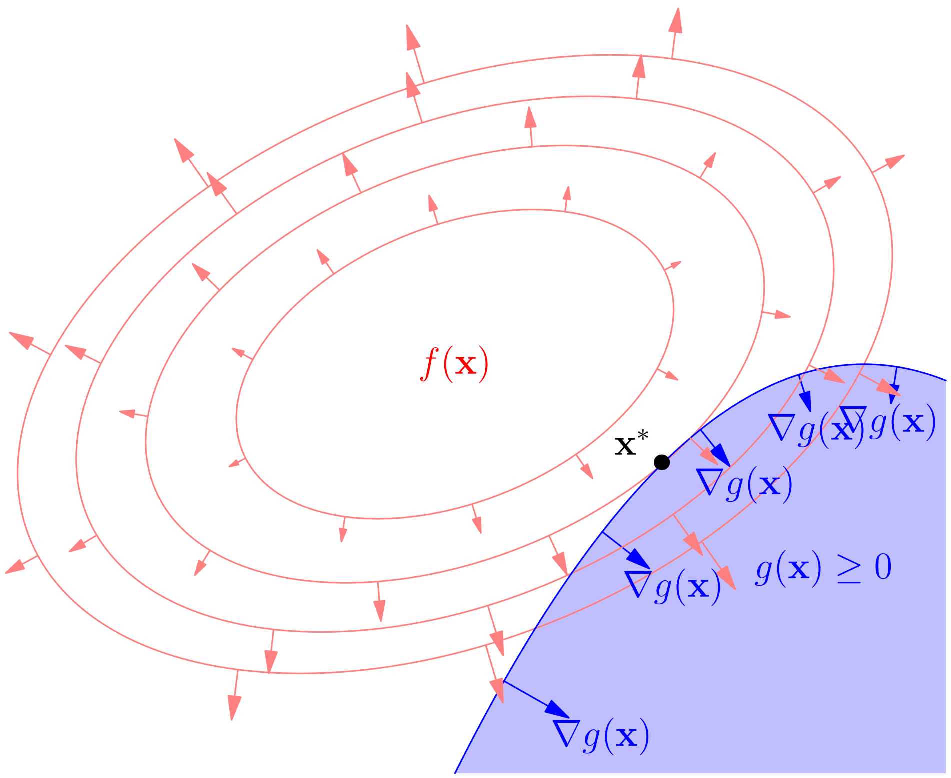
Advanced Machine Learning

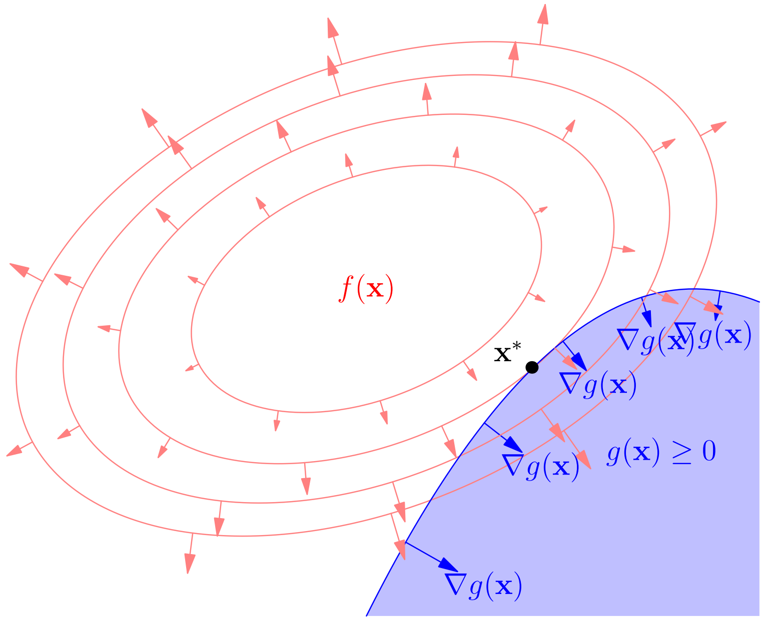
Constrained Optimisation



Lagrangians, Inequalities, KKT, Linear Programming, Quadratic Programming, Duality

Outline

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



Optimisation with Constraints

- There are a number of important applications where we wish to minimise an objective function subject to inequality constraints
- A prominent example of this is support vector machines
- More generally there are a large number of kernel models that involve constraints
- However, constraints are ubiquitous in machine learning (e.g. in Wasserstein GANs)

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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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- Assuming differentiability

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

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

- The second condition is just the constraint

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- The second condition is just the constraint

- But what about first condition: $\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x}) = \alpha\, \boldsymbol{\nabla}_{\boldsymbol{x}} g(\boldsymbol{x})$?

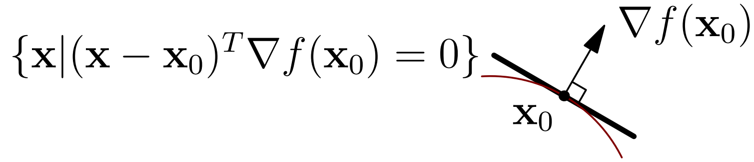
Note on Gradients

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

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

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

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



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

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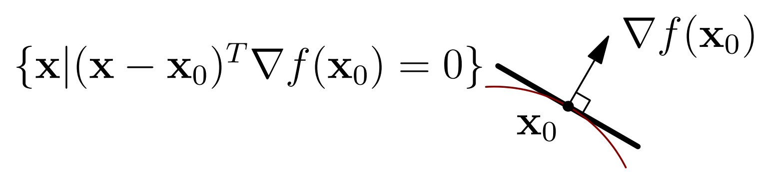

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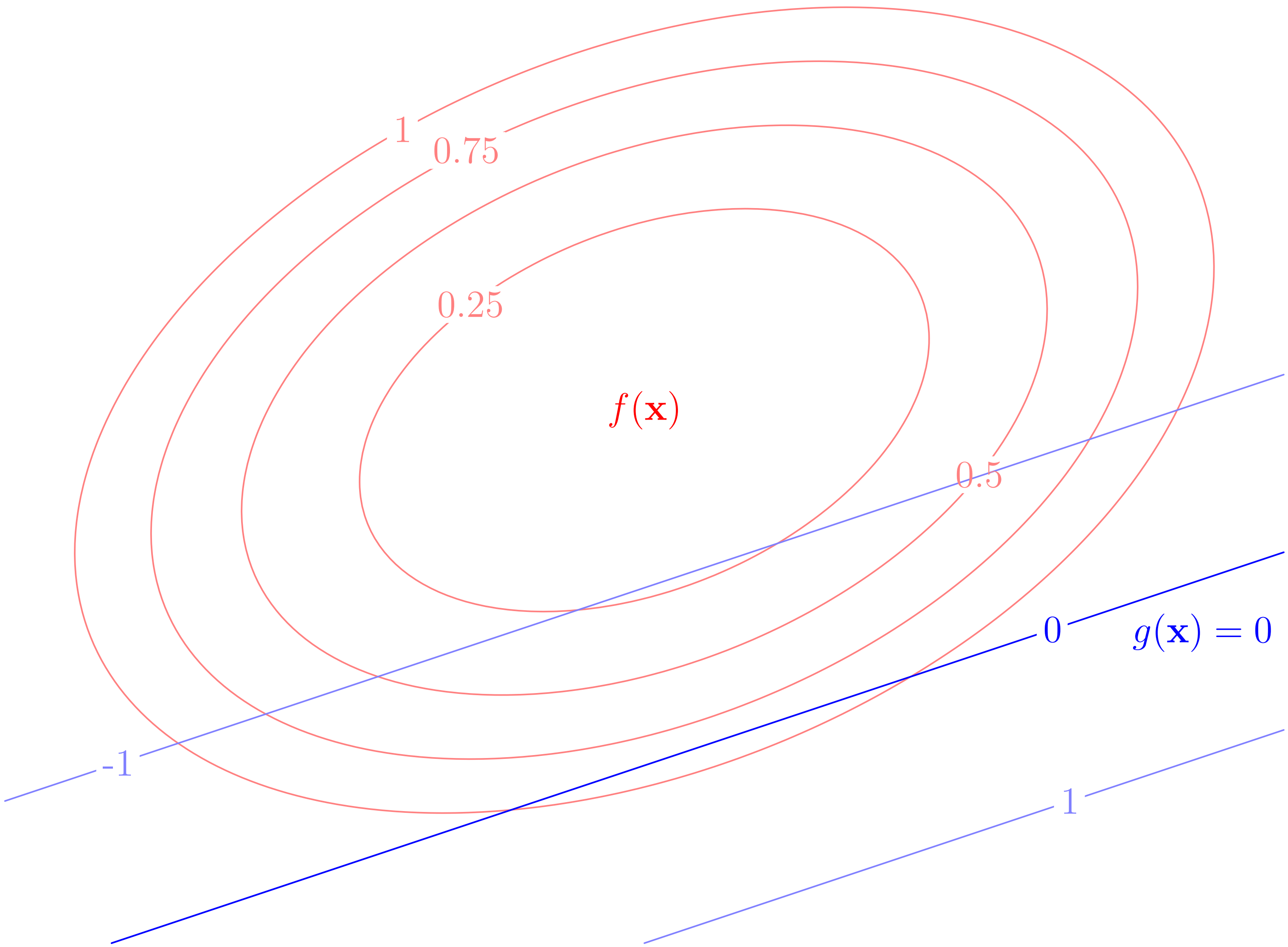
Constrained Optima



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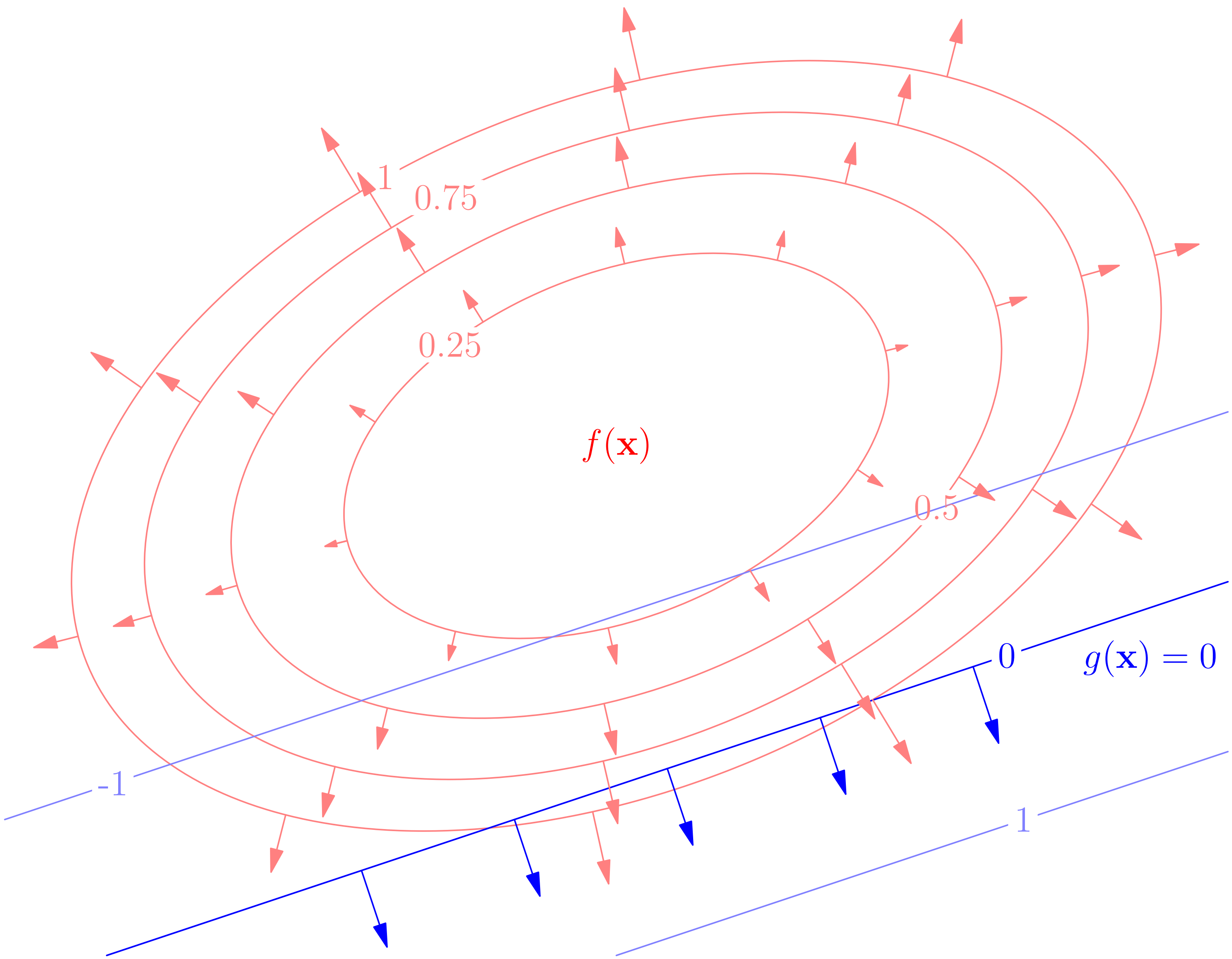

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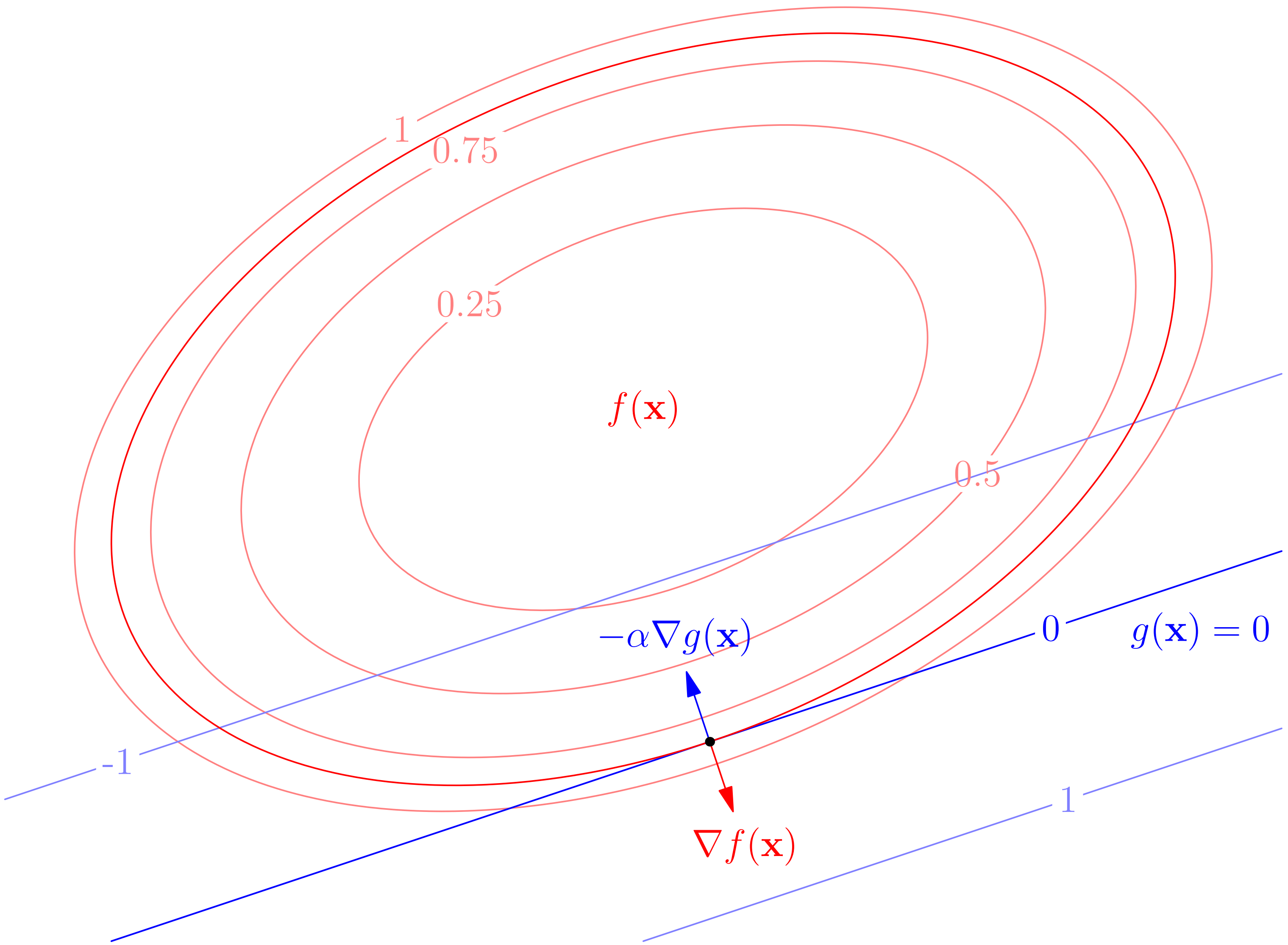

Example

- 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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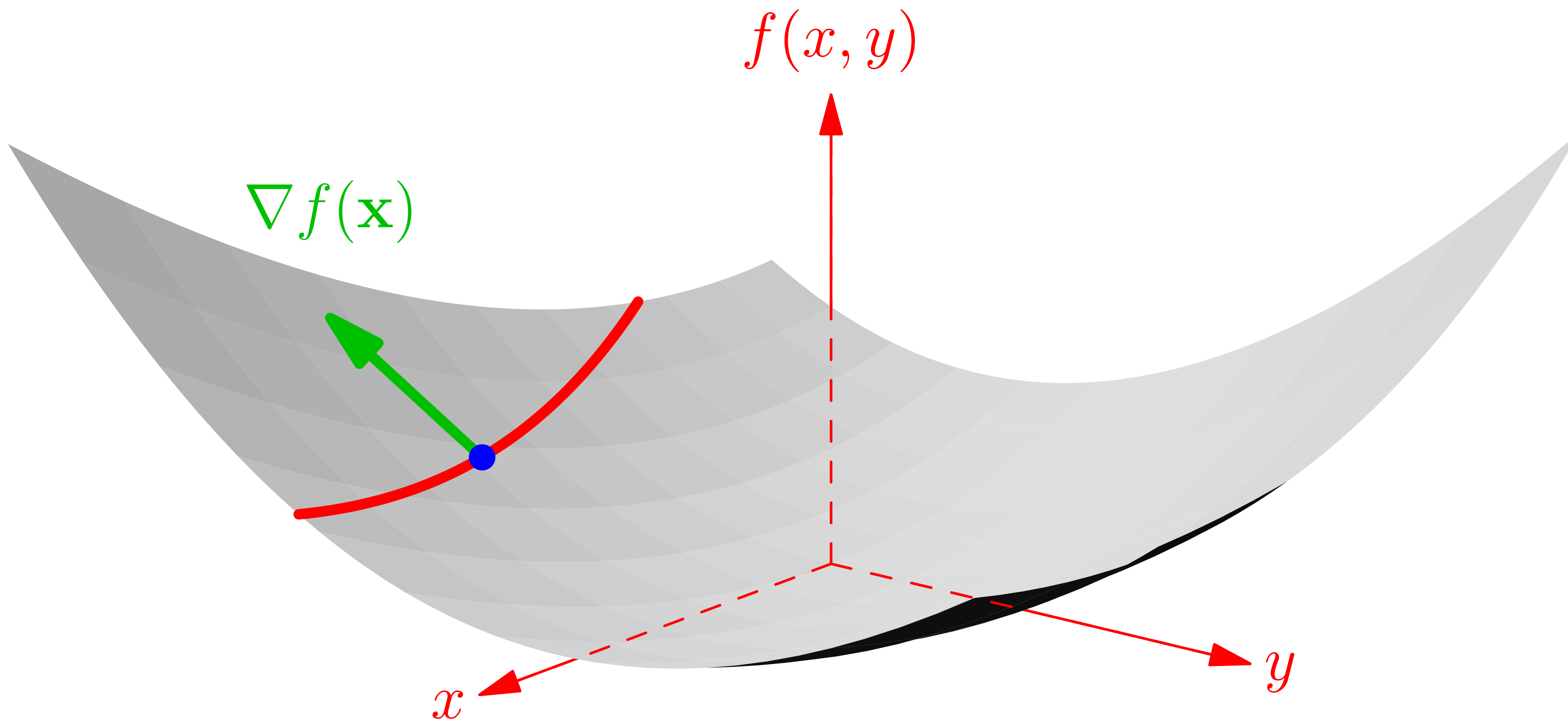
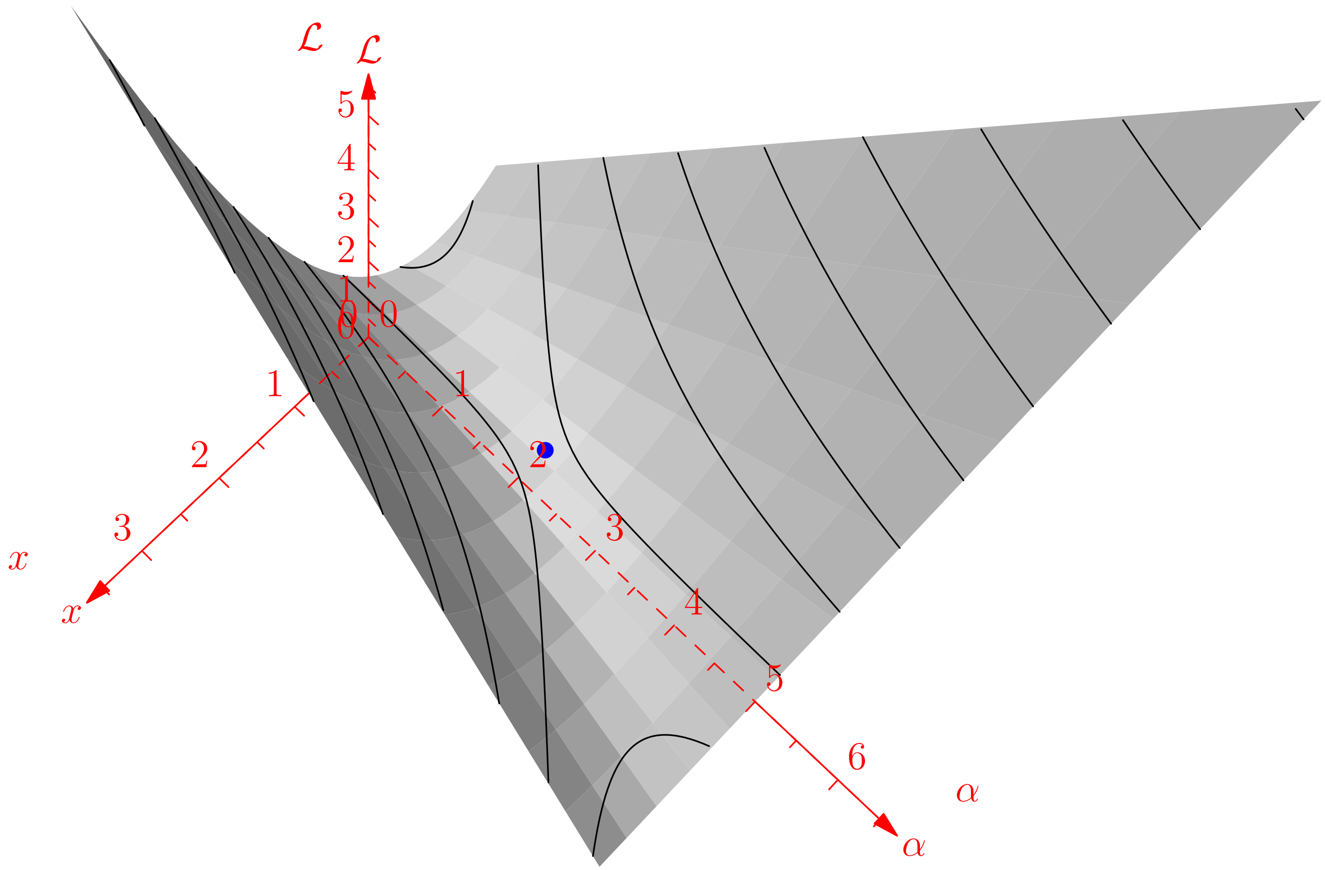
Surface



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

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

- The condition for an optima is $\boldsymbol{\nabla}_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}) = 0$ which implies

$$\boldsymbol{\nabla}_{\boldsymbol{x}} f(\boldsymbol{x}) = \sum_{k=1}^{m} \alpha_k \, \boldsymbol{\nabla}_{\boldsymbol{x}} g_k(\boldsymbol{x})$$

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Example

- 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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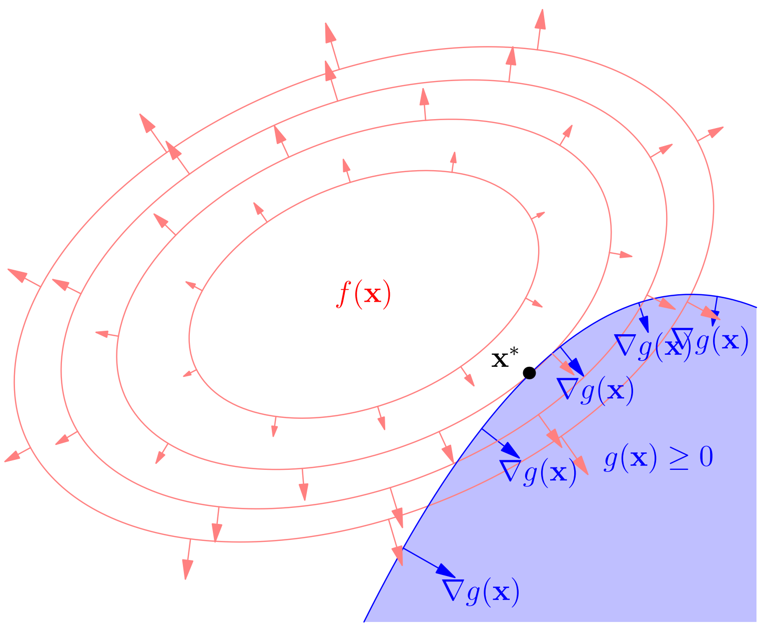

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2. **Inequalities**
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Inequality Constraints

- 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 a minimum, $\boldsymbol{x}^*$, of $f(\boldsymbol{x})$ satisfies $g(\boldsymbol{x}^*) > 0$
    - ∗ We then have an unconstrained optimisation problem
  - ⋆ Otherwise, it satisfies $g(\boldsymbol{x}^*) = 0$
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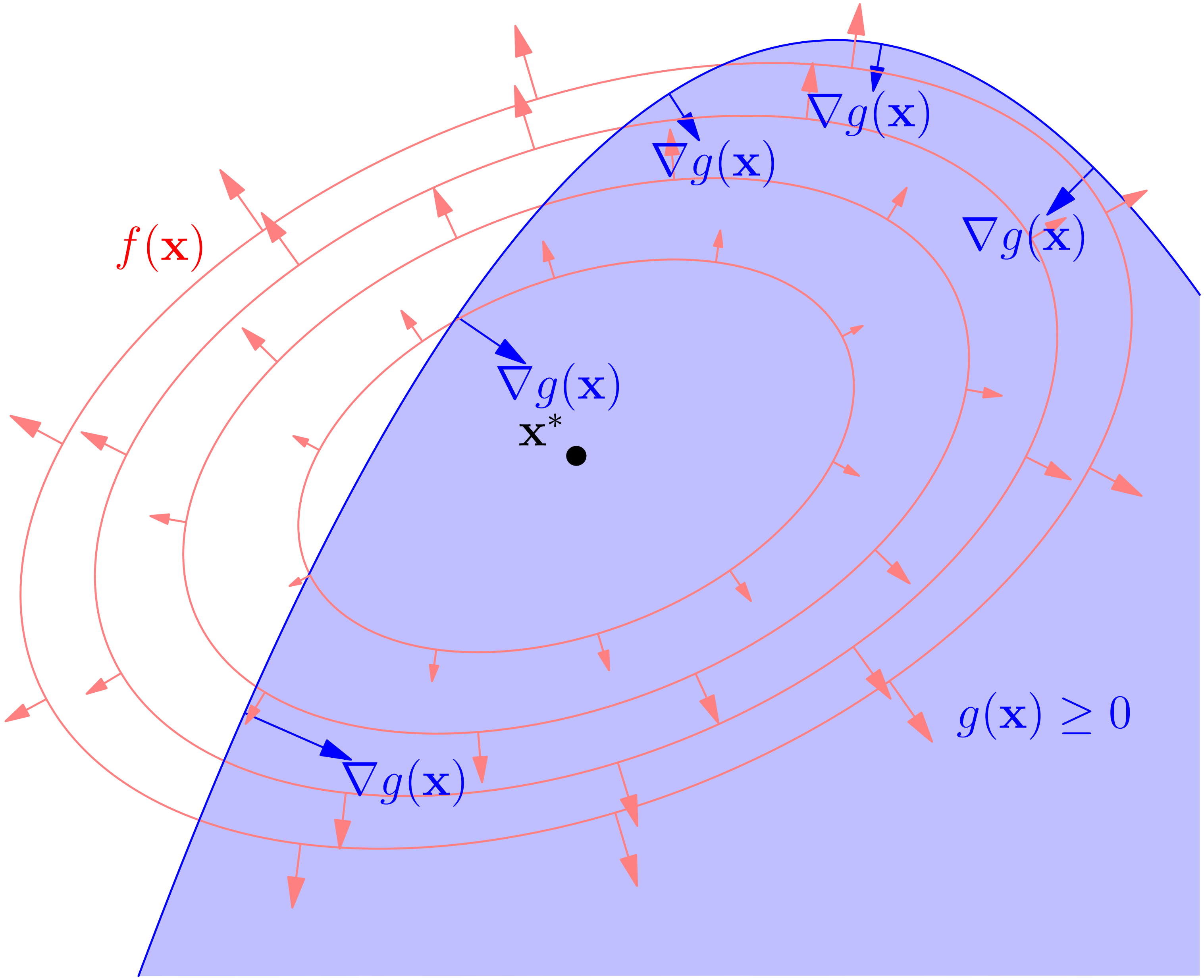
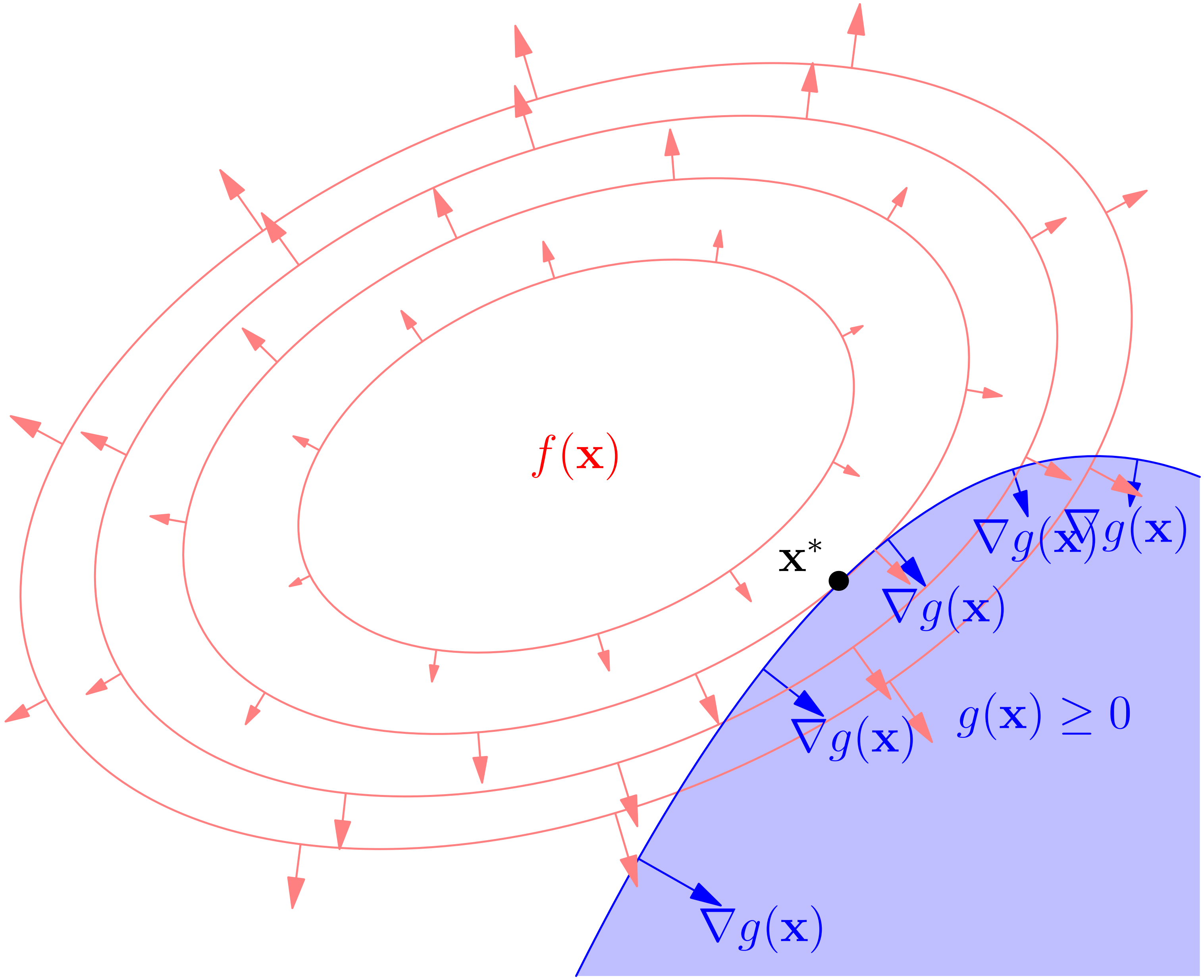
Inside Region



On the Boundary



KKT Conditions

- To minimise $f(\boldsymbol{x})$ subject to $g(\boldsymbol{x}) \geq 0$

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

- Then $\boldsymbol{\nabla}_{\boldsymbol{x}} \mathcal{L} = 0$ or

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- where either
  - ⋆ $\alpha = 0$ and the solutions in the interior or
  - ⋆ $\alpha > 0$ and $g(\boldsymbol{x}) = 0$, i.e. the solution is on the boundary

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KKT Conditions

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Many Inequalities

- Given the problem

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

- We introduce multiple Lagrange multipliers

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

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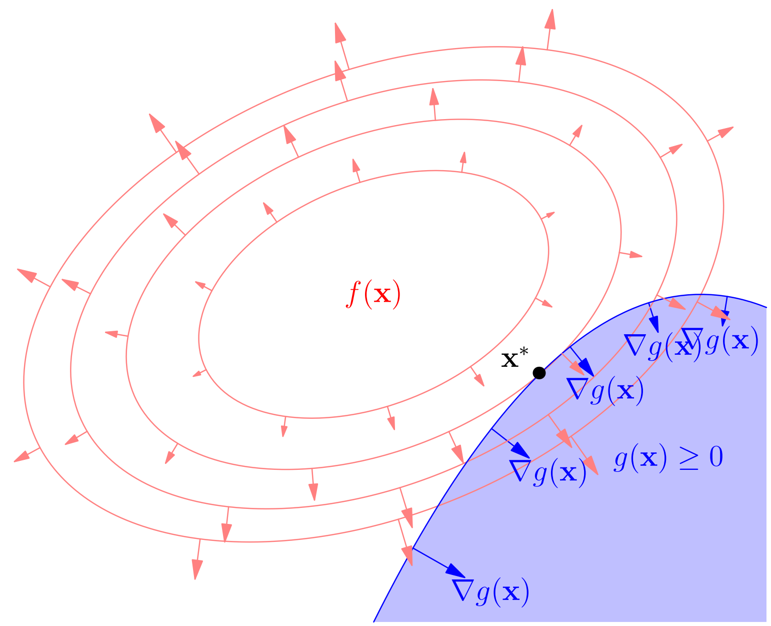
Outline

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



Solving the Lagrangian for x

- Consider minimising a function $f(\boldsymbol{x})$ subject to a set of constraints $g_i(\boldsymbol{x}) = 0$ or $g_i(\boldsymbol{x}) \leq 0$

- We can consider this a double optimisation problem

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where there would be constraints on α_i if we had an inequality constraint

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Dual Problem

- If $f(\boldsymbol{x})$ and $g_i(\boldsymbol{x})$ are simple we can sometimes find a set of variables $\boldsymbol{x}^*(\boldsymbol{\alpha})$ that minimises the Lagrangian

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

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- In linear programming we minimise a linear objective function $\boldsymbol{c}^\mathsf{T}\boldsymbol{x}$ subject to linear constraints $\boldsymbol{g}(\boldsymbol{x}) = \mathbf{M}\,\boldsymbol{x} - \boldsymbol{b} = 0$ (or $\boldsymbol{g}(\boldsymbol{x}) \geq 0$)

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- Suppose we eat potatoes and rice and we want to ensure that we get enough vitamin A and C

	Potatoes	Rice	Daily Requirement
Vitamin A	3	5	20
Vitamin C	5	2	24
Price	5	4	

- We want to buy P kg potatoes and R kg of rice as cheaply as possible subject to fulfilling our vitamin requirement

$$\min_{P,R} 5\,P + 4\,R$$

subject to $\quad P, R \geq 0, \quad 3P + 5R \geq 20 \quad$ and $\quad 5P + 2R \geq 24$

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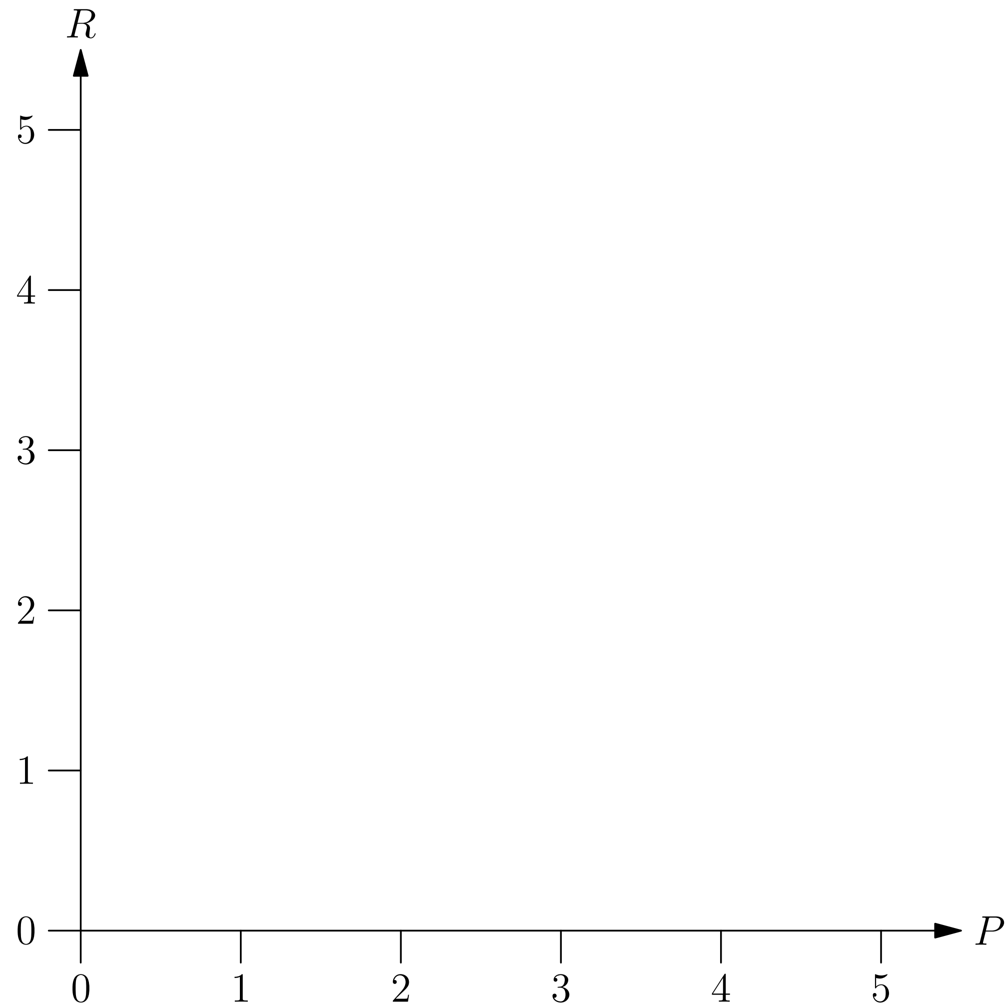

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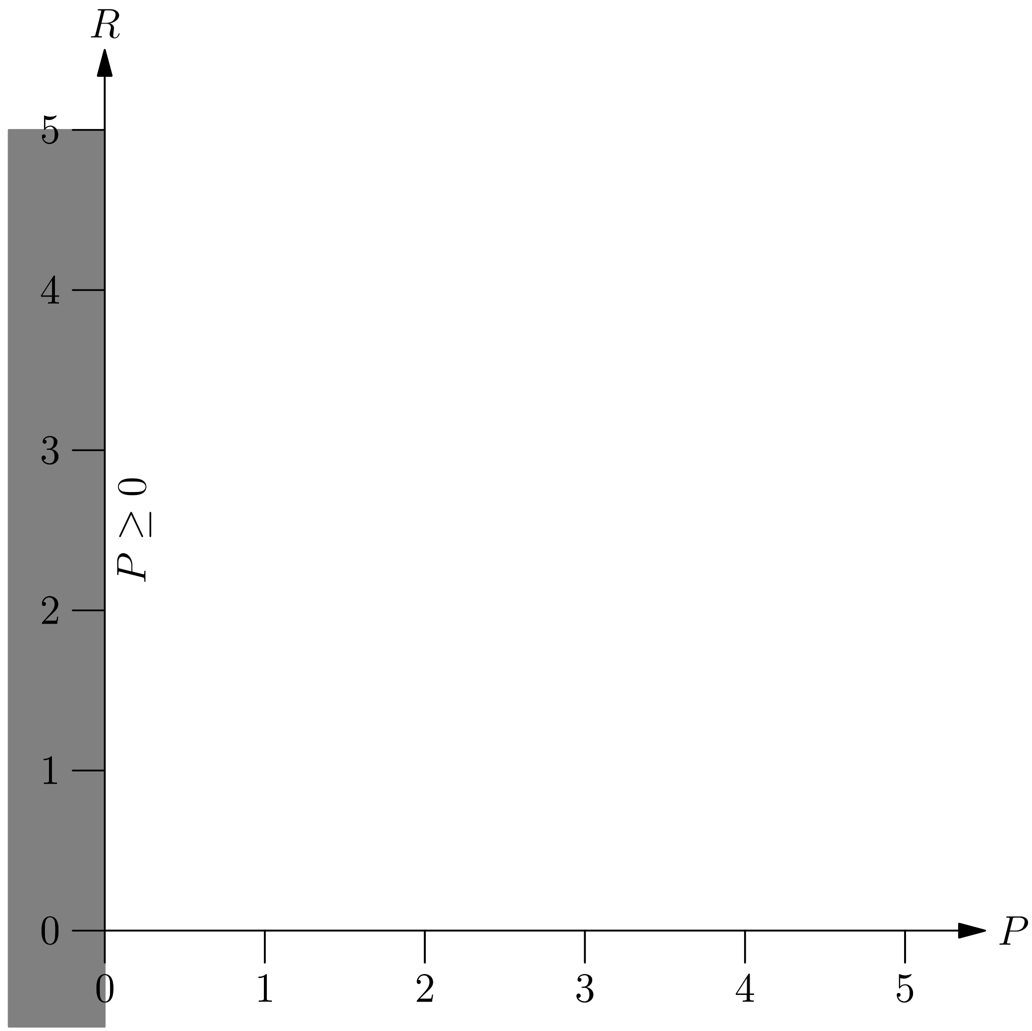

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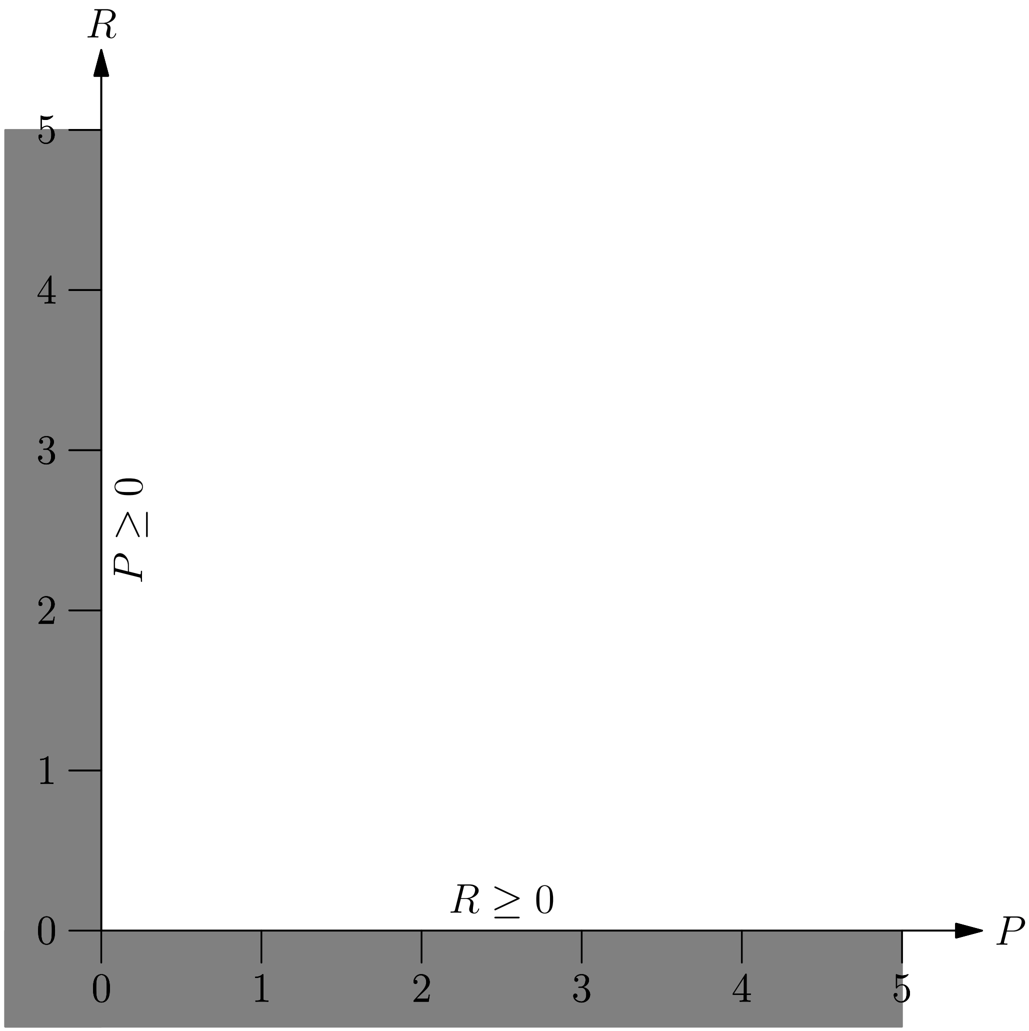

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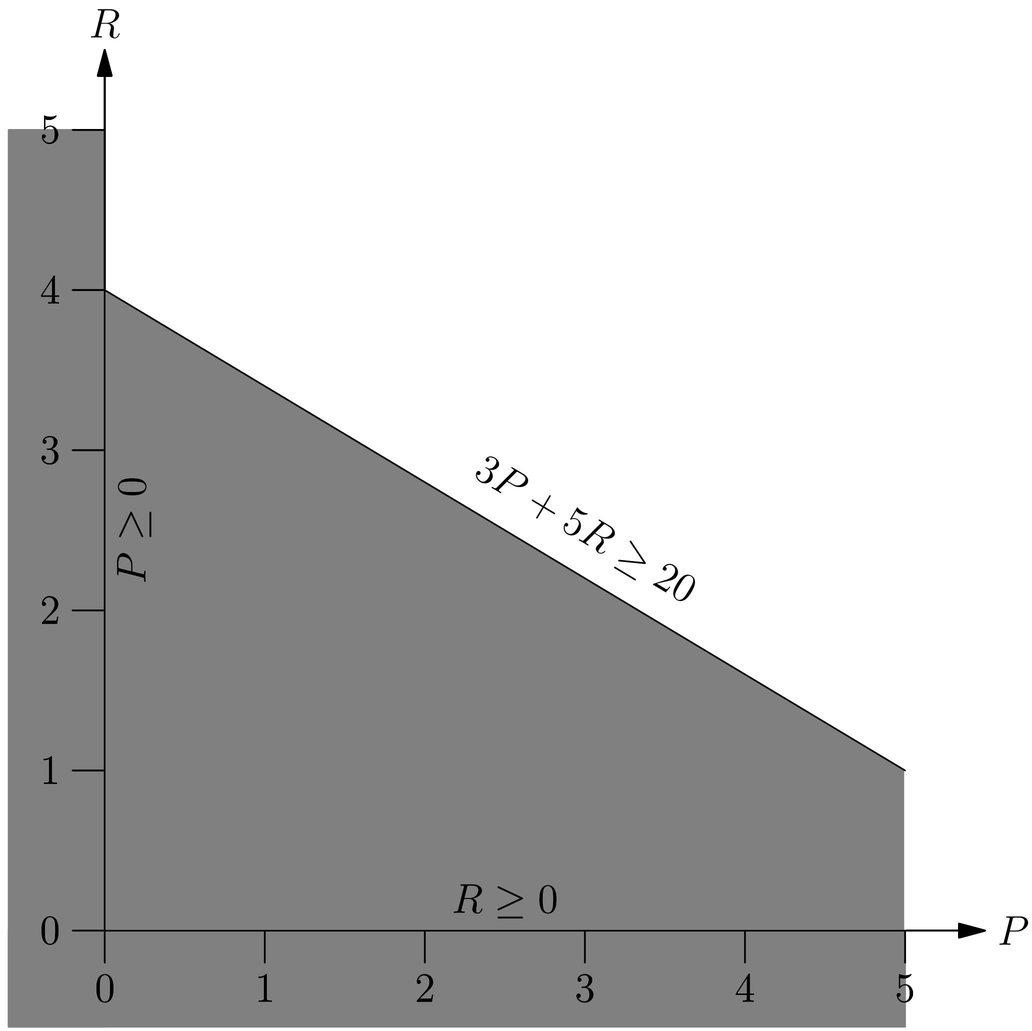

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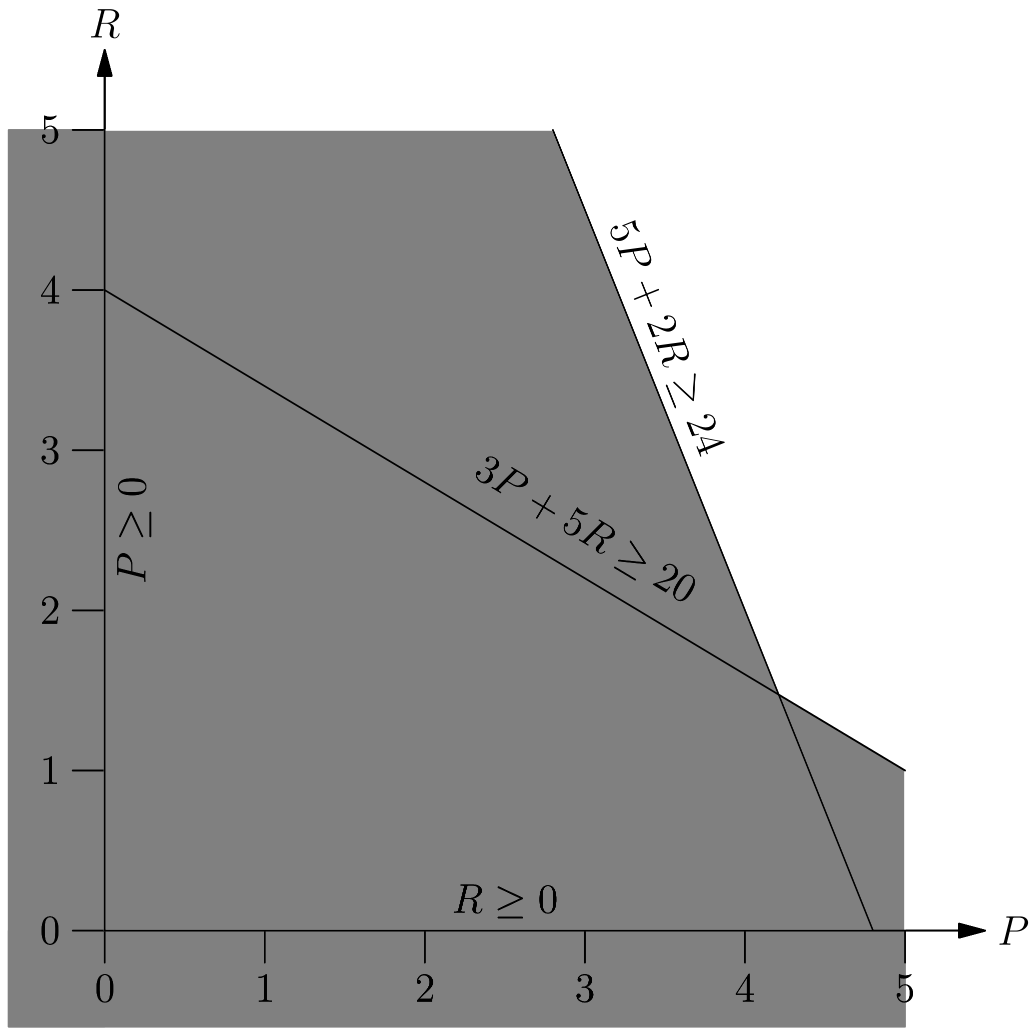

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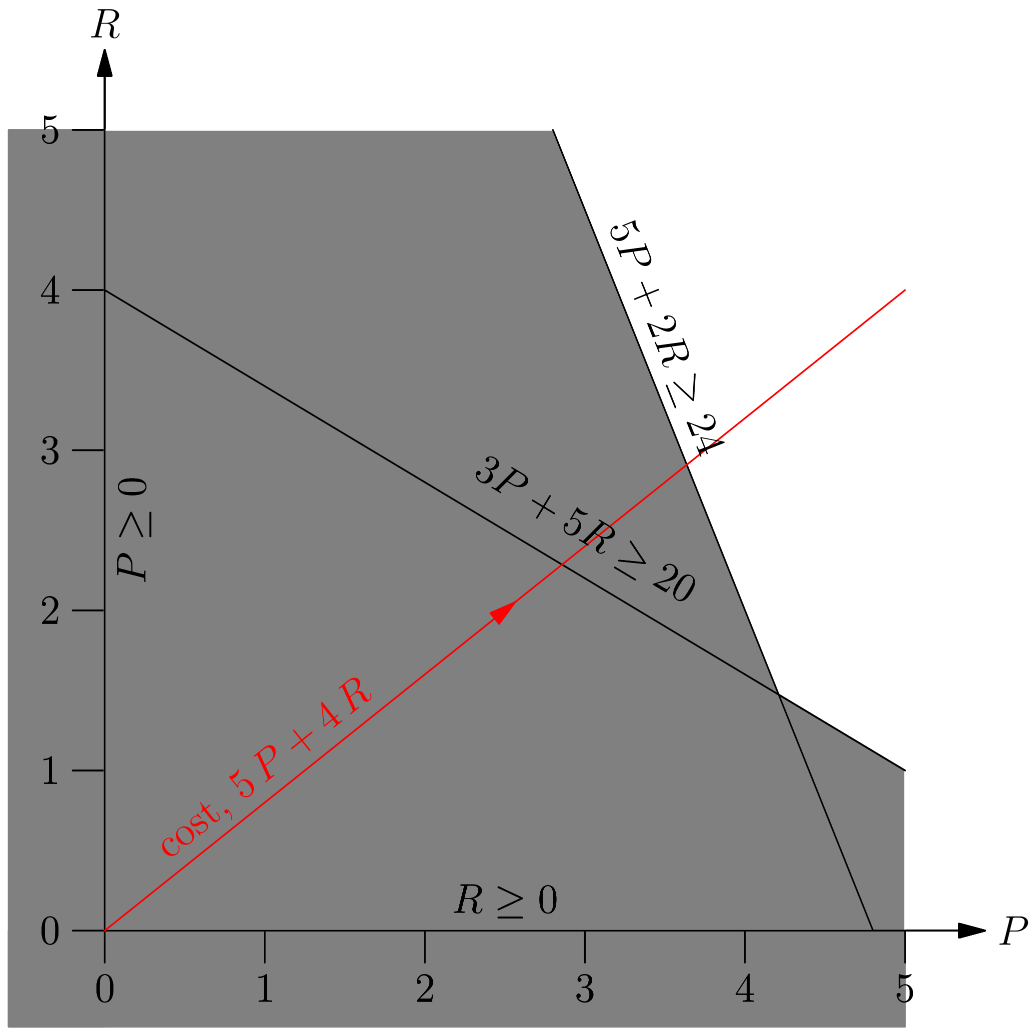

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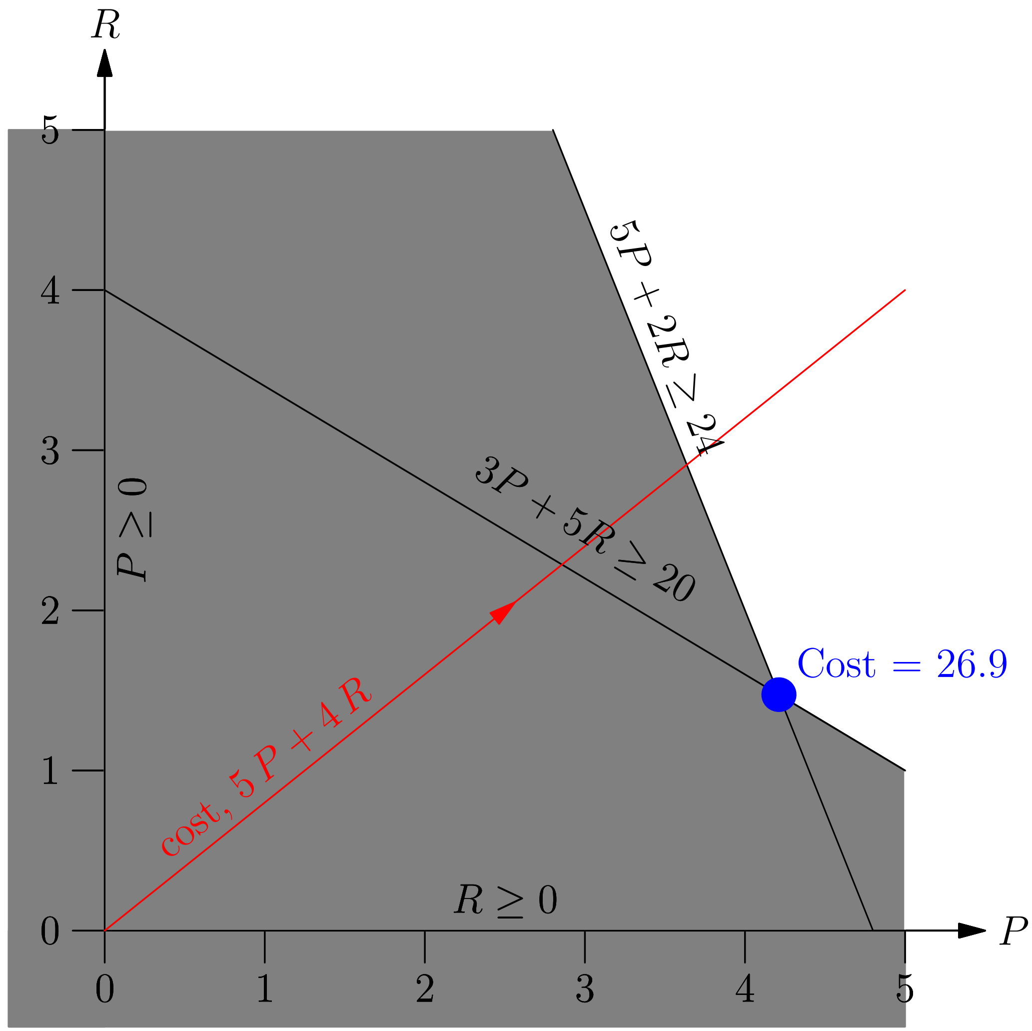

Lagrangian

- We can write the problem as a Lagrange problem

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- subject to $P, R, A, B \geq 0$

- A and C are Lagrange multipliers for vitamin A and C

- We can rearrange the Lagrangian to obtain

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- Consider someone selling vitamins A and C. They want to maximise the price of vitamins A and C, but their prices cannot exceed the price of the vitamins in potatoes or rice

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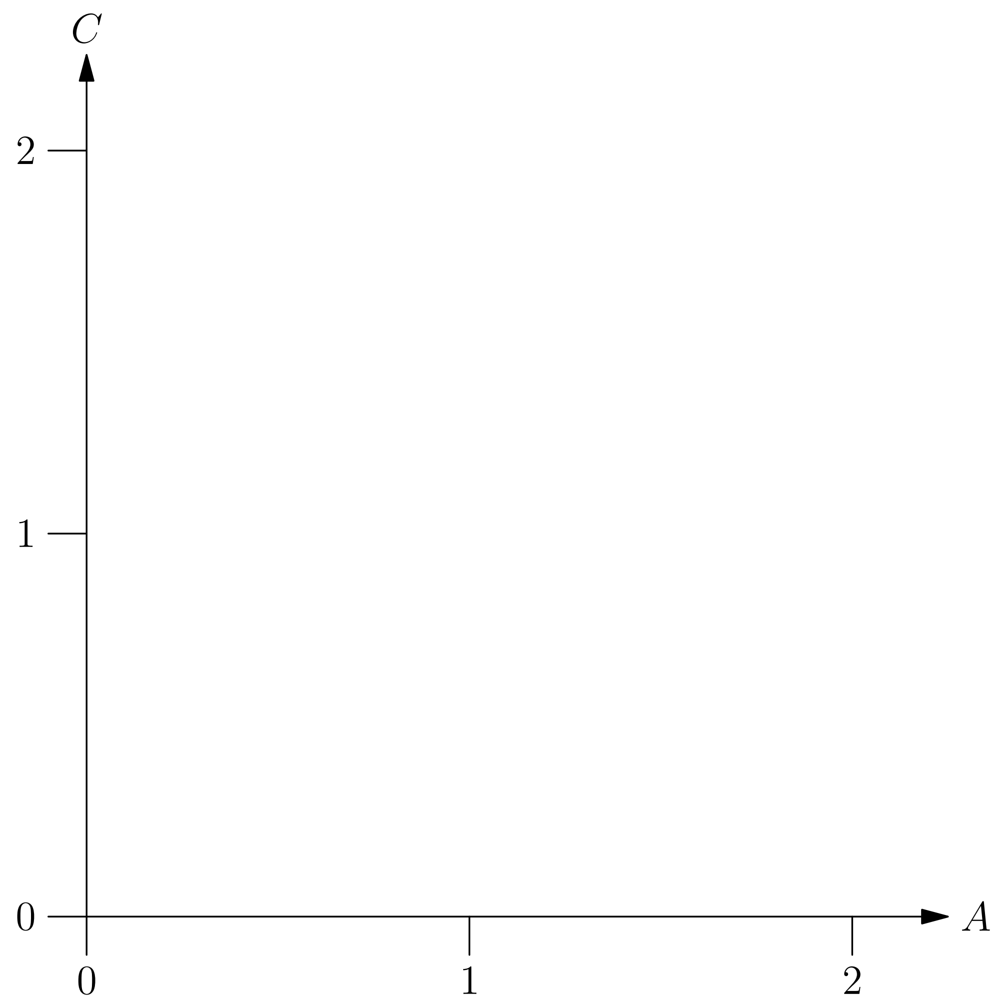

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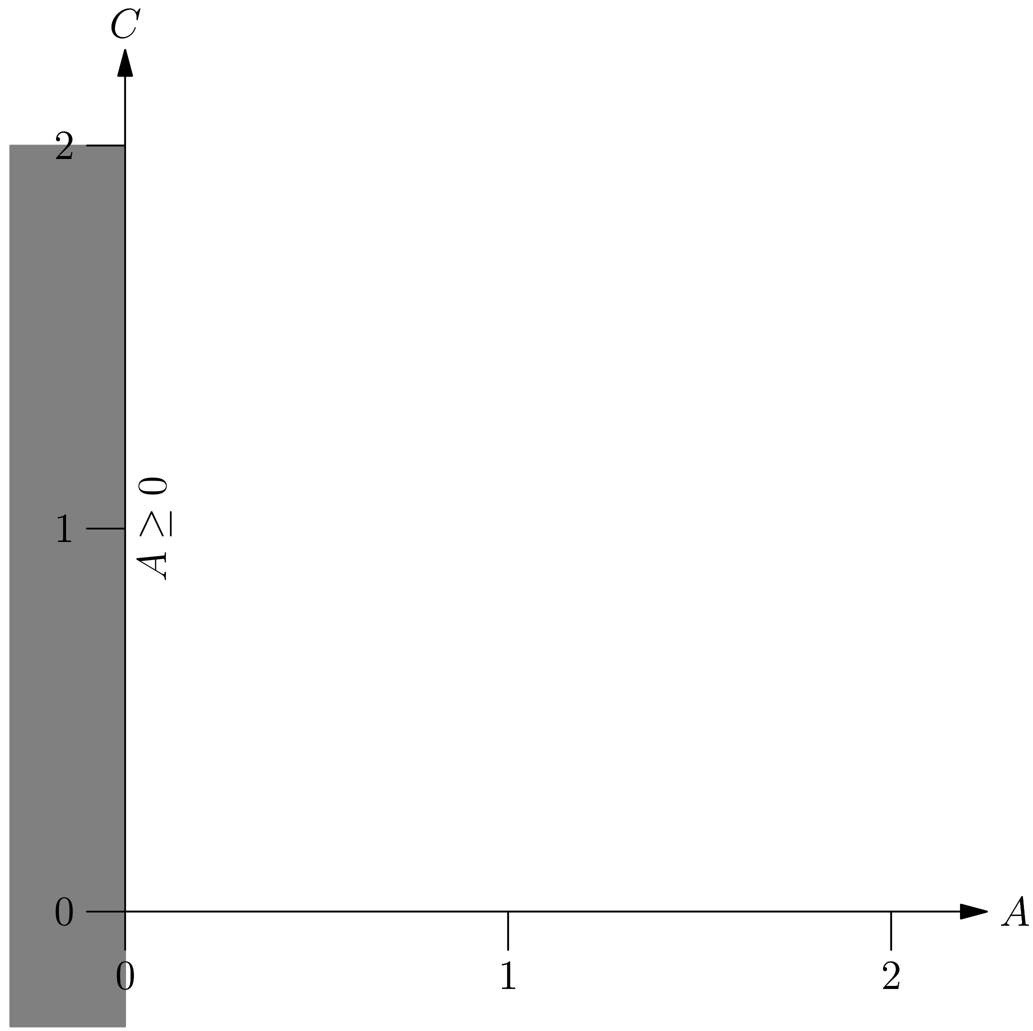

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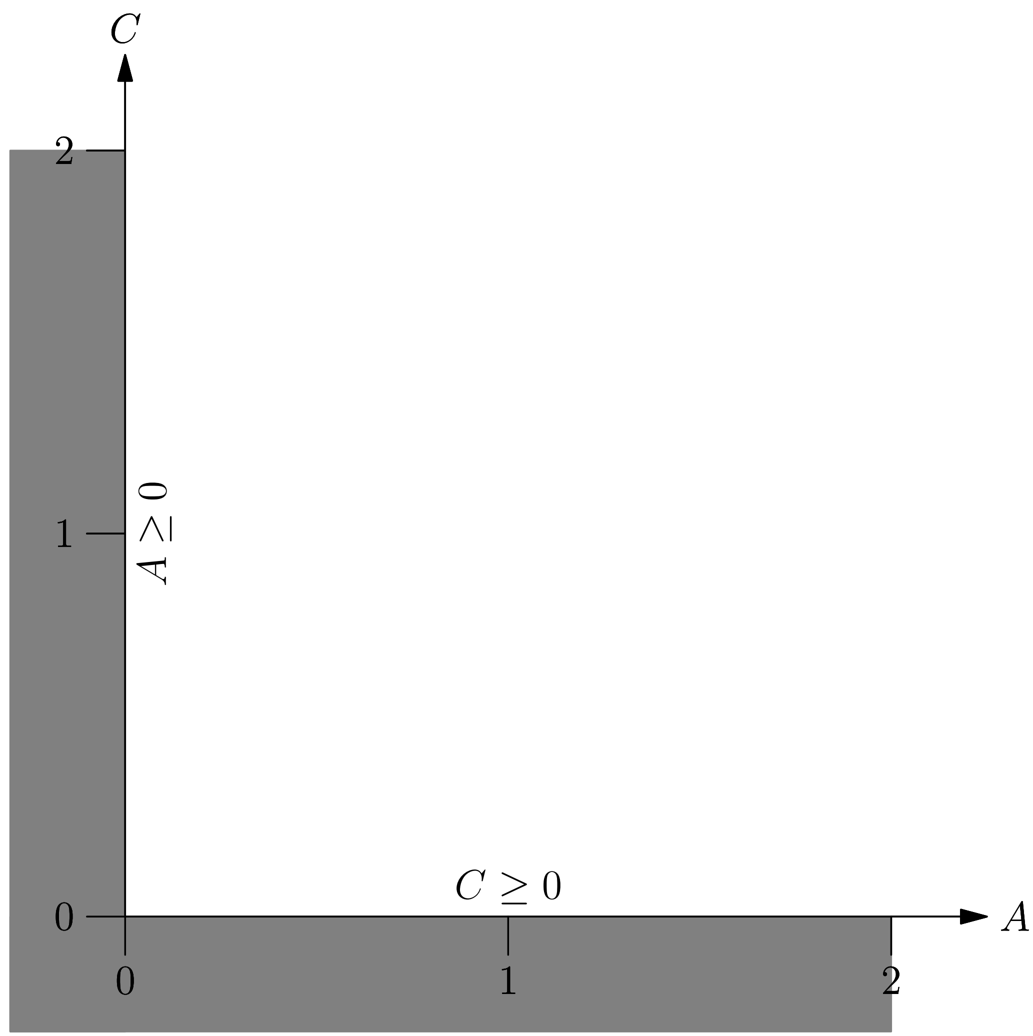

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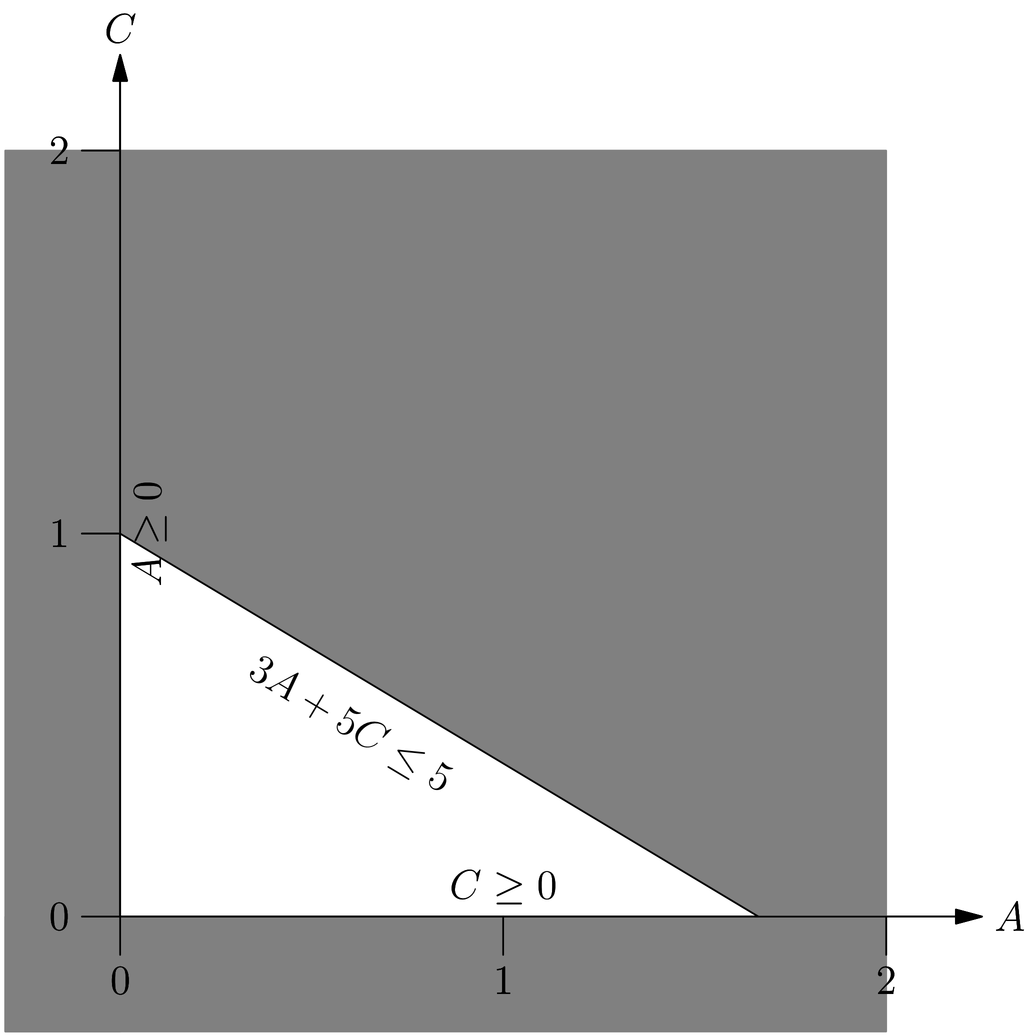

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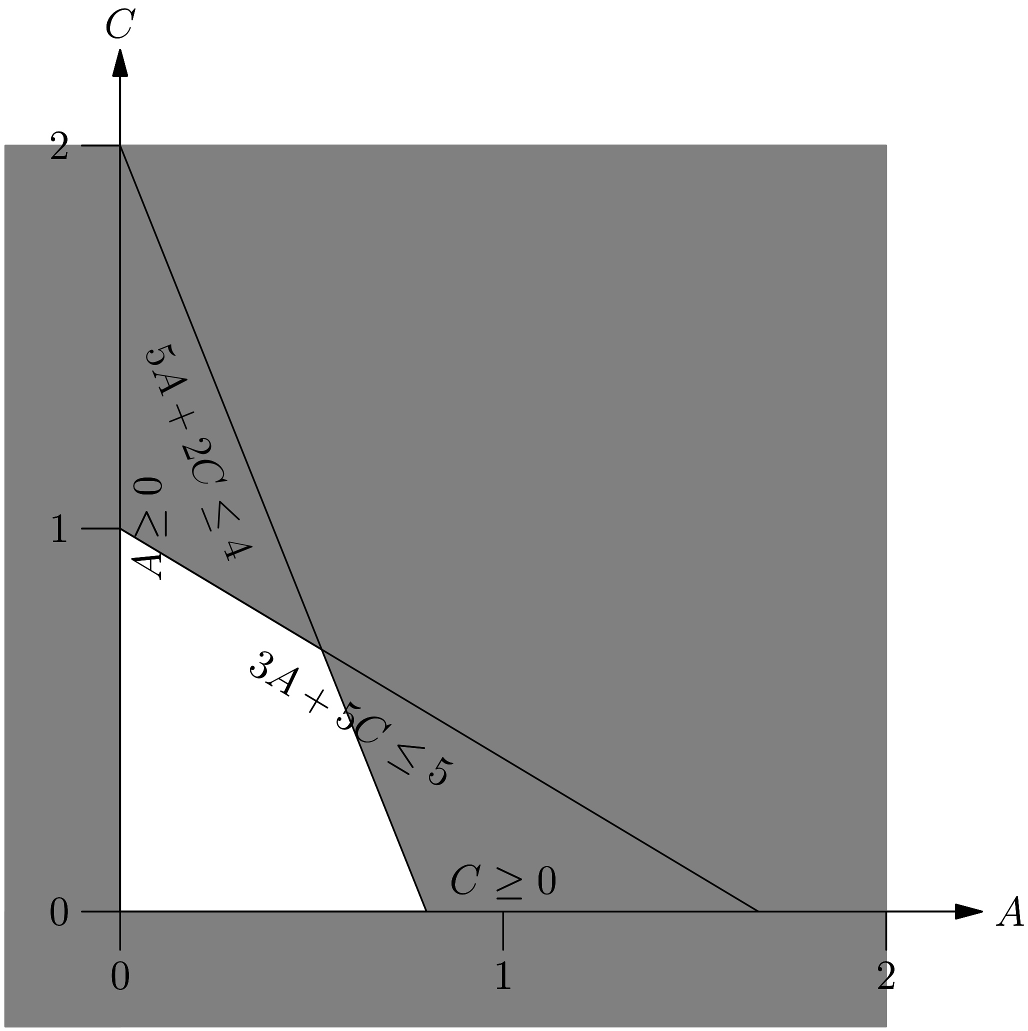

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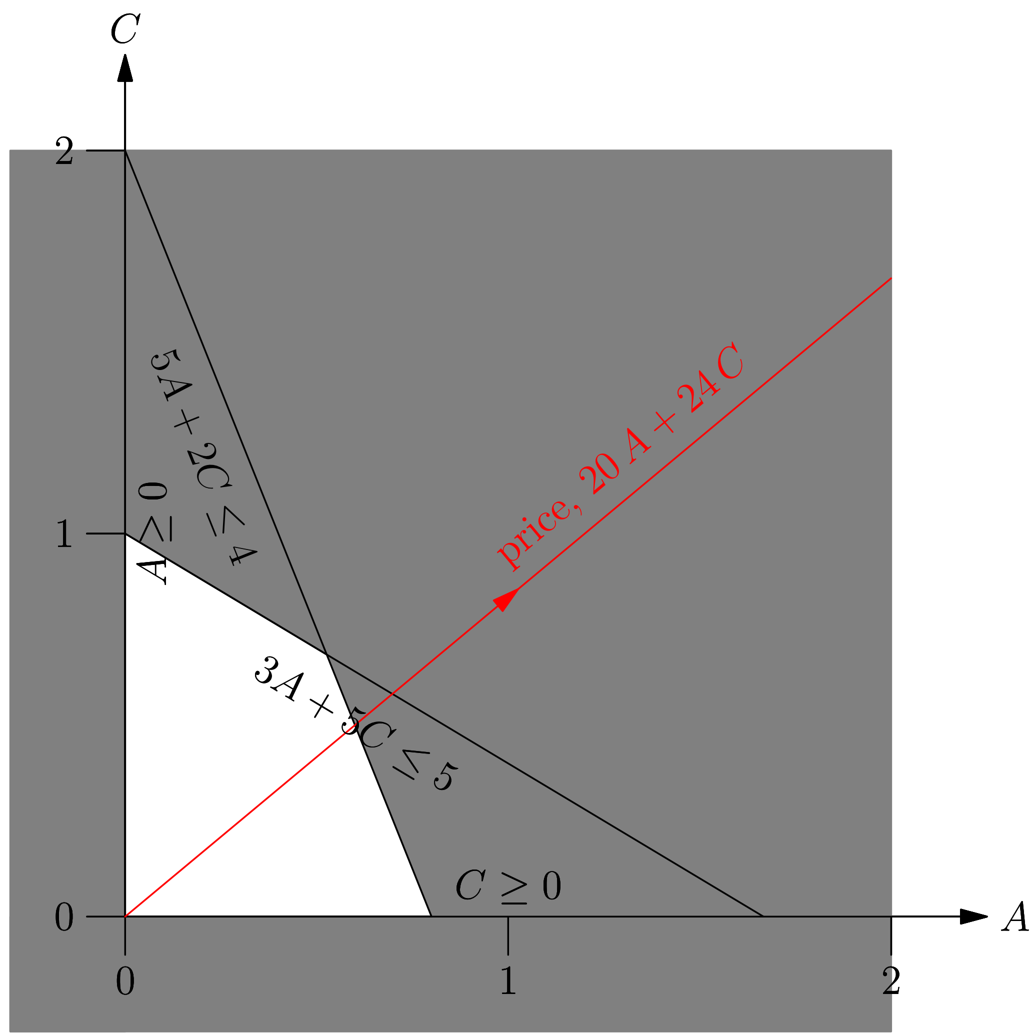

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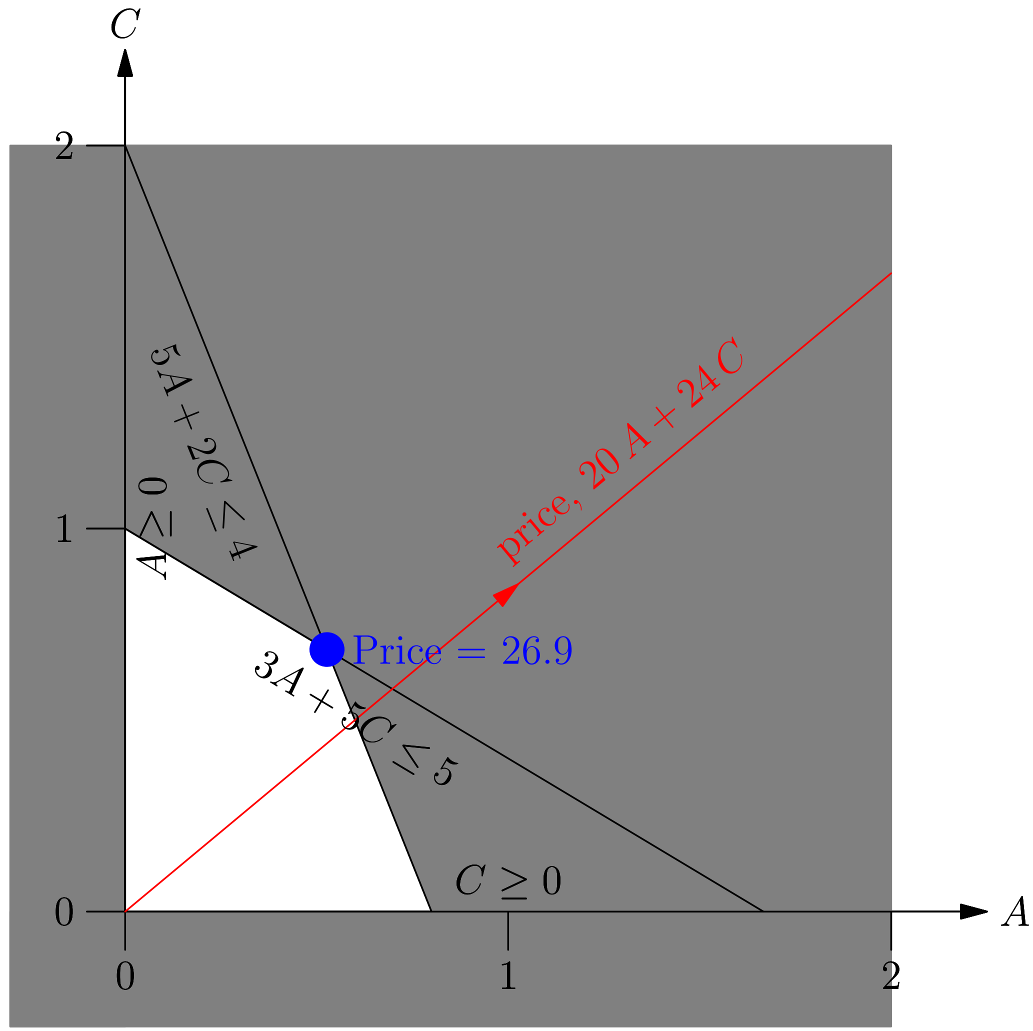

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- Why are we bothered about translating one linear programme into another?
- Sometime one form is massively easier to solve than the other
- This is because the first linear programme depends on the dimensionality of $\boldsymbol{x}$ while the second linear programme depends on the number of constraints (or dimensionality of $\boldsymbol{\alpha}$)
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Quadratic Programme

- A quadratic programme involves minimising a quadratic function $\boldsymbol{x}^\mathsf{T}\mathbf{Q}\boldsymbol{x}$ (with $\mathbf{Q} \succ 0$) subject to linear constraints $\mathbf{M}\,\boldsymbol{x} = \boldsymbol{b}$ (or $\mathbf{M}\,\boldsymbol{x} \leq \boldsymbol{b}$)

- We can define the Lagrangian

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}) = \boldsymbol{x}^\mathsf{T}\mathbf{Q}\,\boldsymbol{x} - \boldsymbol{\alpha}^\mathsf{T}\,(\mathbf{M}\,\boldsymbol{x} - \boldsymbol{b})$$

- where the solution is given by $\max\limits_{\boldsymbol{\alpha}} \min\limits_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha})$

- If the constraints are inequality constraints then $\alpha_i \geq 0$

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Solution to Quadratic Programming Problem

- Using

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}) = \boldsymbol{x}^{\mathsf{T}} \mathbf{Q}\, \boldsymbol{x} - \boldsymbol{\alpha}^{\mathsf{T}} (\mathbf{M}\, \boldsymbol{x} - \boldsymbol{b})$$

- Then

$$\boldsymbol{\nabla}_{\boldsymbol{x}} \mathcal{L}(\boldsymbol{x}, \boldsymbol{\alpha}) = 2\, \mathbf{Q}\, \boldsymbol{x} + \mathbf{M}^{\mathsf{T}} \boldsymbol{\alpha}$$

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

$$\boldsymbol{x}^* = \frac{1}{2} \mathbf{Q}^{-1} \mathbf{M}^{\mathsf{T}} \boldsymbol{\alpha}$$

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Lessons

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- This is particularly useful for problems with unique solutions (it will work when there are multiple solutions, but finding many saddle points is a pain)
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