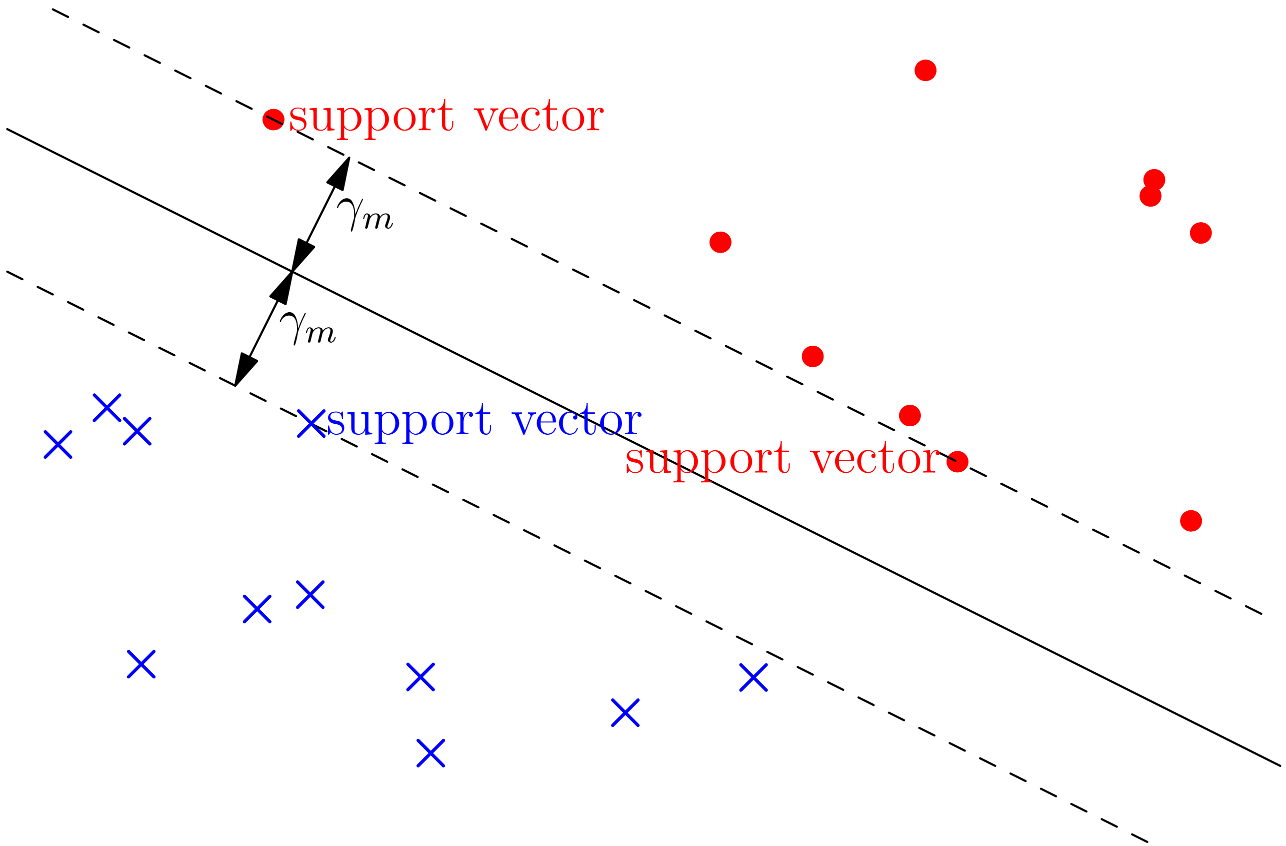

Finding Maximum Margin Hyperplane

- We showed to find the maximum margin hyper-plane we can solve

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

(I've got rid of the hats on $\boldsymbol{w}$ and b because life is too short)

- This is a quadratic programme (a quadratic function with linear constraints)
- Quadratic programmes have a unique solution
- This is generally true of convex function optimisation

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Extended Feature Spaces

- If we map into an extended feature space

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

  $r \gg p$

- The optimisation problem becomes

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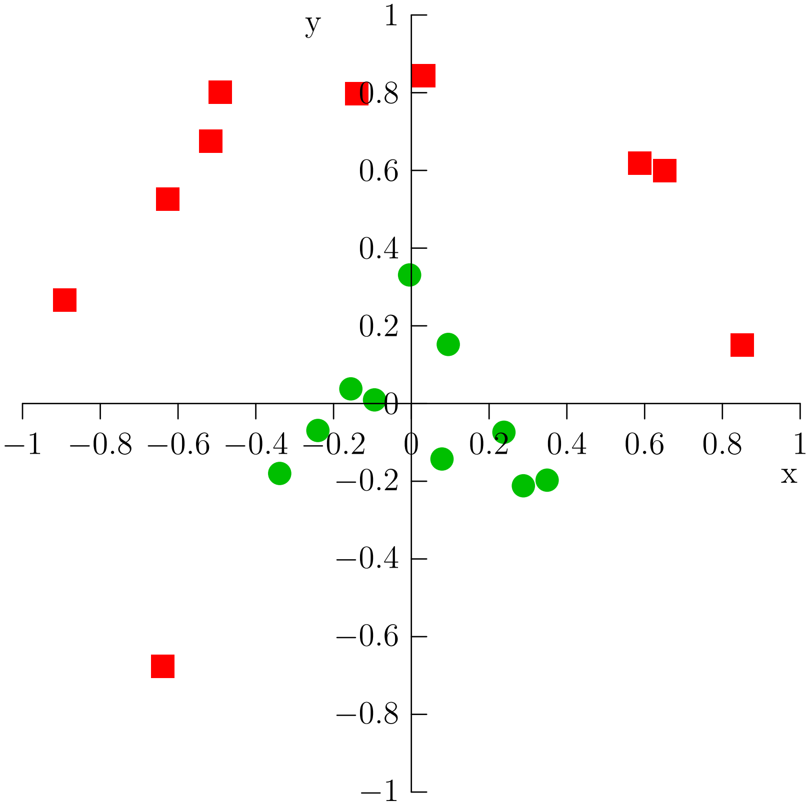
Non-linearly Separation of Data

$$\boldsymbol{x} = \begin{pmatrix} x \\ y \end{pmatrix} \to \vec{\phi}(\boldsymbol{x}) \begin{pmatrix} 2\,x\,y \\ x^2 \\ y^2 \end{pmatrix}$$



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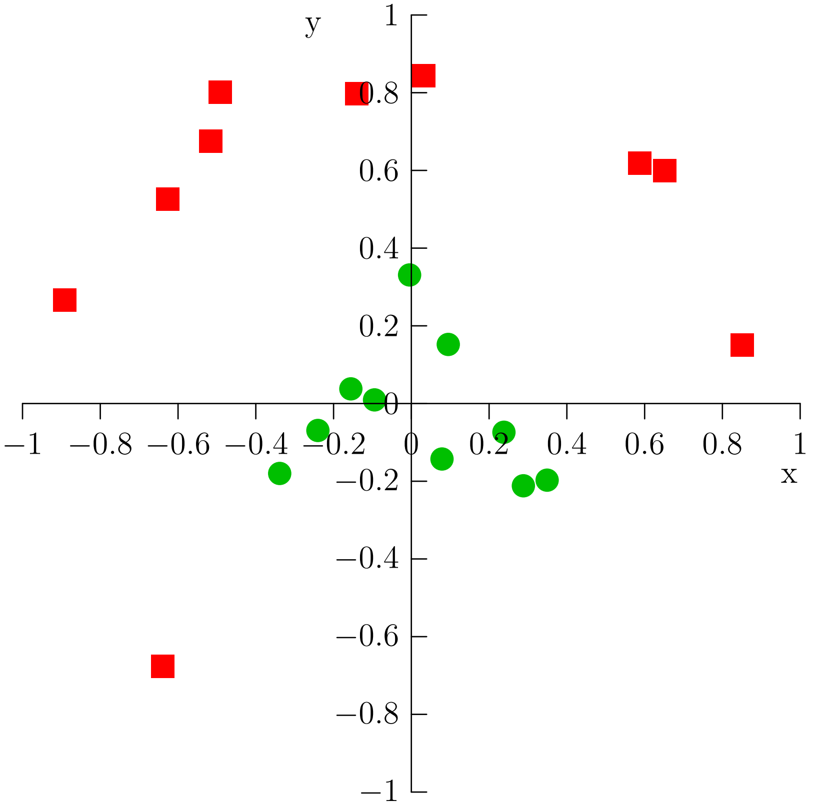

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$\longrightarrow$

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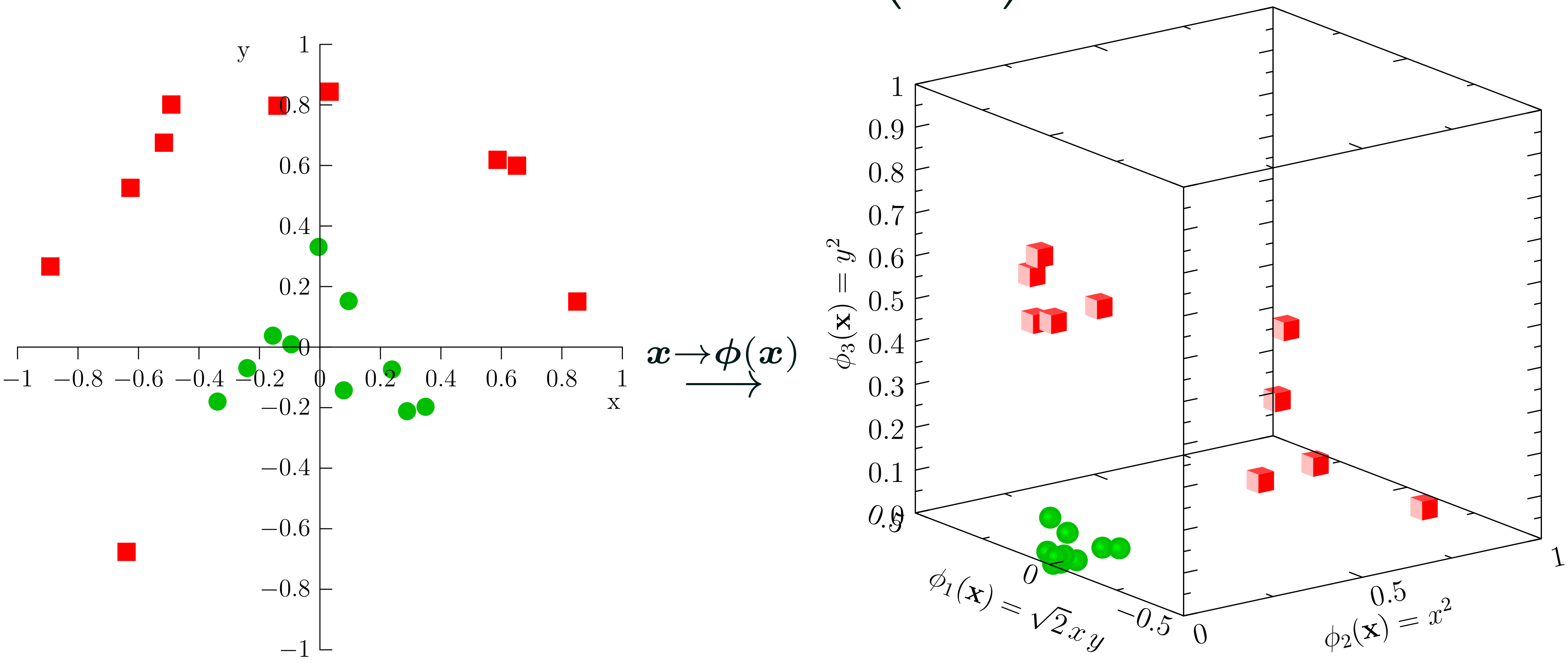

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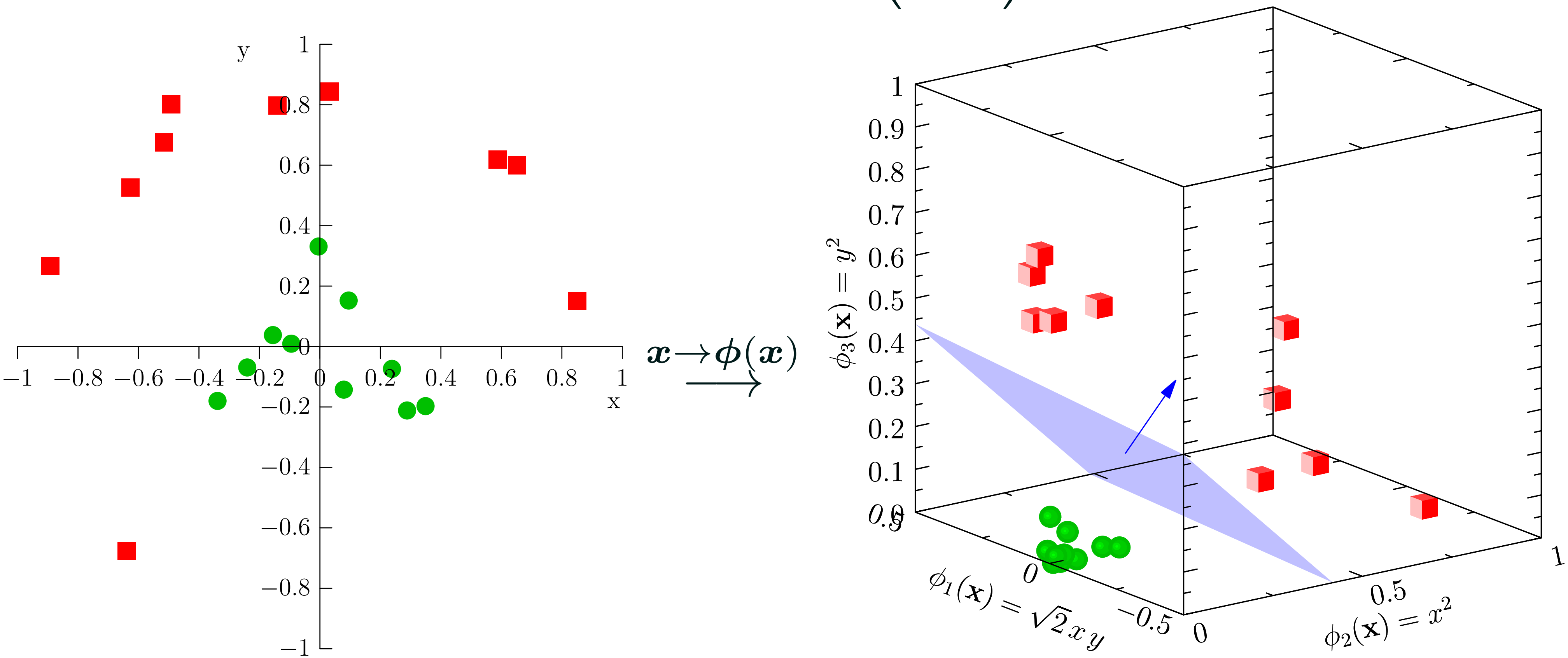

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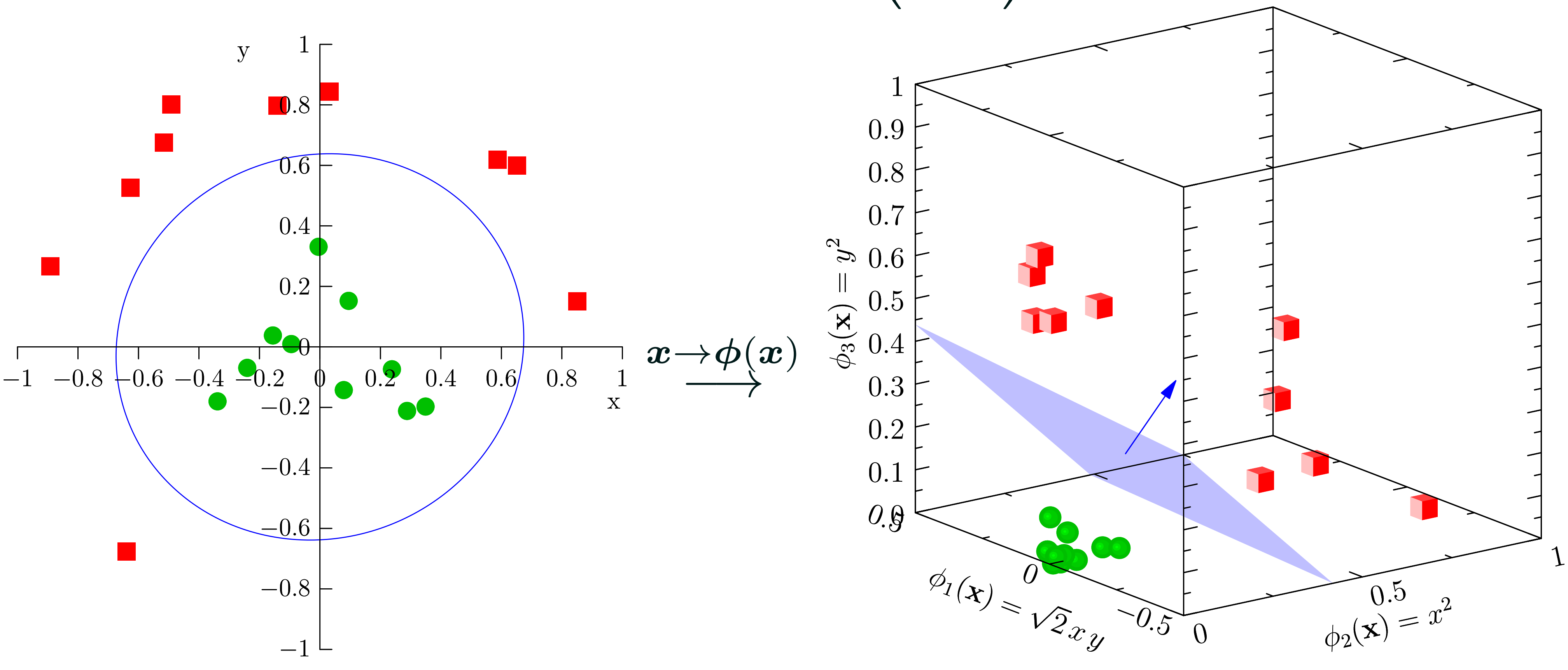

Constrained Optimisation

- Recall that when we try to solve an optimisation problem with constraints we can add Lagrange multipliers

- The optimisation problem becomes

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- Is equivalent to finding the extremal point of the Lagrangian

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

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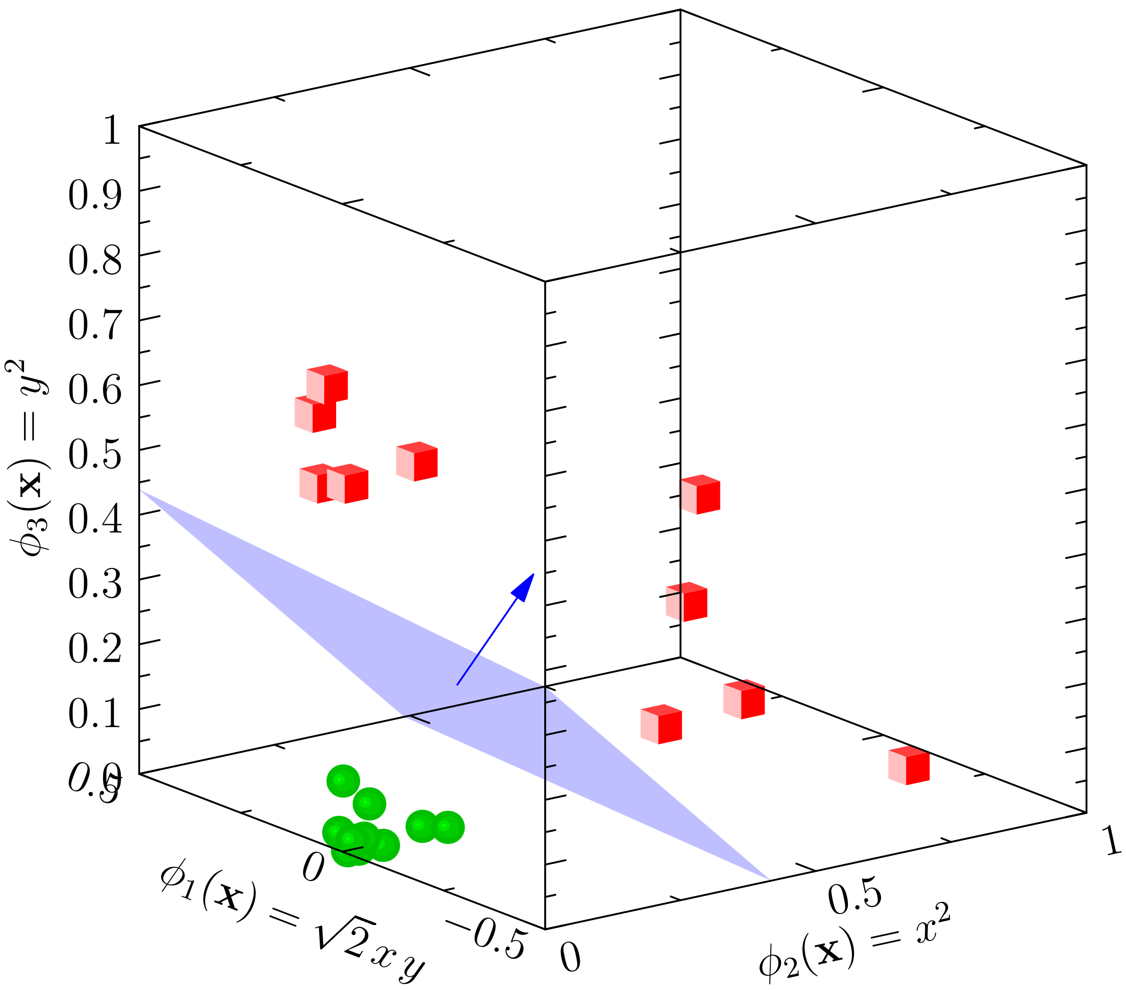

Solving Constrained Optimisation Problems

- Suppose we have a problem

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{subject to } g(\boldsymbol{x}) = 0$$

- A standard procedure is to define the Lagrangian

$$\mathcal{L}(\boldsymbol{x}, \alpha) = f(\boldsymbol{x}) - \alpha\, g(\boldsymbol{x})$$

  where α is known as a Lagrange multiplier

- In the extended space $(\boldsymbol{x}, \alpha)$ we have to solve

$$\max_{\alpha} \min_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \alpha)$$

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Conditions on Optimum

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$$\max_{\alpha} \min_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \alpha) \quad \text{where} \quad \mathcal{L}(\boldsymbol{x}, \alpha) = f(\boldsymbol{x}) - \alpha\, g(\boldsymbol{x})$$

- Assuming differentiability

$$\boldsymbol{\nabla}_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \alpha) = \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x}) - \alpha\, \boldsymbol{\nabla}_{\boldsymbol{x}} g(\boldsymbol{x}) = 0$$

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- The second condition is just the constraint

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Note on Gradients

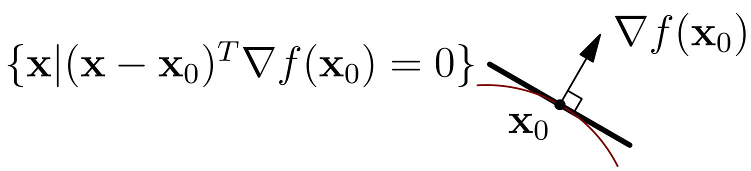
- Note that for any function $f(\boldsymbol{x})$ we can Taylor expand around $\boldsymbol{x}_0$

$$f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + (\boldsymbol{x} - \boldsymbol{x}_0)^{\mathsf{T}} \boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_0)^{\mathsf{T}} \mathbf{H} (\boldsymbol{x} - \boldsymbol{x}_0) + \ldots$$

  where $\mathbf{H}$ is a matrix of second derivative known as the Hessian

- If we consider points perpendicular to $\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x}_0)$ which go through $\boldsymbol{x}_0$ these will have values

$$f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + O(\|\boldsymbol{x} - \boldsymbol{x}_0\|^2)$$



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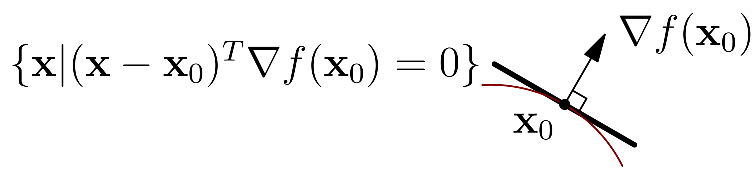

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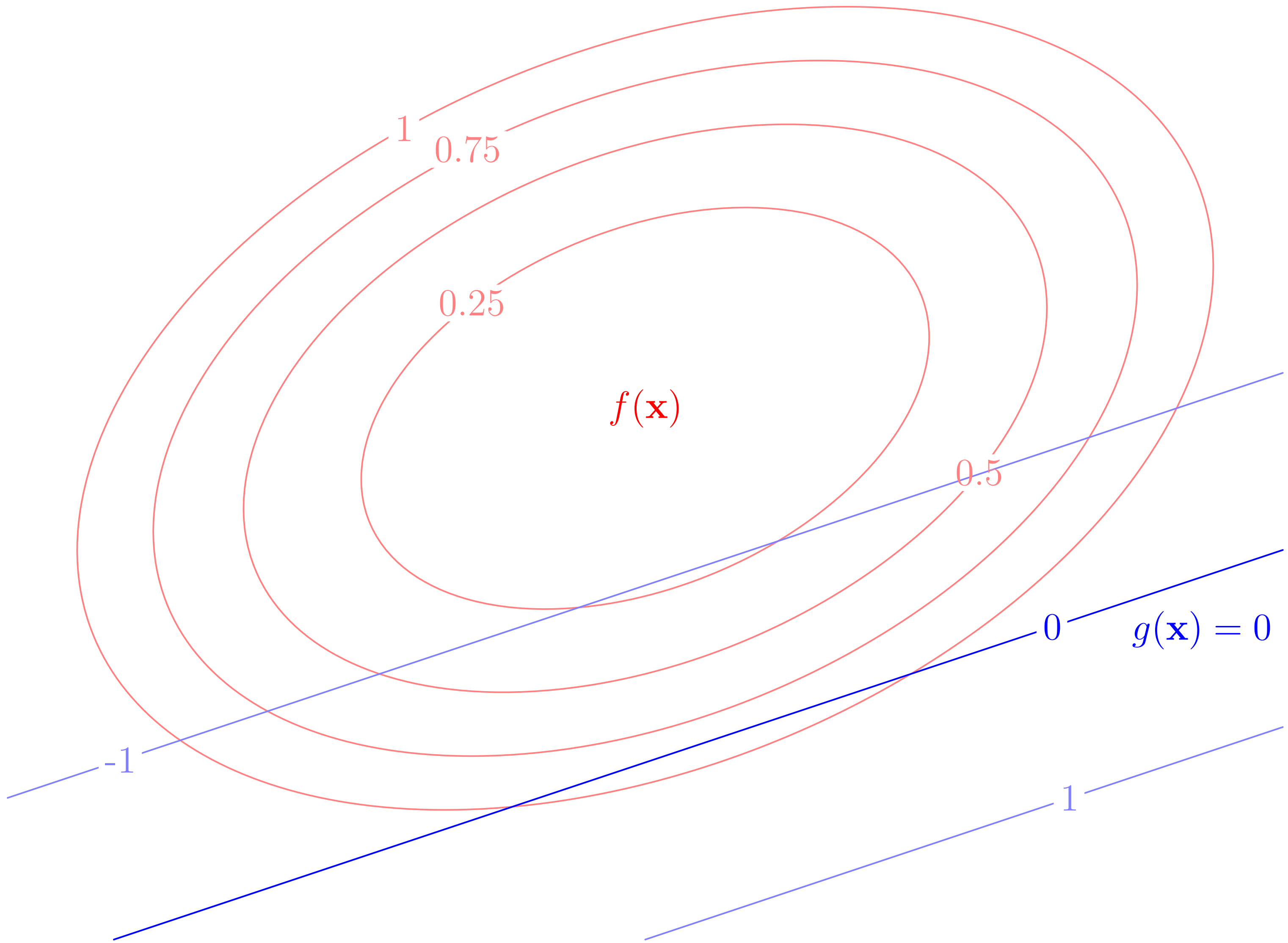

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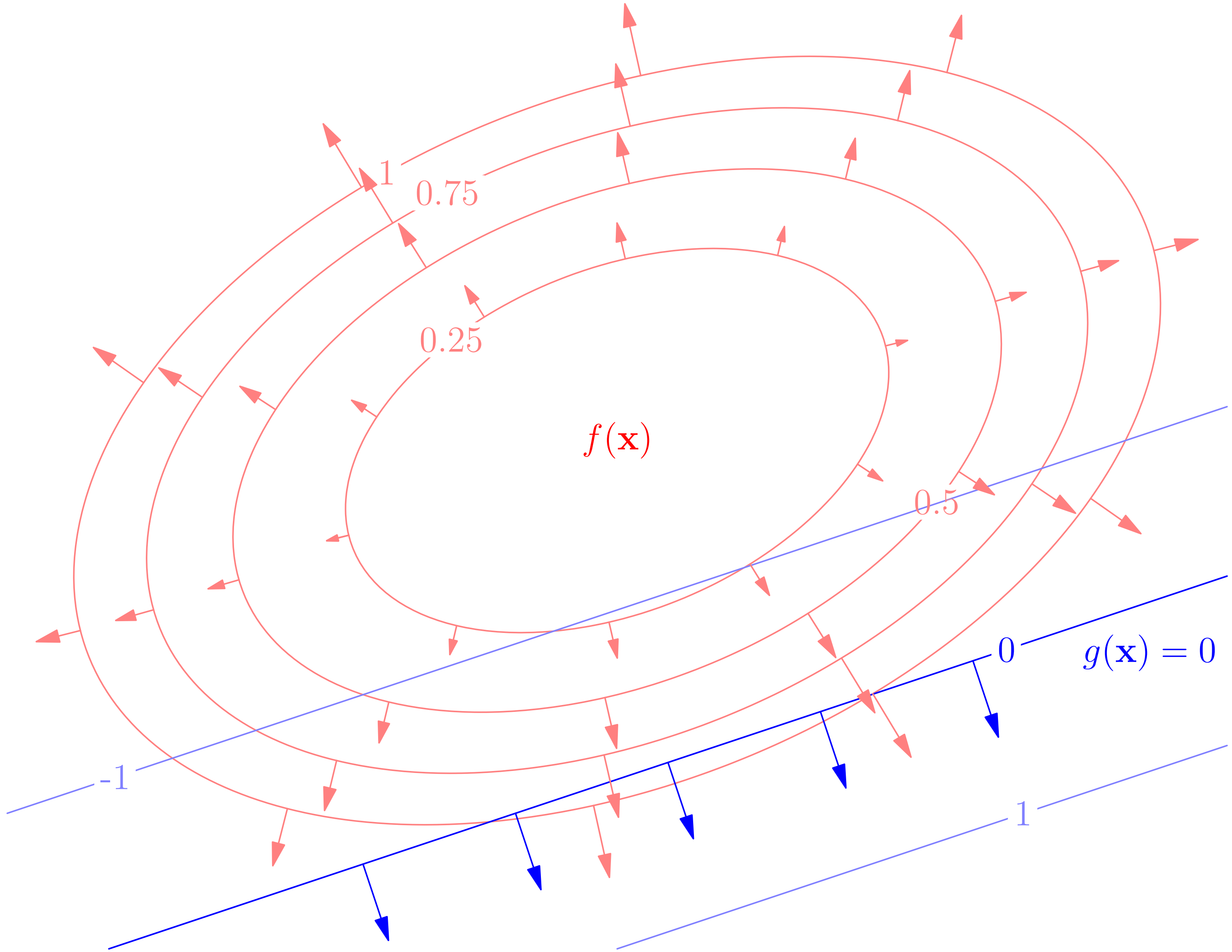

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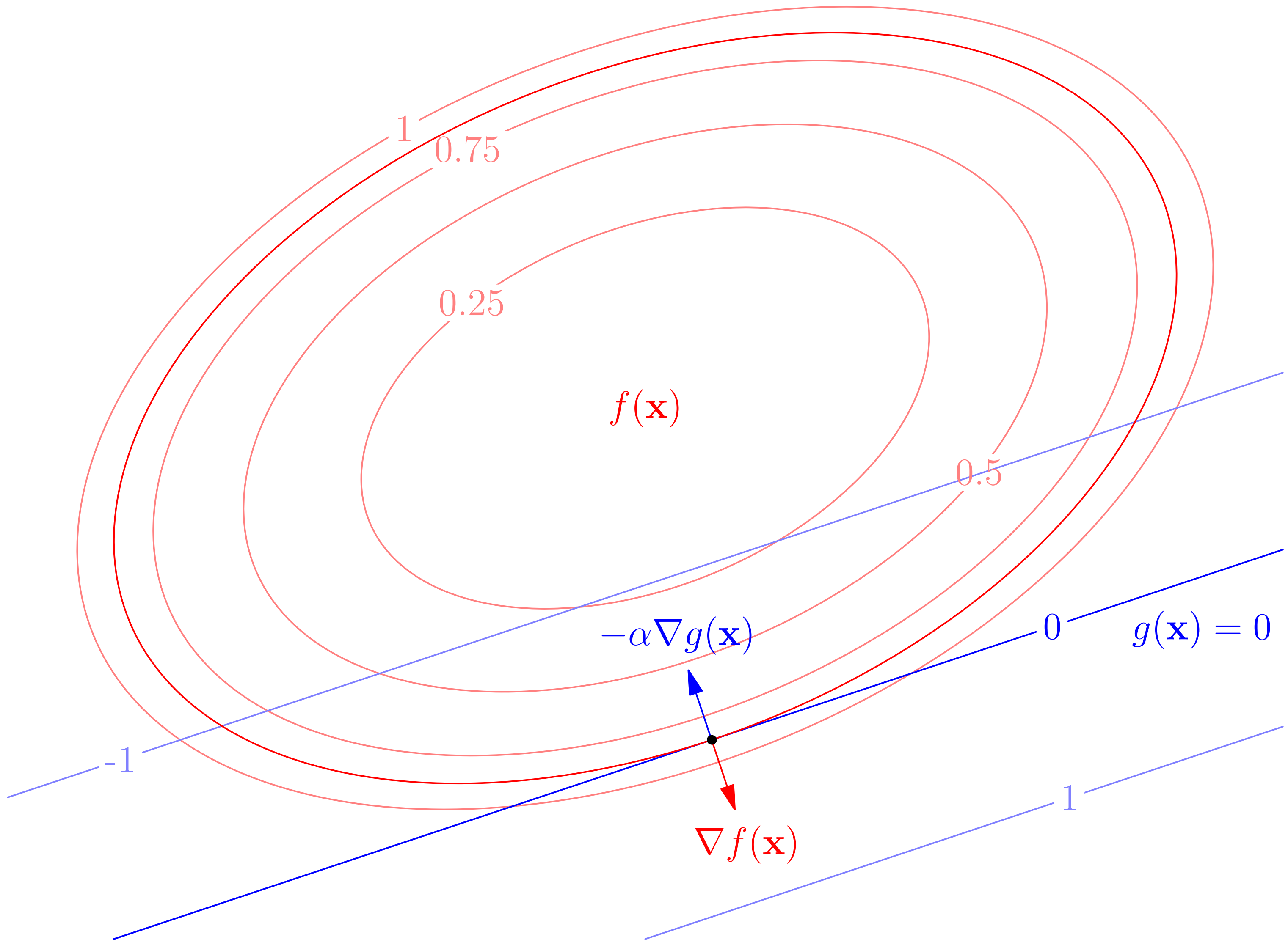

Example

- Minimise $f(\boldsymbol{x}) = x^2 + 2\,y^2 - x\,y$
- Subject to $g(\boldsymbol{x}) = x - 2\,y - 3 = 0$
- Writing $\mathcal{L} = f(\boldsymbol{x}) - \alpha\,g(\boldsymbol{x})$
- Condition for minima is $\boldsymbol{\nabla}_{\boldsymbol{x}}\mathcal{L} = 0$

$$\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x}) = \begin{pmatrix} 2\,x - y \\ -x + 4\,y \end{pmatrix} = \alpha \boldsymbol{\nabla}_{\boldsymbol{x}} g(\boldsymbol{x}) = \alpha \begin{pmatrix} 1 \\ -2 \end{pmatrix}$$

and $\frac{\partial \mathcal{L}}{\partial \alpha} = g(\boldsymbol{x}) = x - 2\,y - 3 = 0$

- Solving simultaneous equations gives minima at $(x, y) = (\frac{3}{4}, -\frac{9}{8})$ with $\alpha = \frac{21}{8}$

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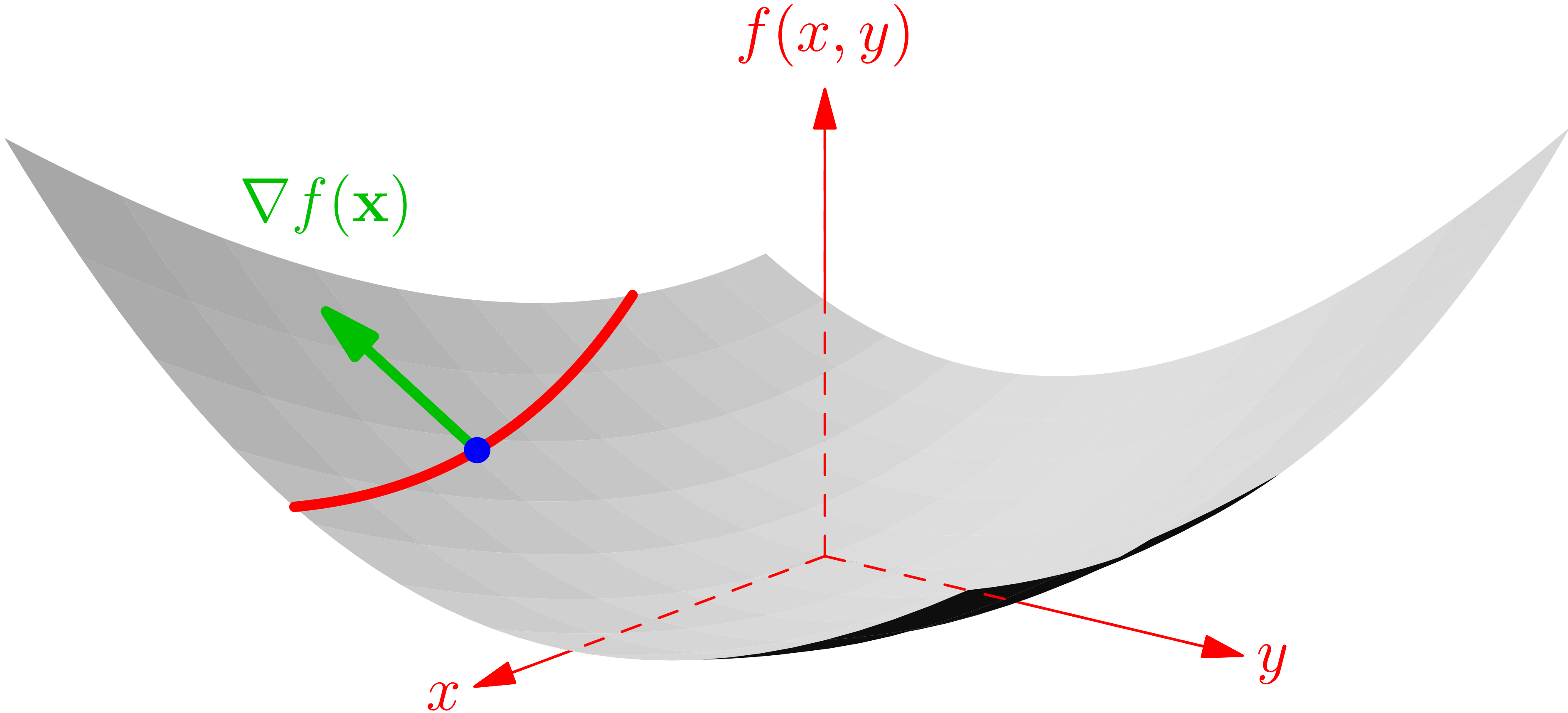
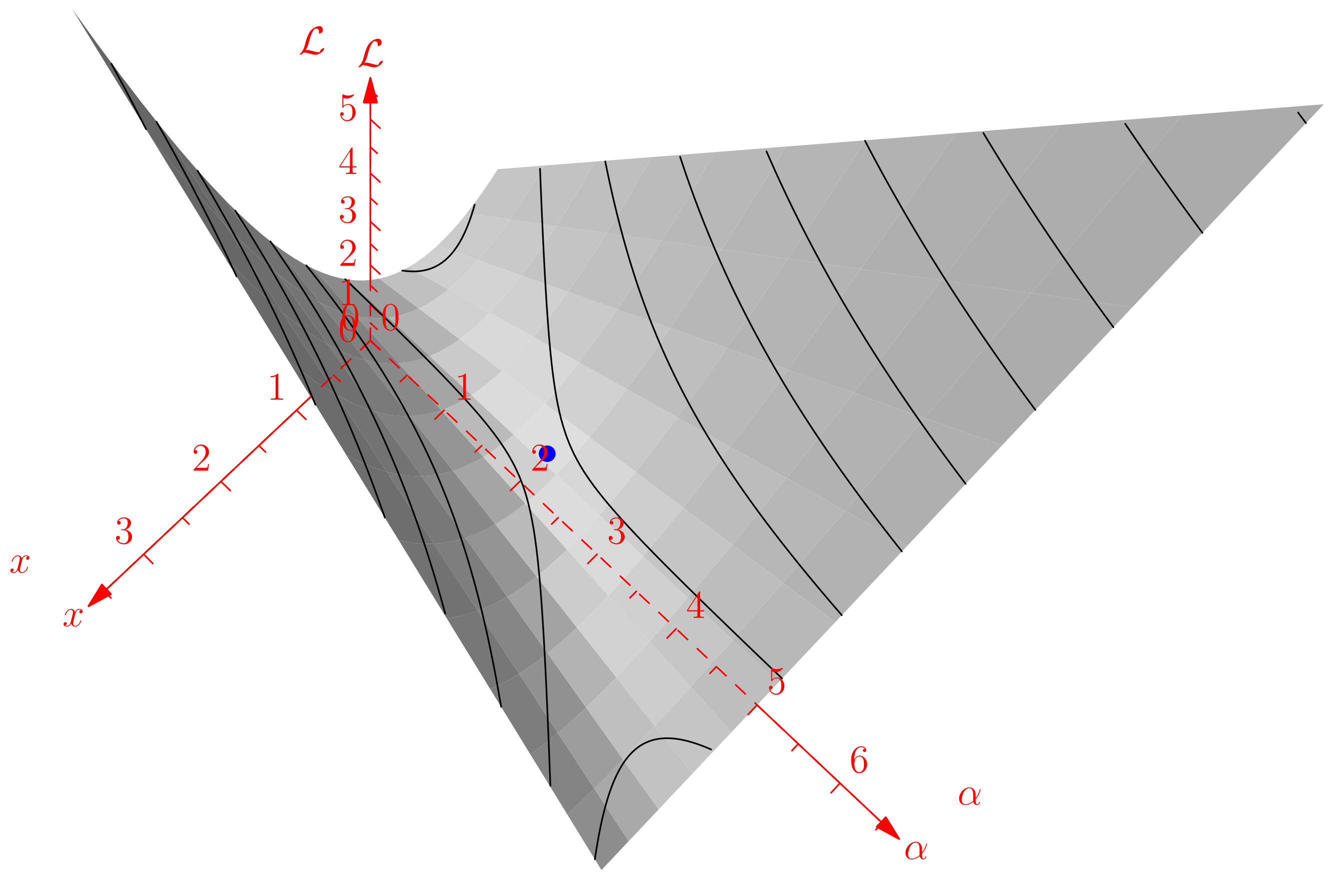
Surface



Saddle-Point $y = -9/8$



Multiple Constraints

- Given an optimisation problem with multiple constraints

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{subject to } g_k(\boldsymbol{x}) = 0 \text{ for } k = 1,\, 2,\, \ldots,\, m$$

- We introduce multiple Lagrange multipliers

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}) = f(\boldsymbol{x}) - \sum_{k=1}^{m} \alpha_k \, g_k(\boldsymbol{x})$$

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- Minimise $f(\boldsymbol{x}) = x^2 + 2\,y^2 + 5\,z^2 - x\,y - x\,z$ subject to $g_1(\boldsymbol{x}) = x - 2\,y - z - 3 = 0$ and $g_2(\boldsymbol{x}) = 2\,x + 3\,y + z - 2 = 0$

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Inequality Constraints

- Suppose we have the problem

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) \quad \text{subject to } g(\boldsymbol{x}) \geq 0$$

- Looks much more complicated, but
- Only two things can happen
  - ⋆ Either the minimum of $f(\boldsymbol{x})$, $\boldsymbol{x}^*$, satisfies $g(\boldsymbol{x}^*) > 0$
    - ∗ We then have an unconstrained optimisation problem
  - ⋆ Otherwise, it satisfies $g(\boldsymbol{x}^*) = 0$
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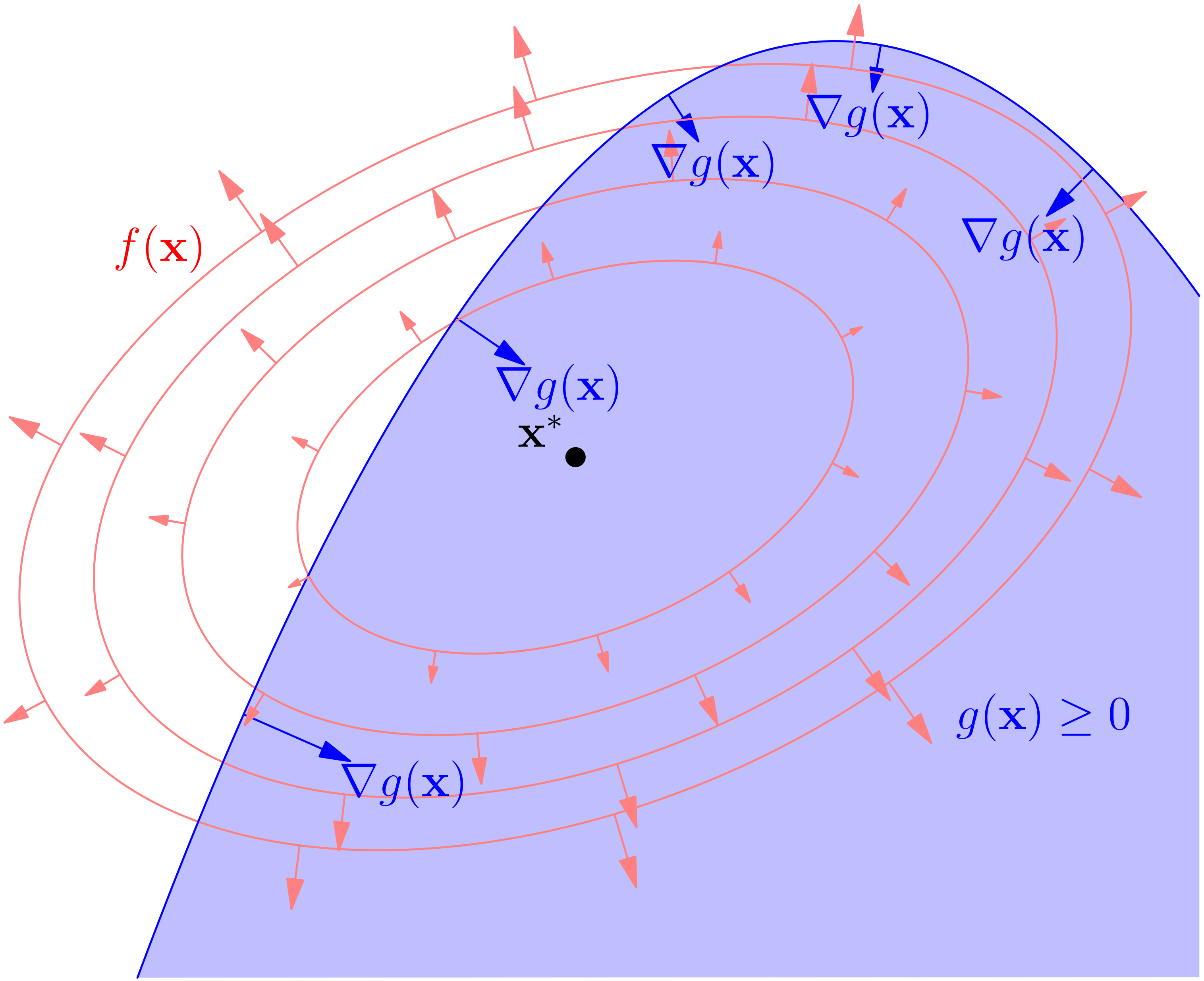
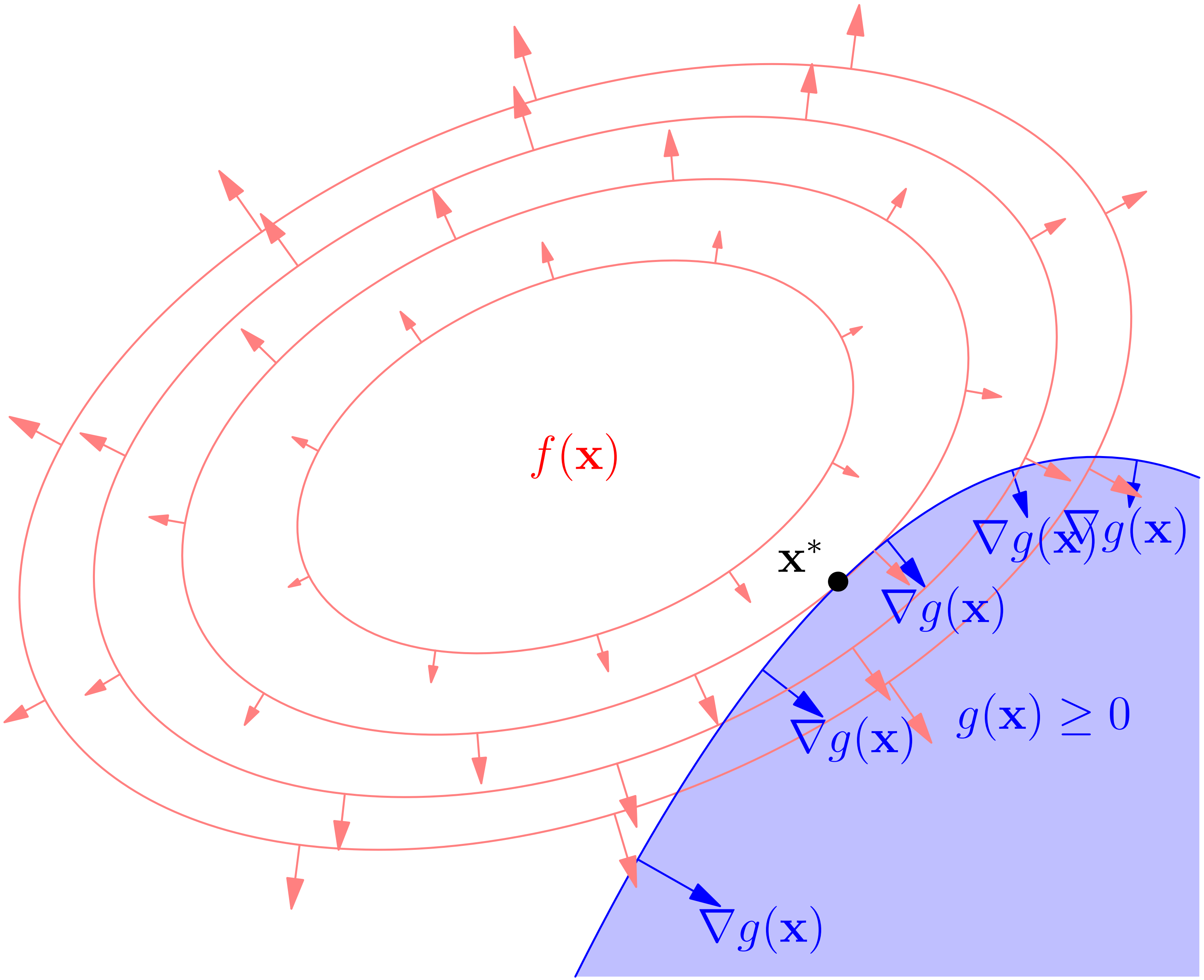


On the Boundary



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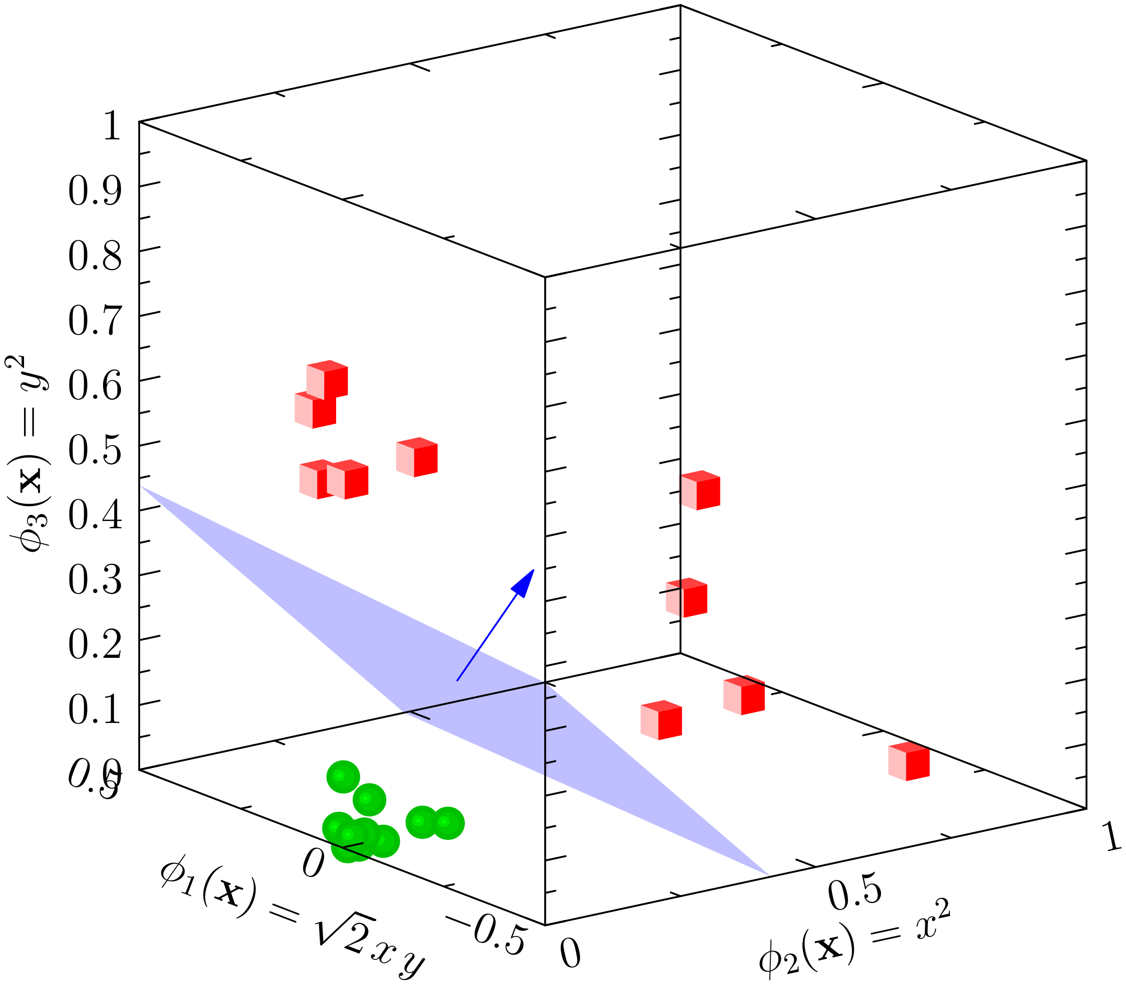
Outline

1. Recap
2. Constrained Optimisation
3. **Duality**



Back to the SVM

- We showed that the quadratic programming problem can be written as

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- Substituting in $\boldsymbol{w}^*$ the optimisation condition becomes

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- Subject to $\sum_{k=1}^{m} \alpha_k \, y_k = 0$ and $\alpha_k \geq 0$ for all k
- This is also a quadratic programming problem!
- It is known as the *dual* form and depends on the number of training examples (it is solved by a standard package)
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Duality

- We can either work in the n-dimensional weight space

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

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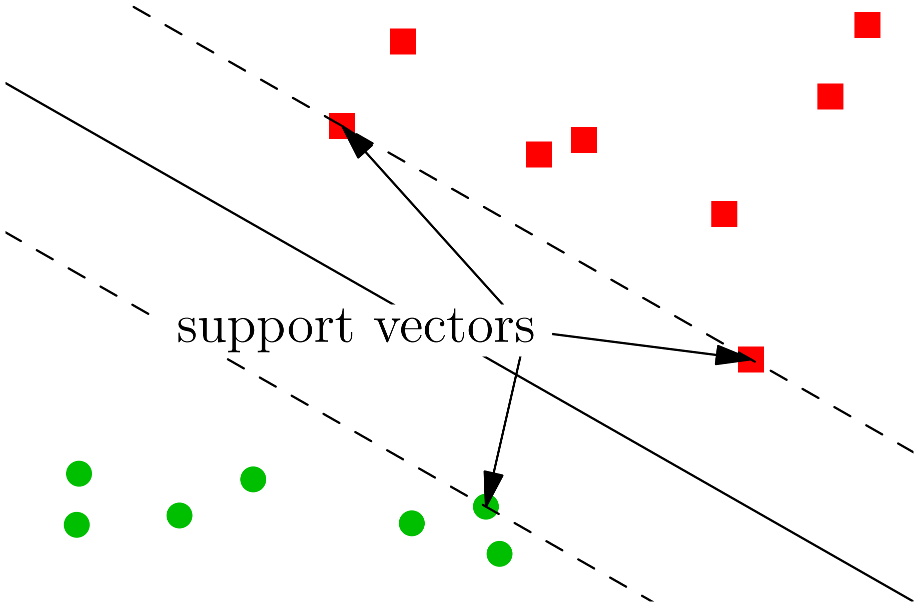
- These data points are known as *support vectors*



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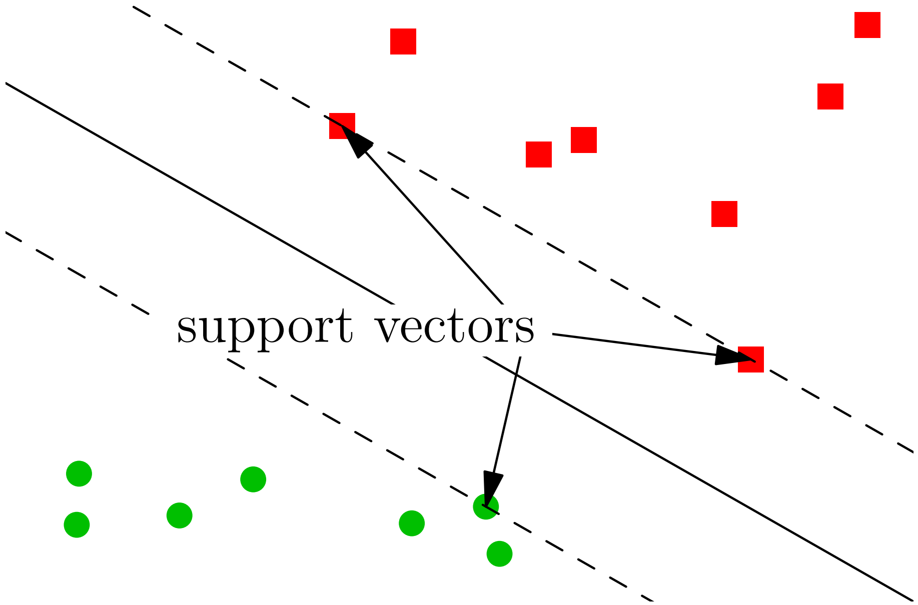

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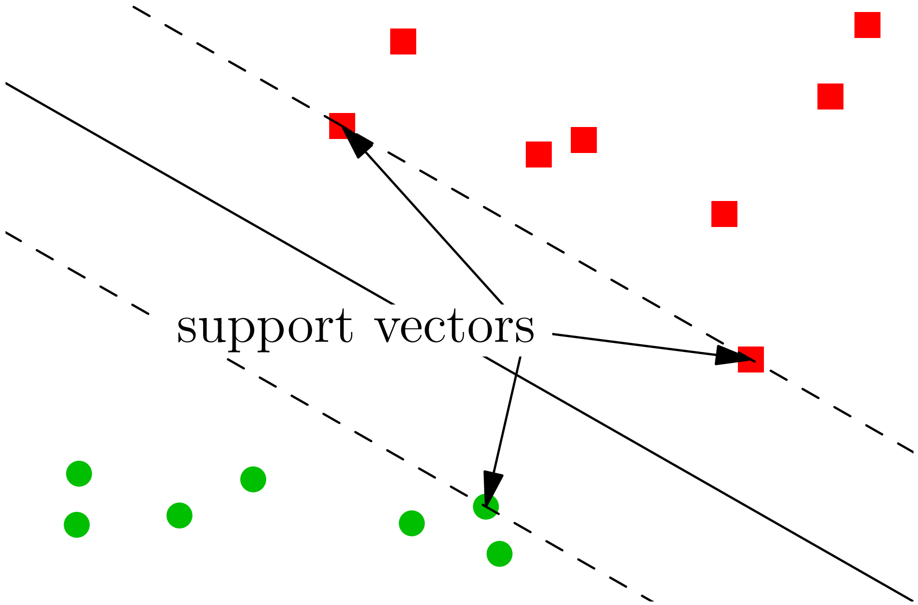

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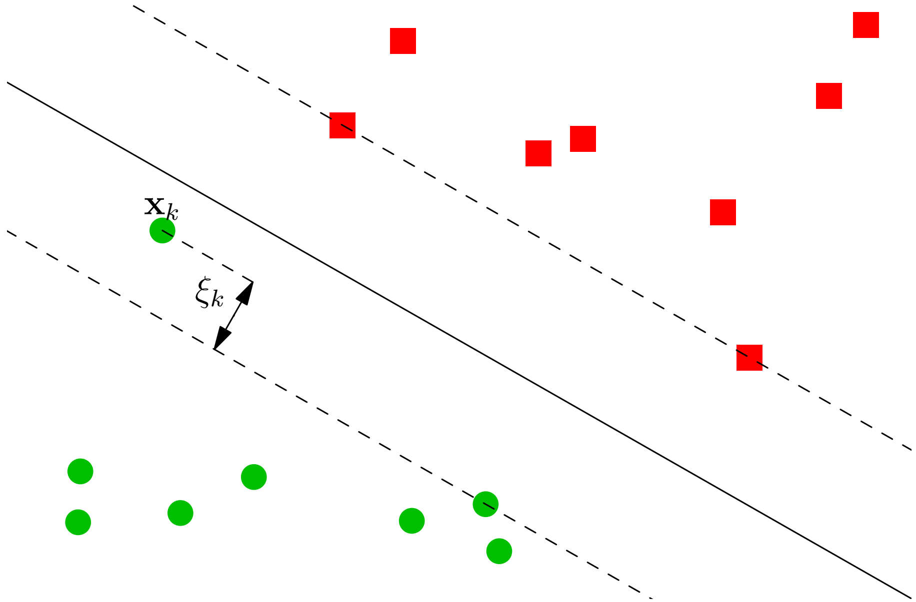
Soft Margins

- Recall we can relax constraints by introducing *slack variables*, $\xi_k \geq 0$



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

- Minimise $\frac{\|\boldsymbol{w}\|^2}{2} + C\sum_{k=1}^{m} \xi_k$
- subject to $\xi_k \geq 0$

Soft Margins

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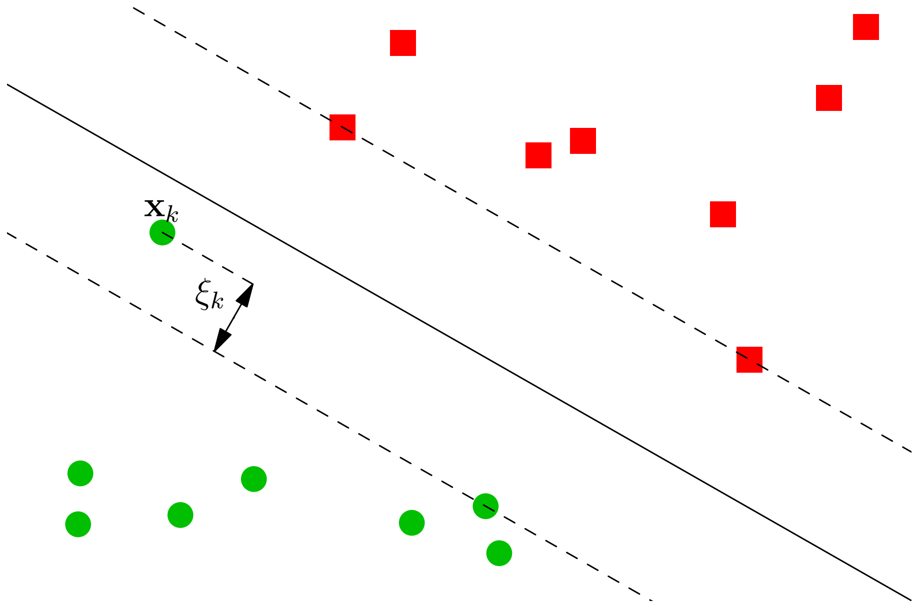

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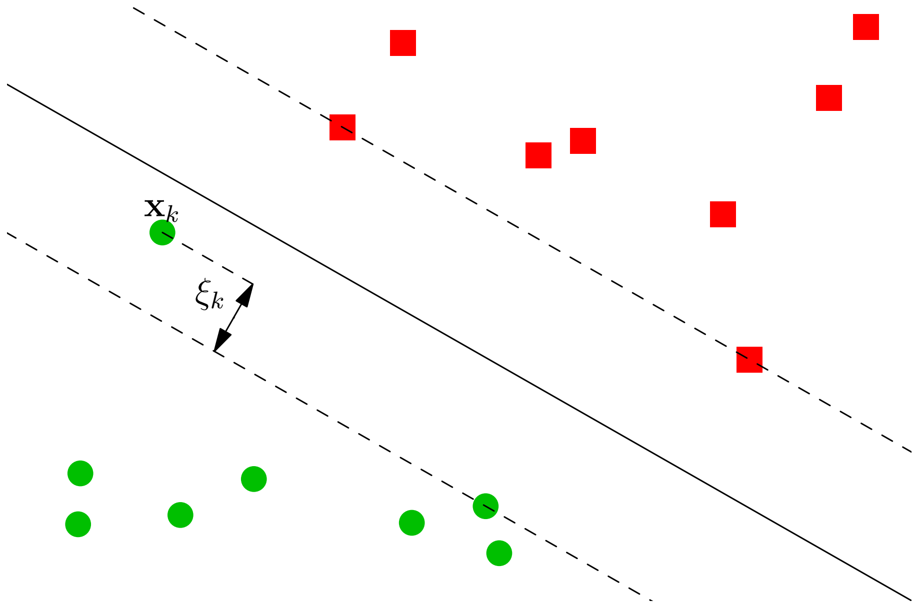

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Extended Feature Space

- In the extended feature space

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- Giving the dual problems

$$\max_{\boldsymbol{\alpha}} \sum_{k=1}^{m} \alpha_k - \frac{1}{2} \sum_{k,l=1}^{m} \alpha_k\, \alpha_l\, y_k\, y_l\, \vec{\phi}(\boldsymbol{x}_k)^{\mathsf{T}}\, \vec{\phi}(\boldsymbol{x}_l) \quad \text{with } \sum_{k=1}^{m} \alpha_k\, y_k = 0 \;\&\; \alpha_k \geq 0$$

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Classifying New Data

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- We can solve for the maximum-margin hyper-plane either in the primal form (space of weights and bias) or the dual form (space of Lagrange multipliers)
- In the dual form the solution only depends on the dot product $\boldsymbol{x}_i^{\mathsf{T}}\boldsymbol{x_j}$ or $\vec{\phi}(\boldsymbol{x}_i)^{\mathsf{T}}\vec{\phi}(\boldsymbol{x}_j)$
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