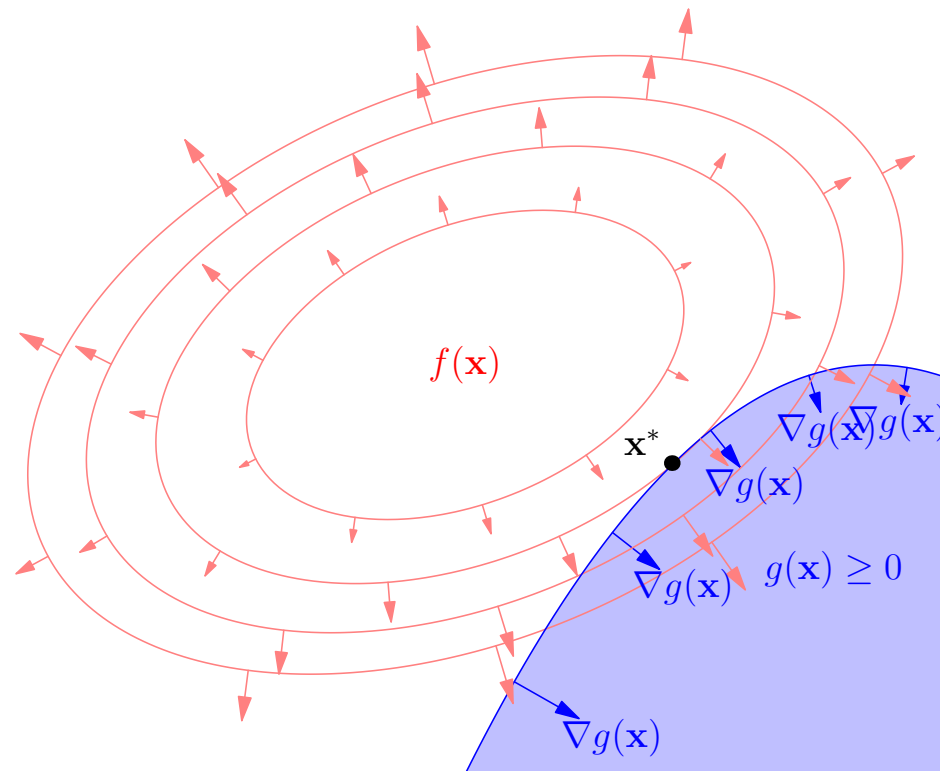


Advanced Machine Learning

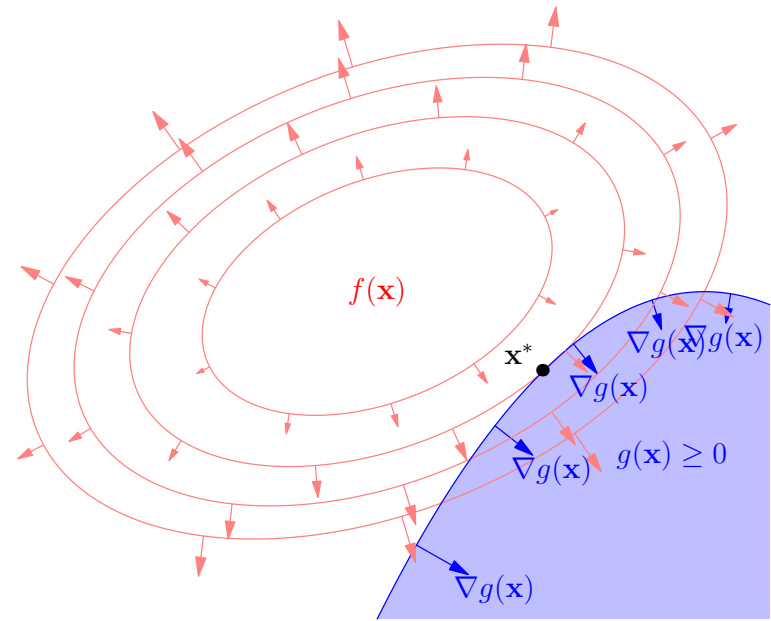
Constrained Optimisation



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

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

- A standard procedure is to define the Lagrangian

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

where α is known as a Lagrange multiplier

- In the extended space (\mathbf{x}, α) we have to solve

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- The second condition is just the constraint
- But what about first condition: $\nabla_{\mathbf{x}} f(\mathbf{x}) = \alpha \nabla_{\mathbf{x}} g(\mathbf{x})$?

Note on Gradients

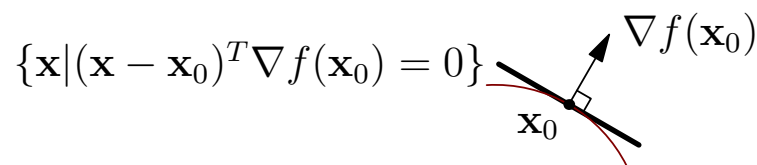
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where \mathbf{H} is a matrix of second derivative known as the Hessian

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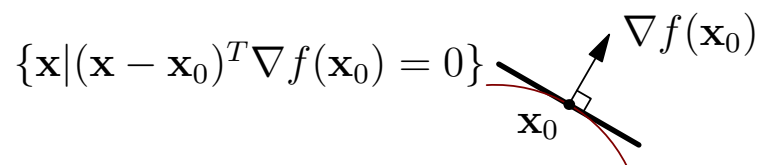
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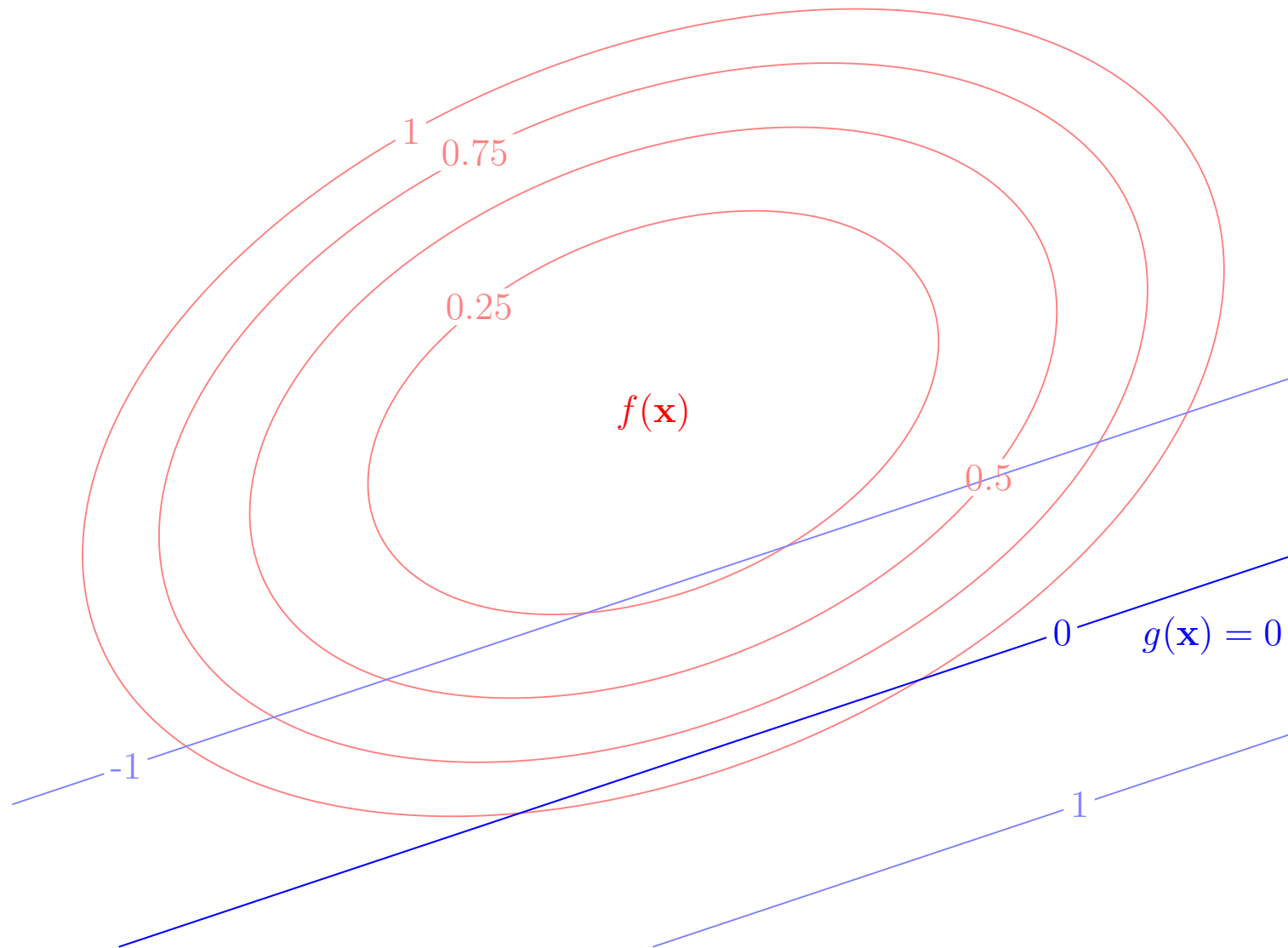
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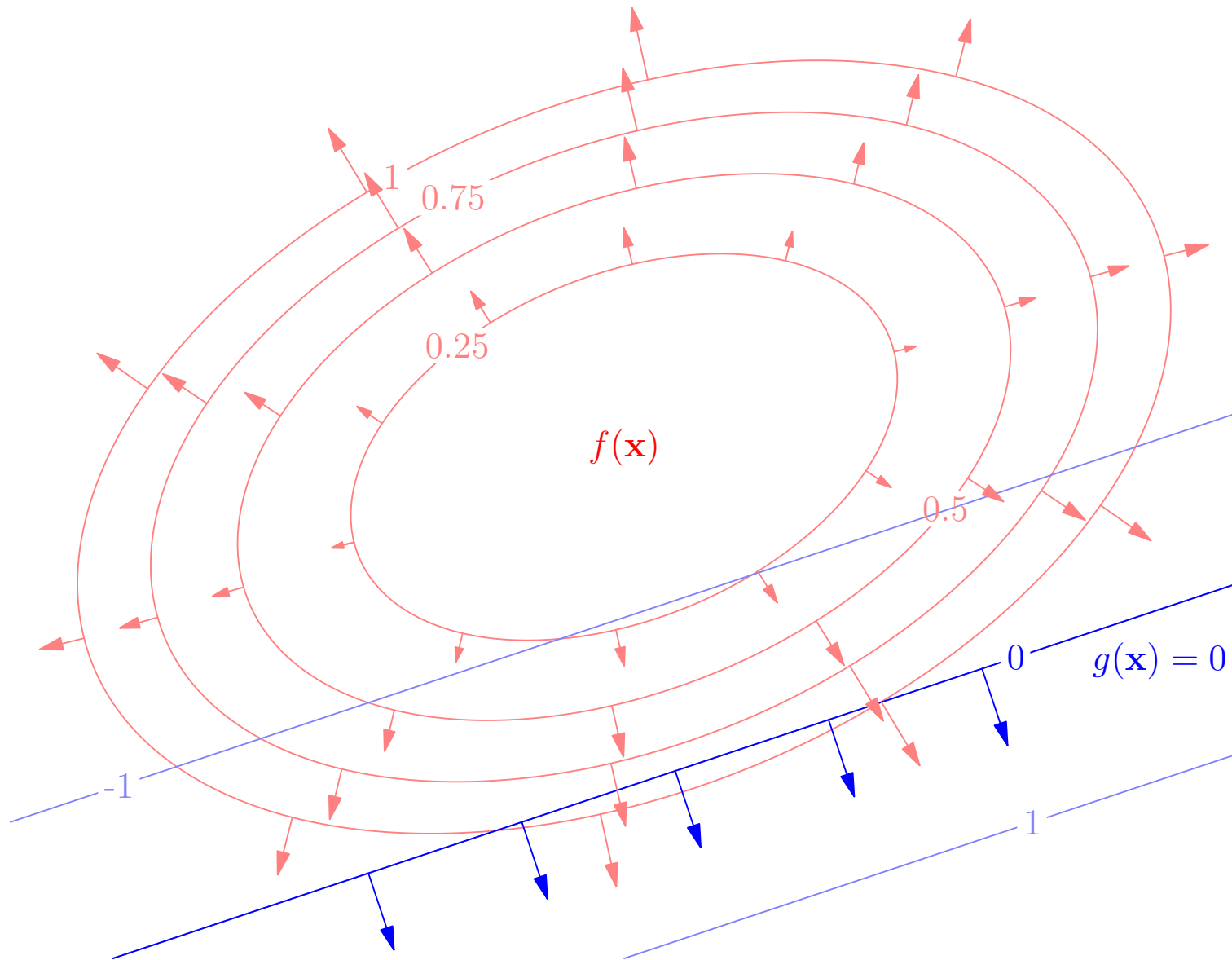


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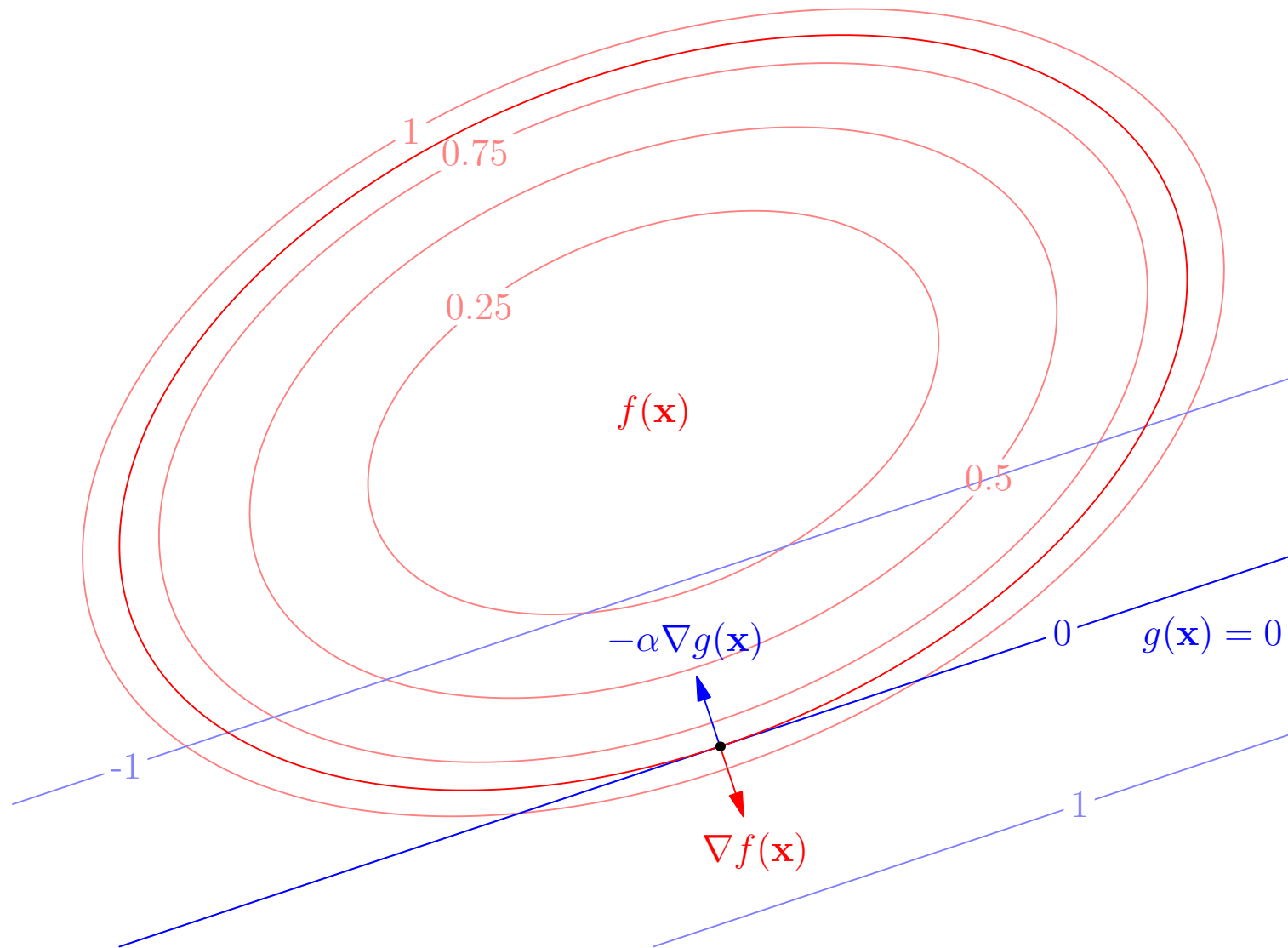
Constrained Optima



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Example

- Minimise $f(\mathbf{x}) = x^2 + 2y^2 - xy$
- Subject to $g(\mathbf{x}) = x - 2y - 3 = 0$
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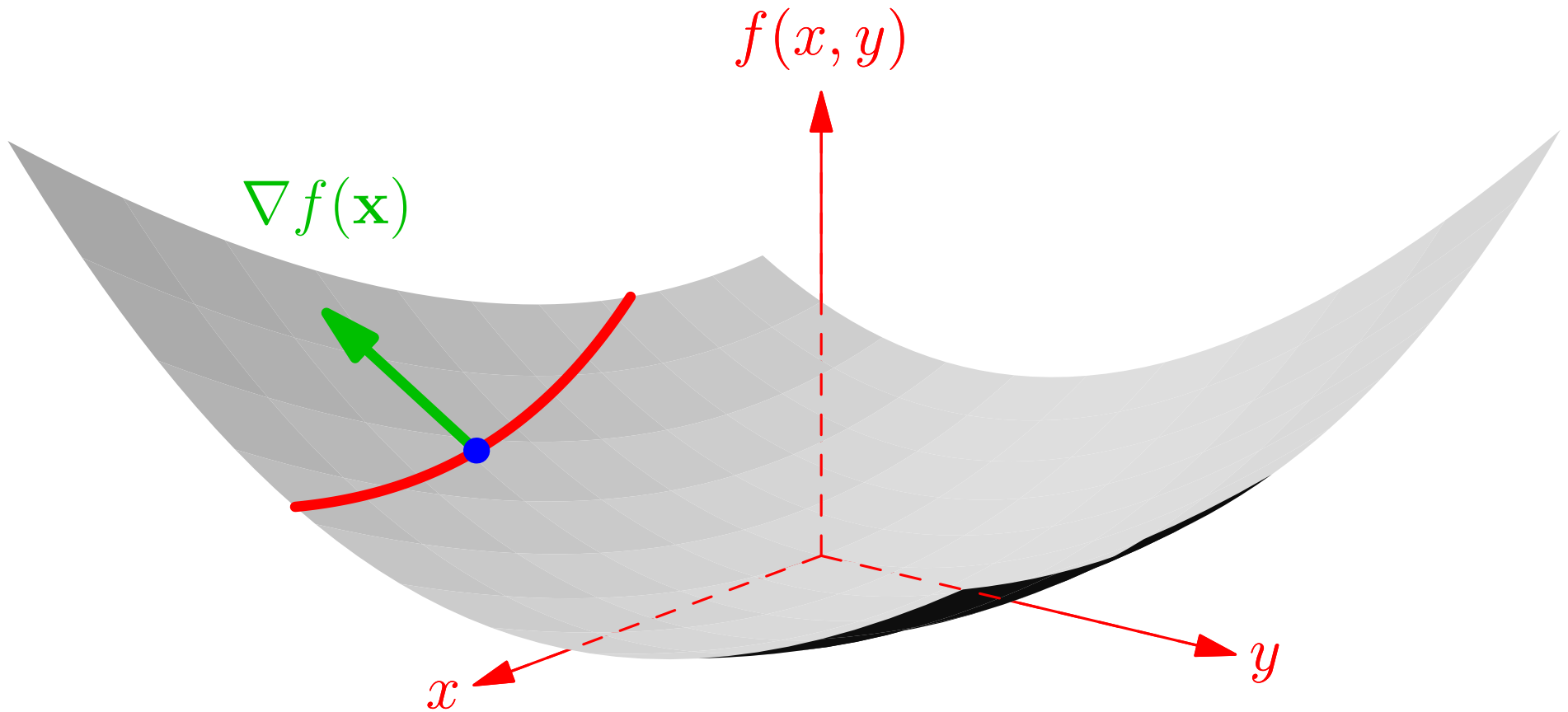
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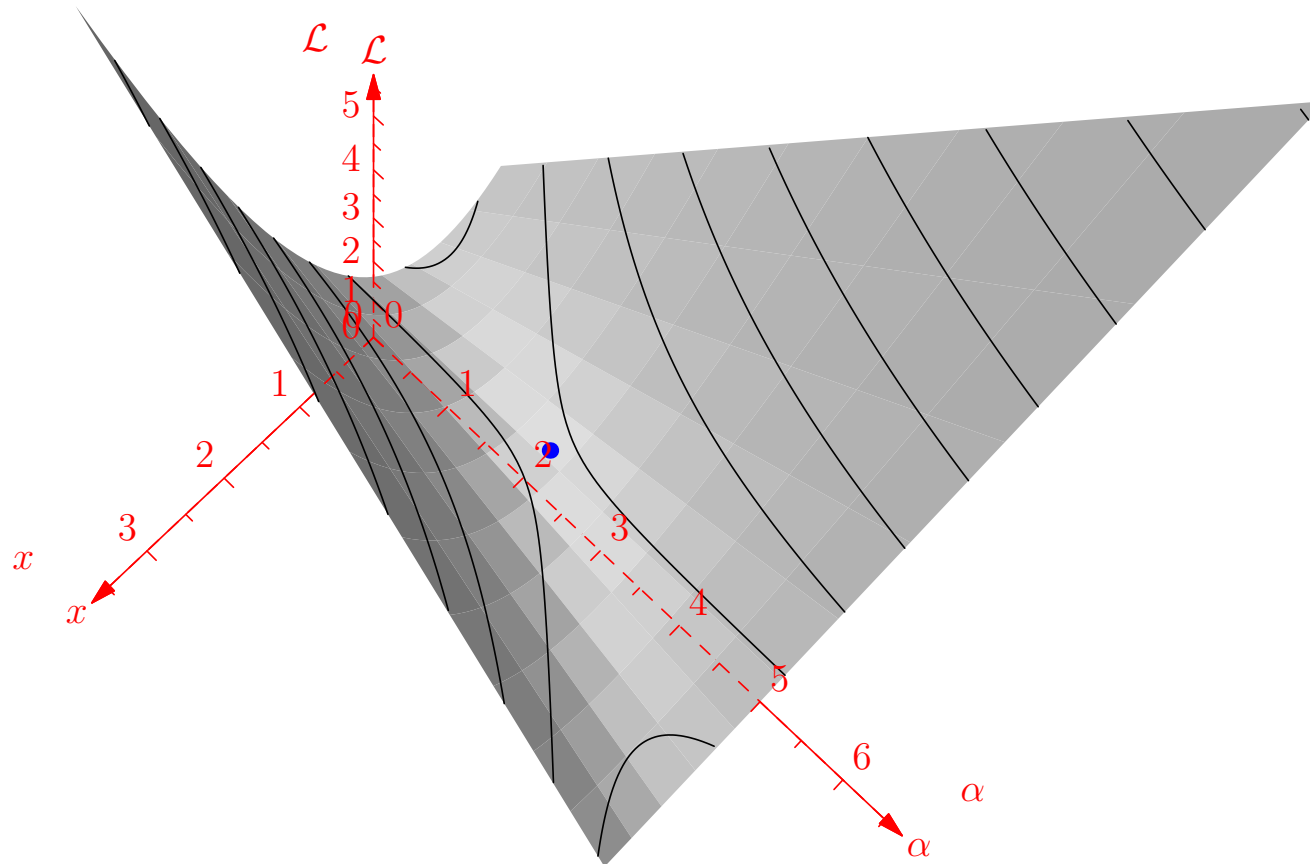
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Surface



Saddle-Point $y = -9/8$



Multiple Constraints

- Given an optimisation problem with multiple constraints

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

- We introduce multiple Lagrange multipliers

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

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- Minimise $f(\mathbf{x}) = x^2 + 2y^2 + 5z^2 - xy - xz$ subject to $g_1(\mathbf{x}) = x - 2y - z - 3 = 0$ and $g_2(\mathbf{x}) = 2x + 3y + z - 2 = 0$
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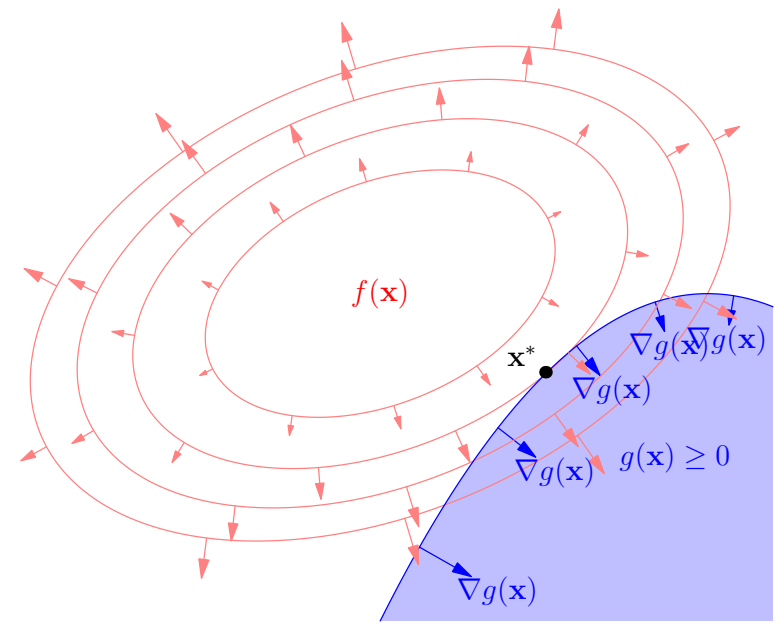
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2. **Inequalities**
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Inequality Constraints

- Suppose we have the problem

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

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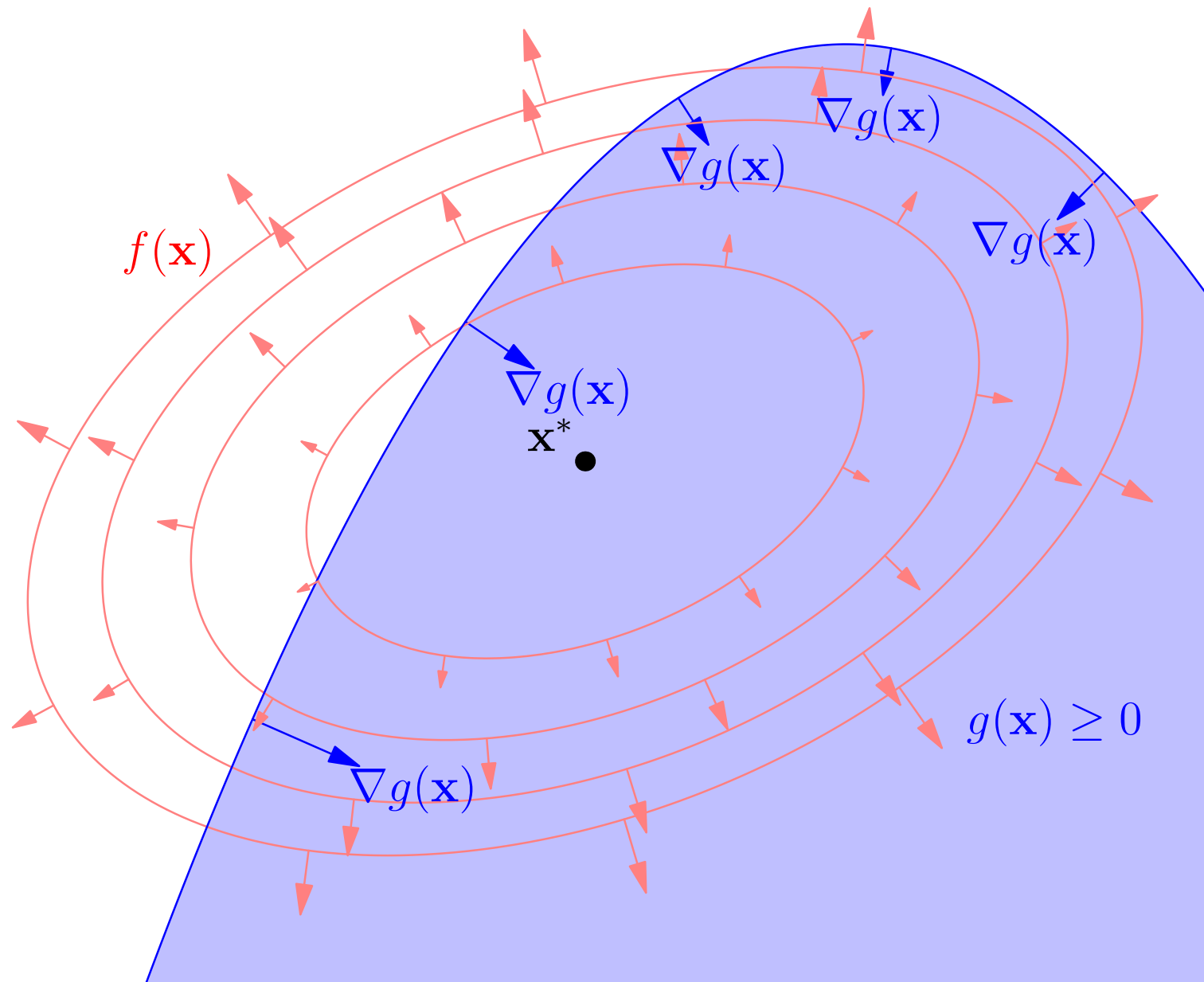
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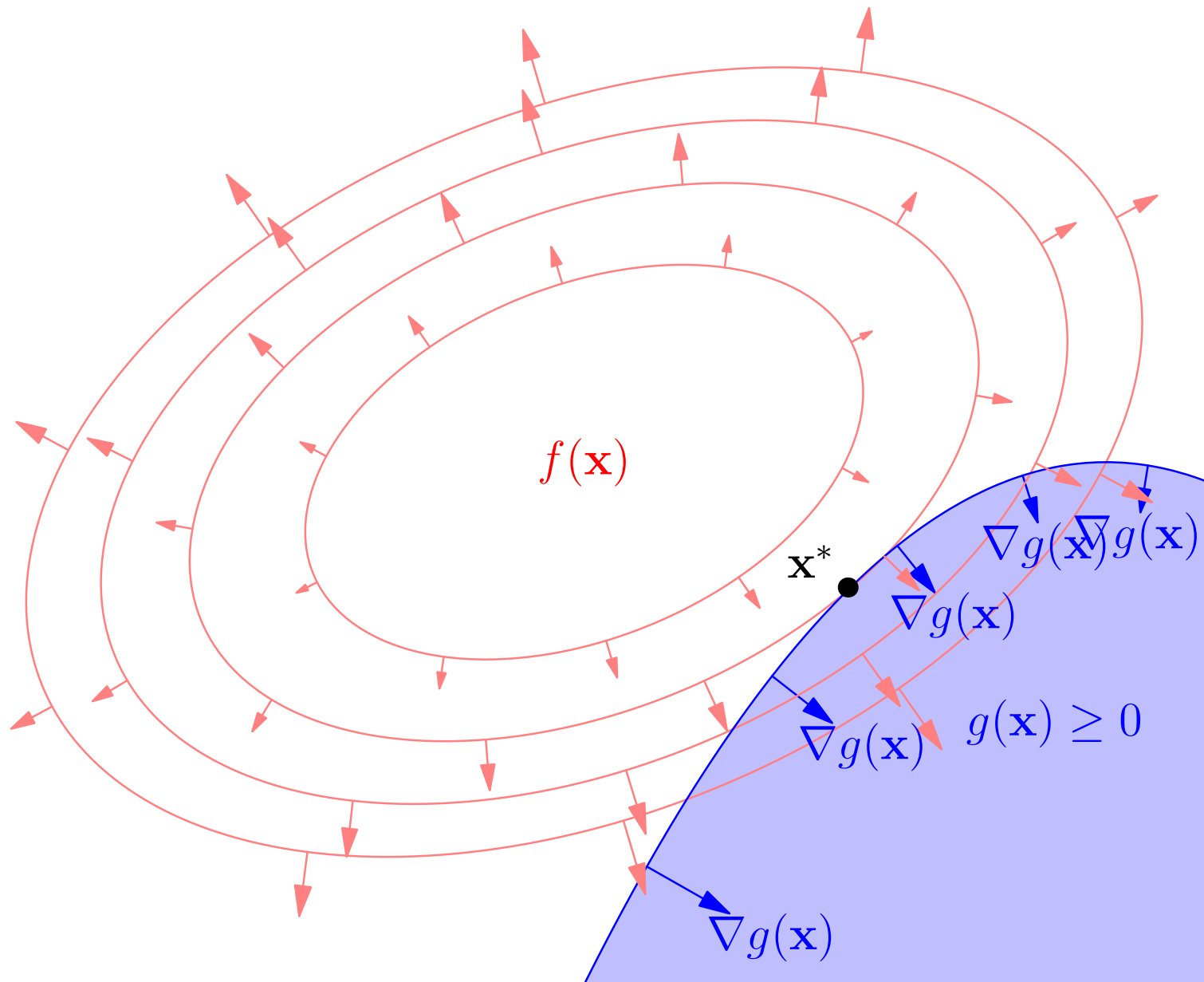
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Inside Region



On the Boundary



KKT Conditions

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

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- where either
 - ★ $\alpha = 0$ and the solutions in the interior or
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Many Inequalities

- Given the problem

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

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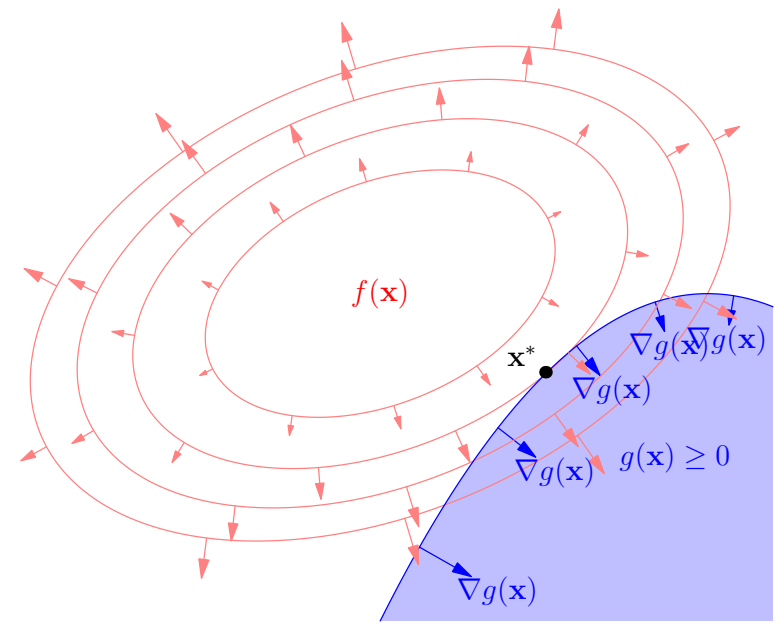
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Outline

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



Solving the Lagrangian for \mathbf{x}

- Consider minimising a function $f(\mathbf{x})$ subject to a set of constraints $g_i(\mathbf{x}) = 0$ or $g_i(\mathbf{x}) \leq 0$
- We can consider this a double optimisation problem

$$\max_{\alpha} \min_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \alpha) = \max_{\alpha} \min_{\mathbf{x}} \left(f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x}) \right)$$

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Dual Problem

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

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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

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

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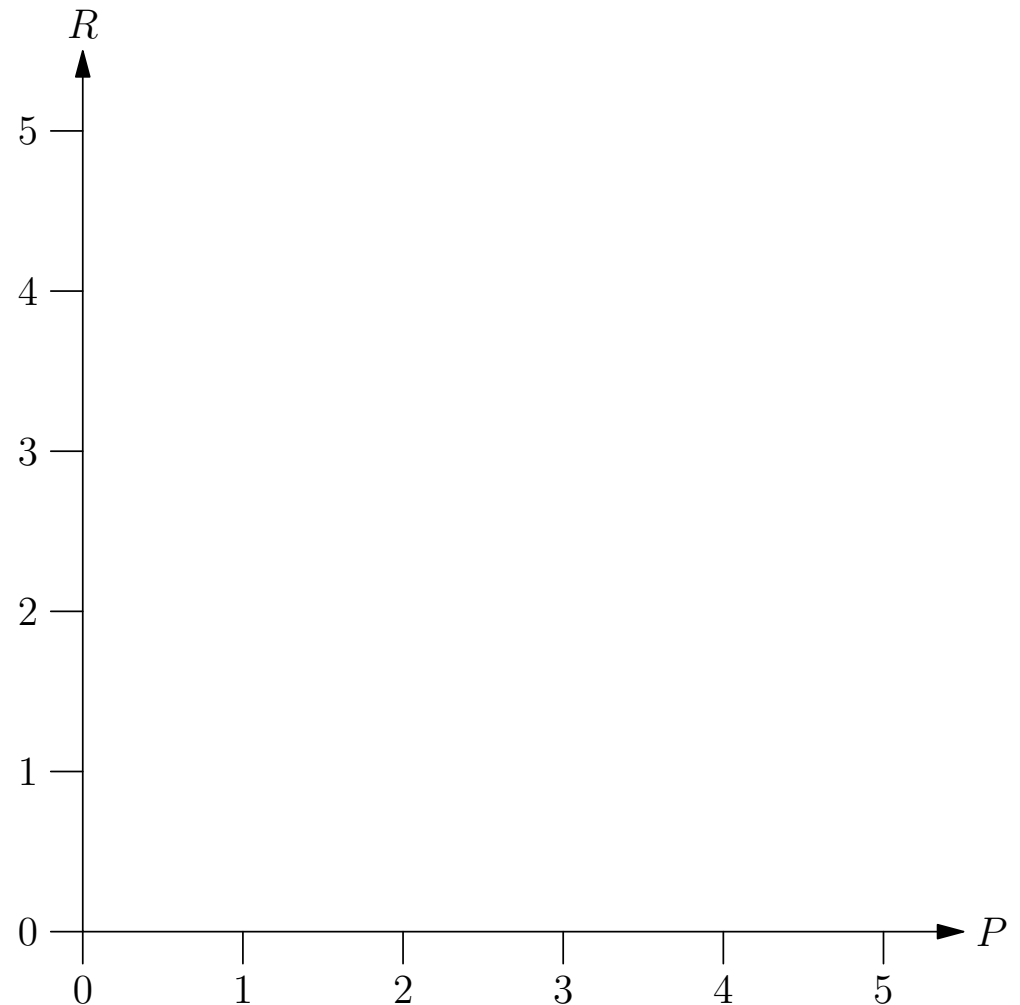
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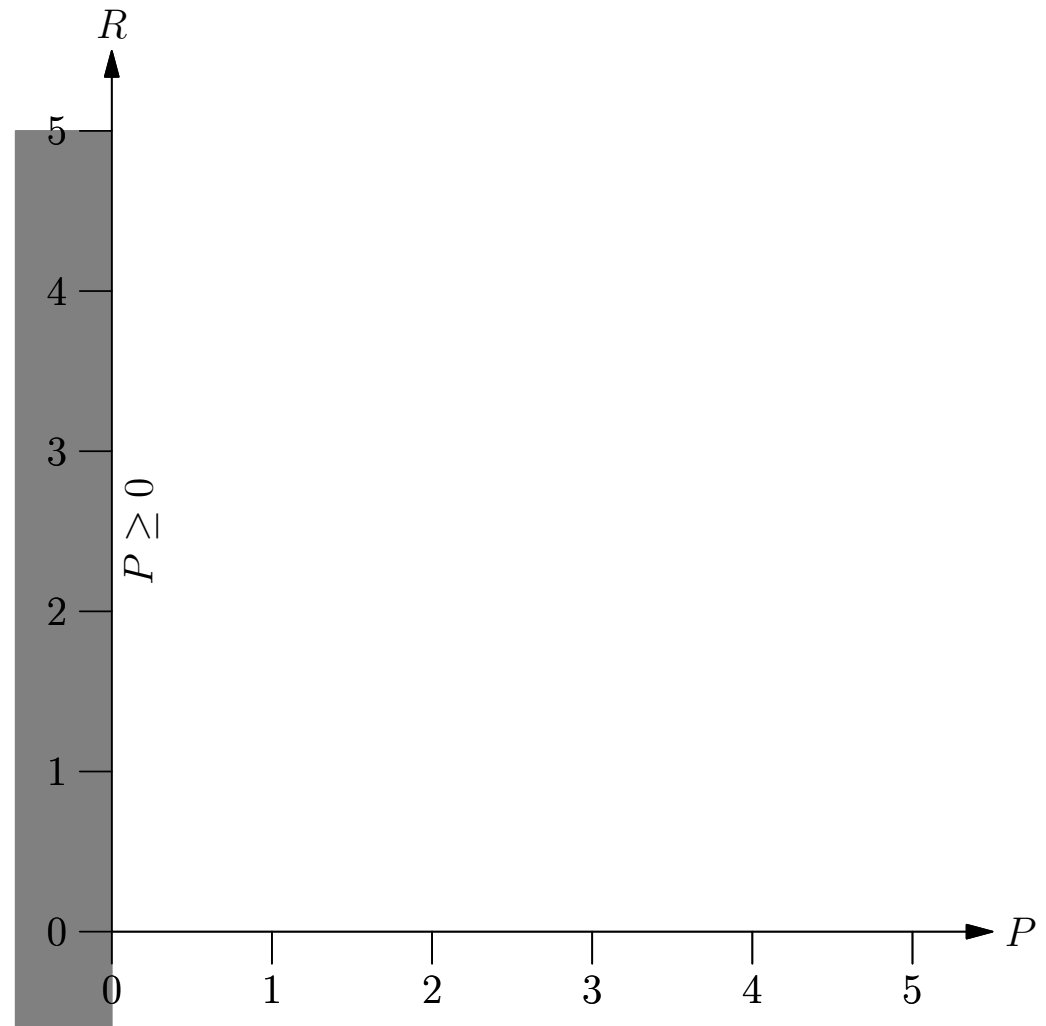
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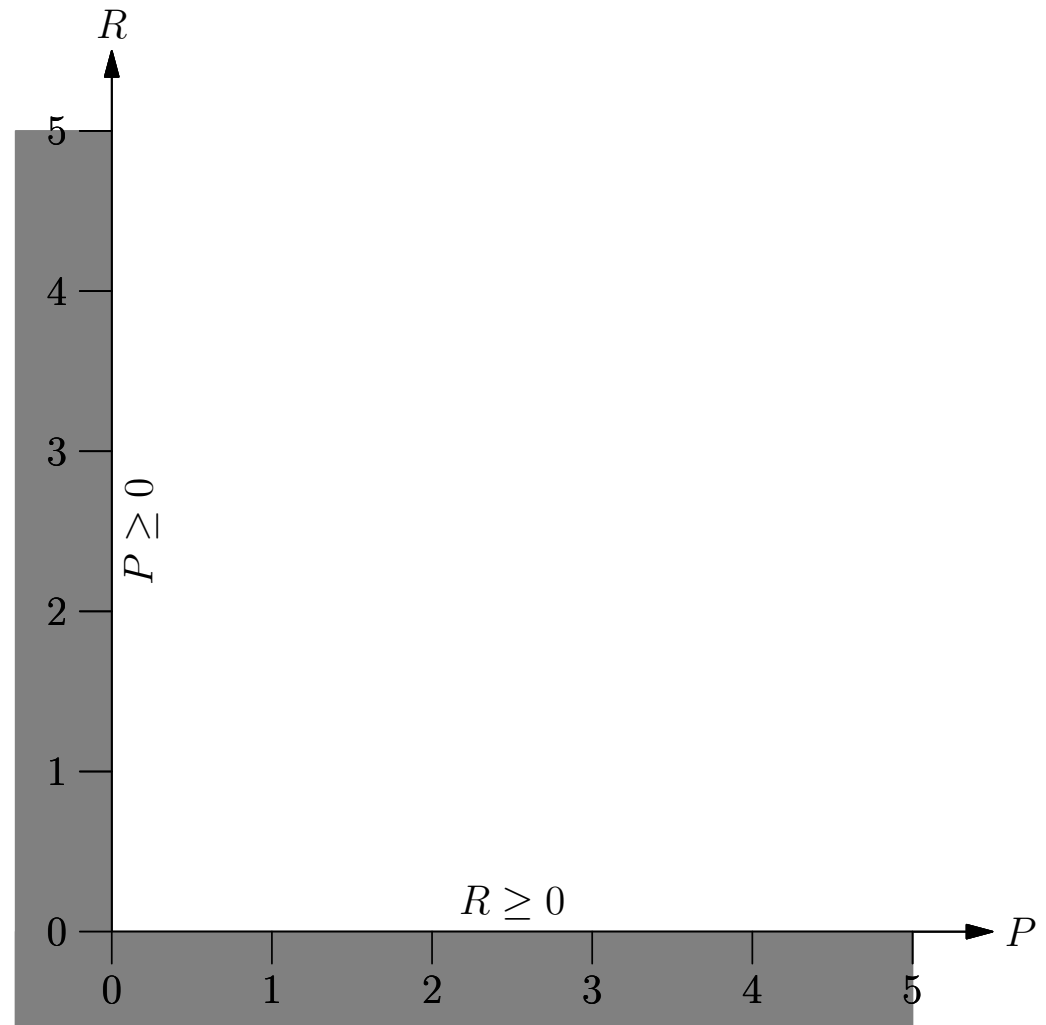
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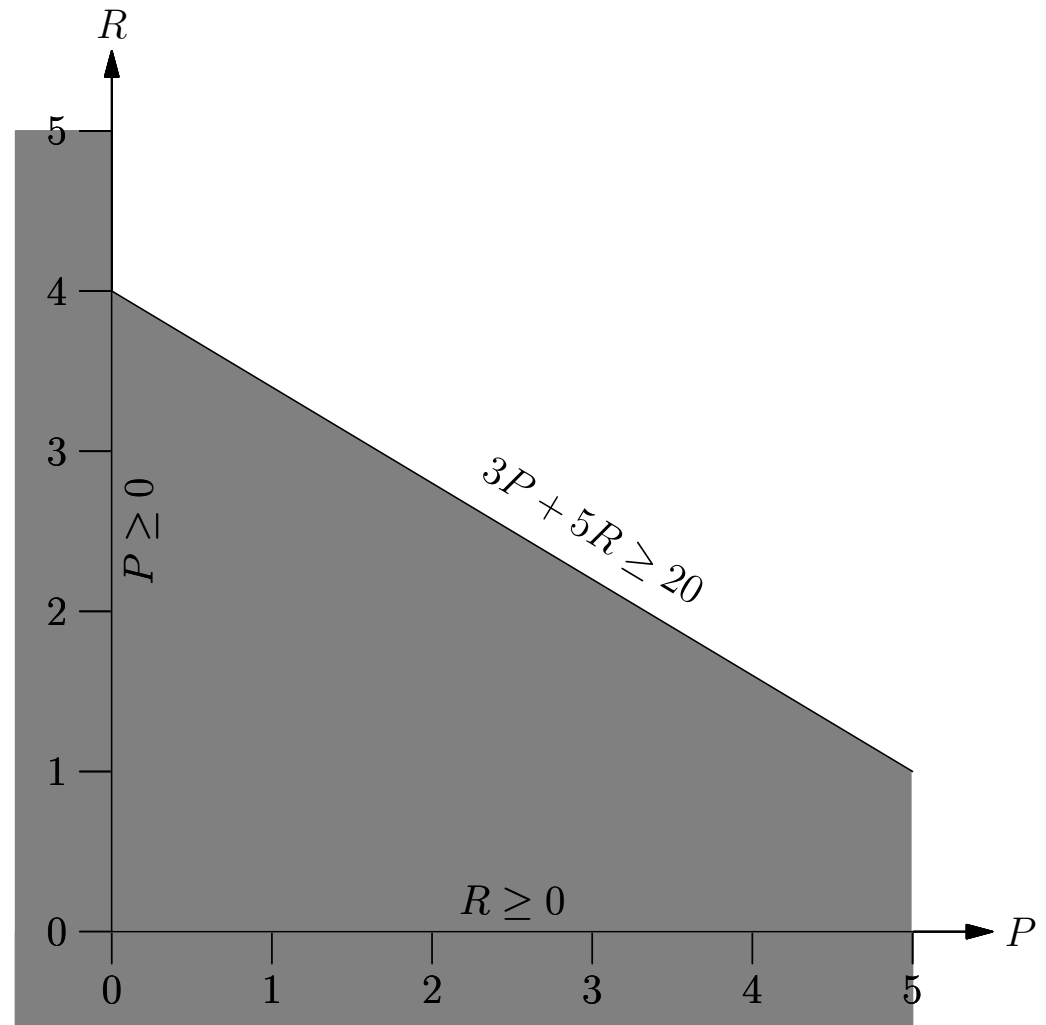
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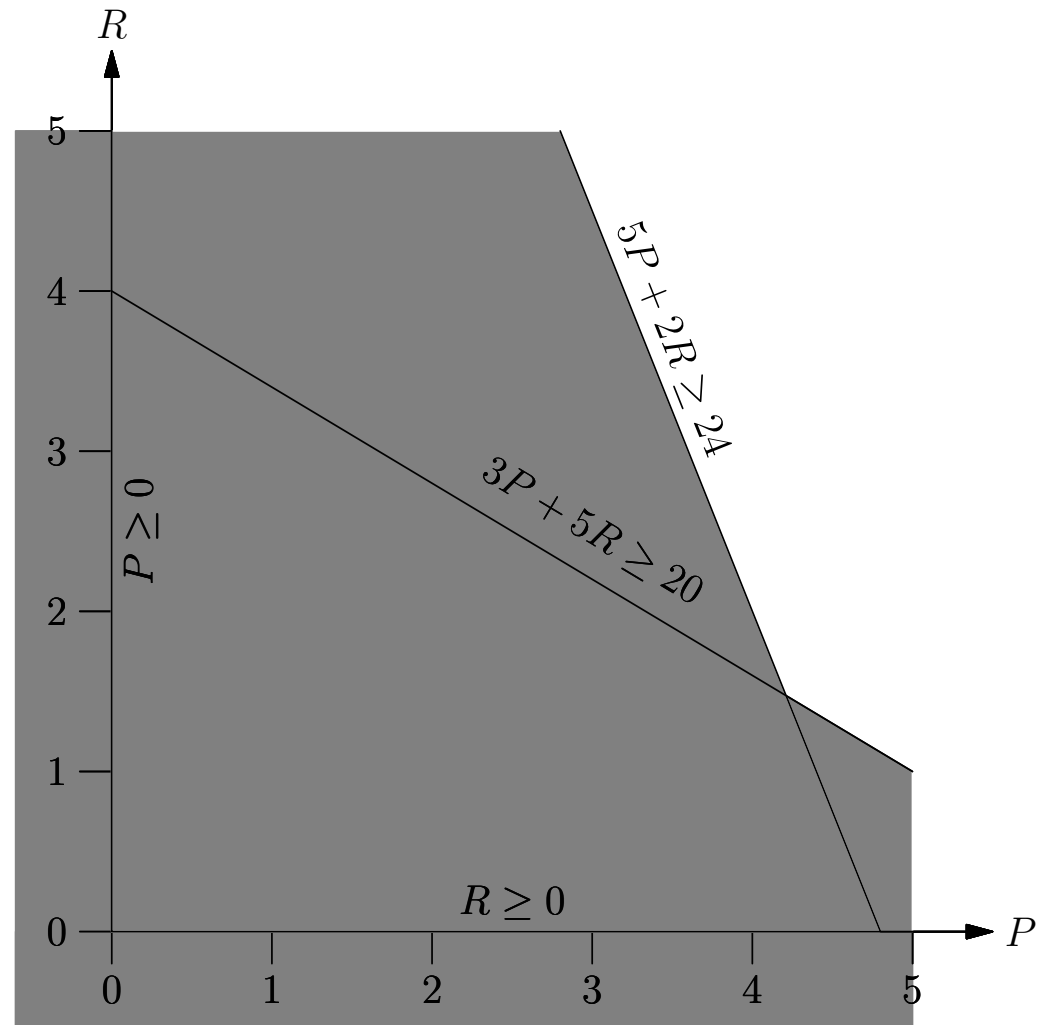
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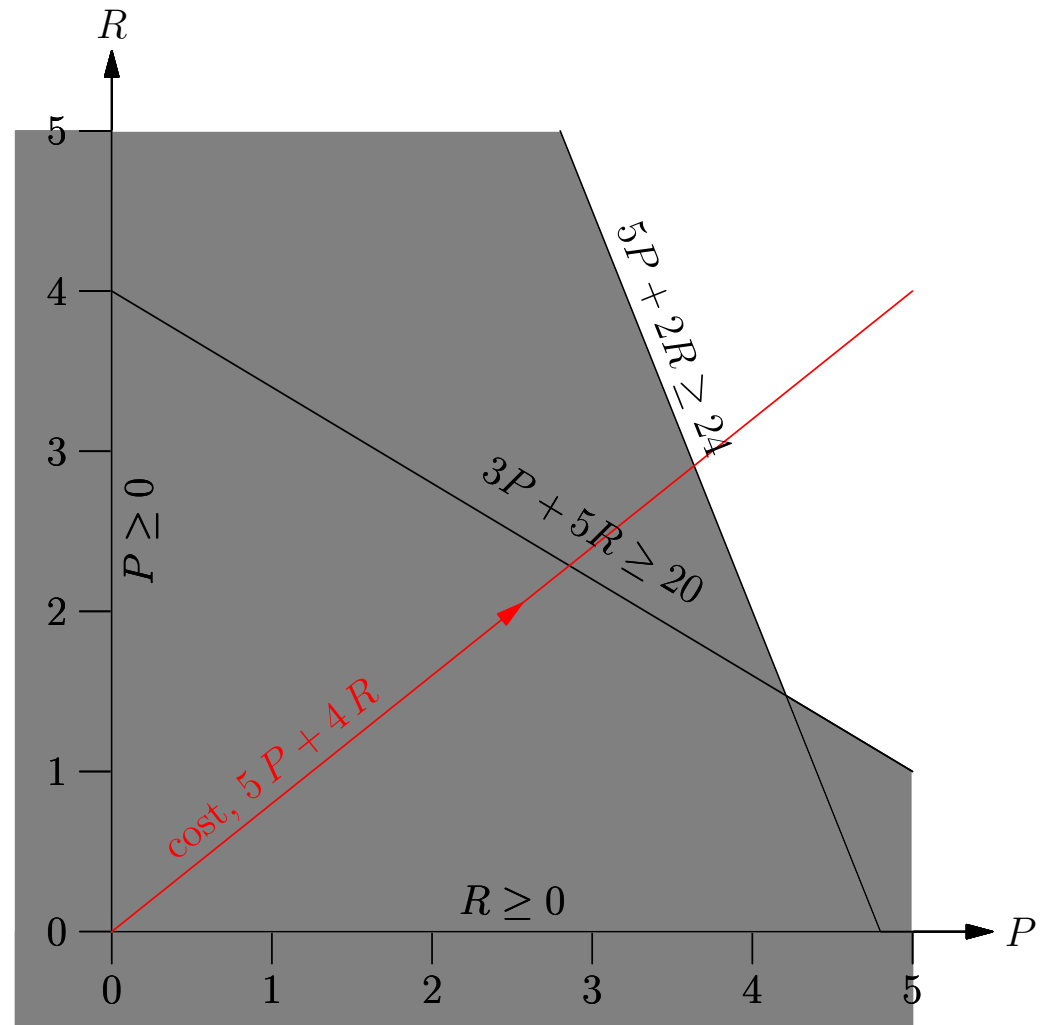
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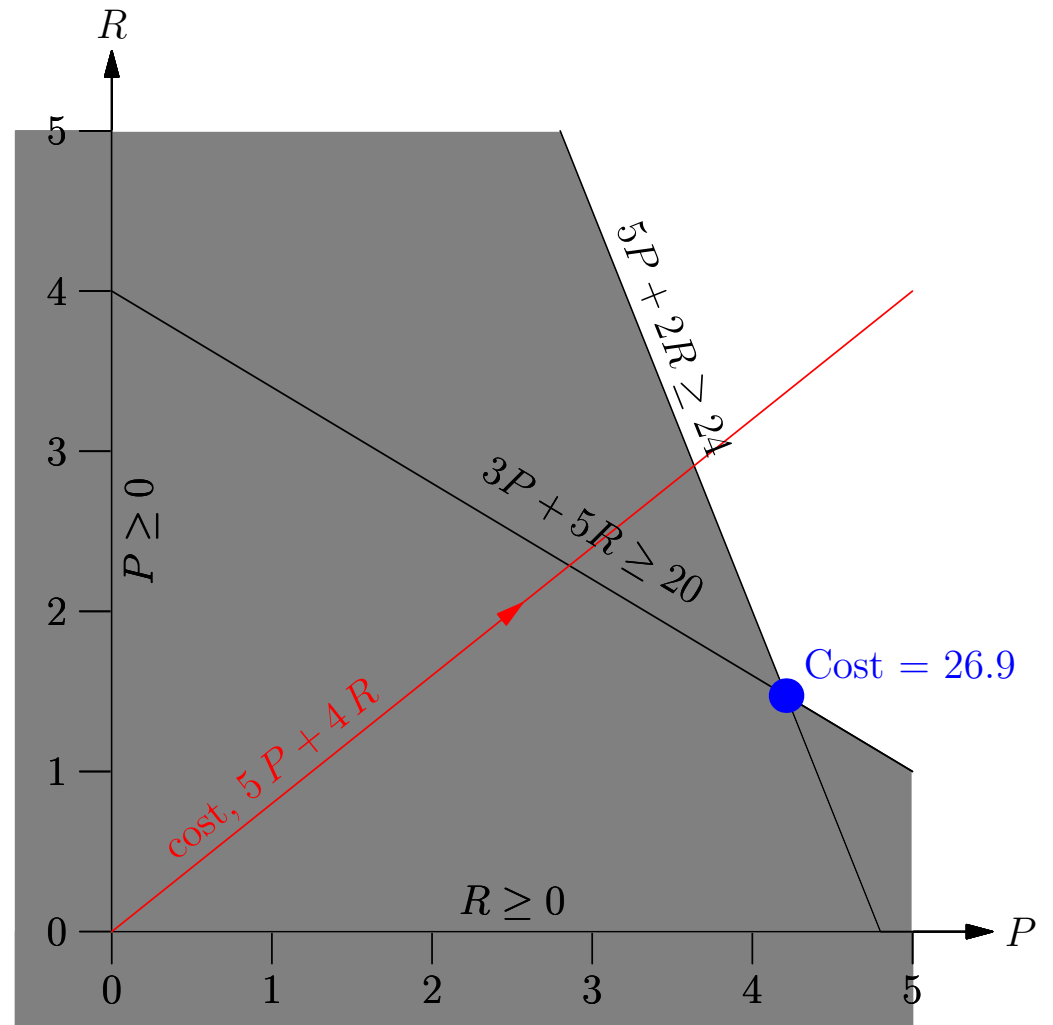
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- We can write the problem as a Lagrange problem

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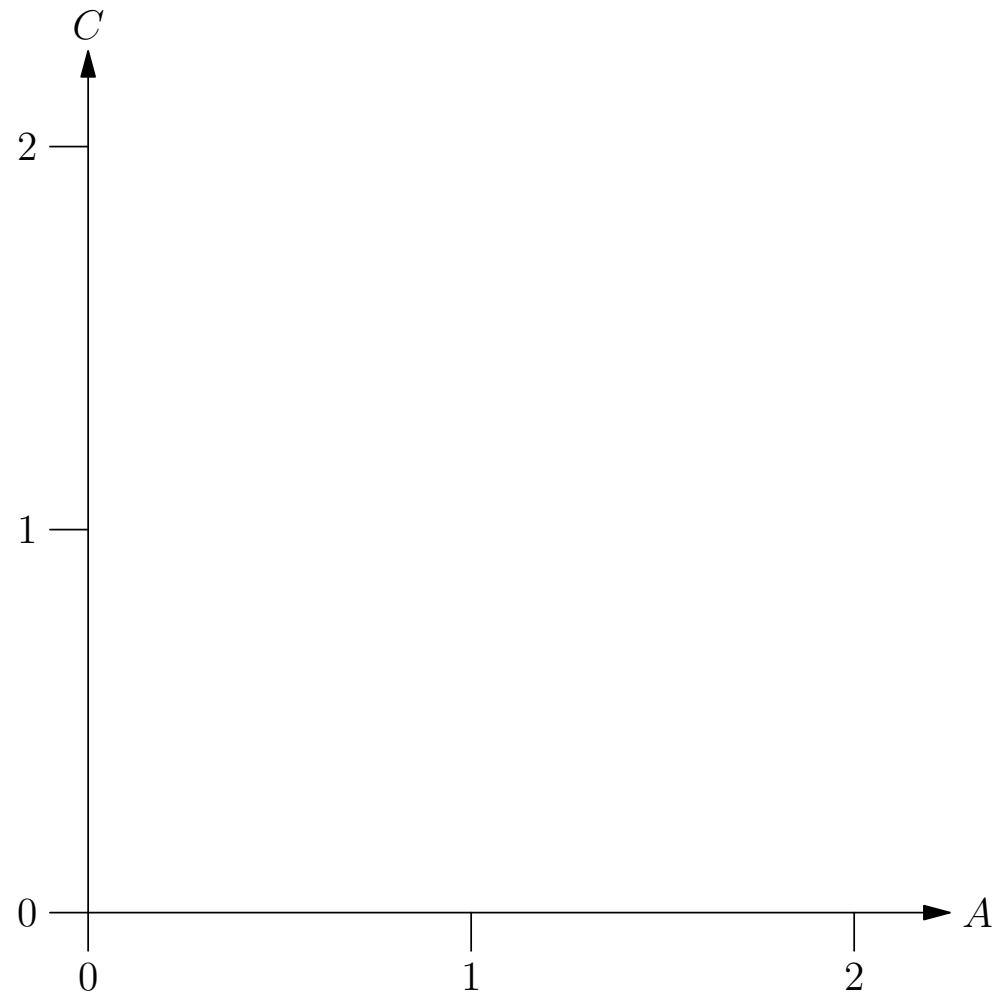
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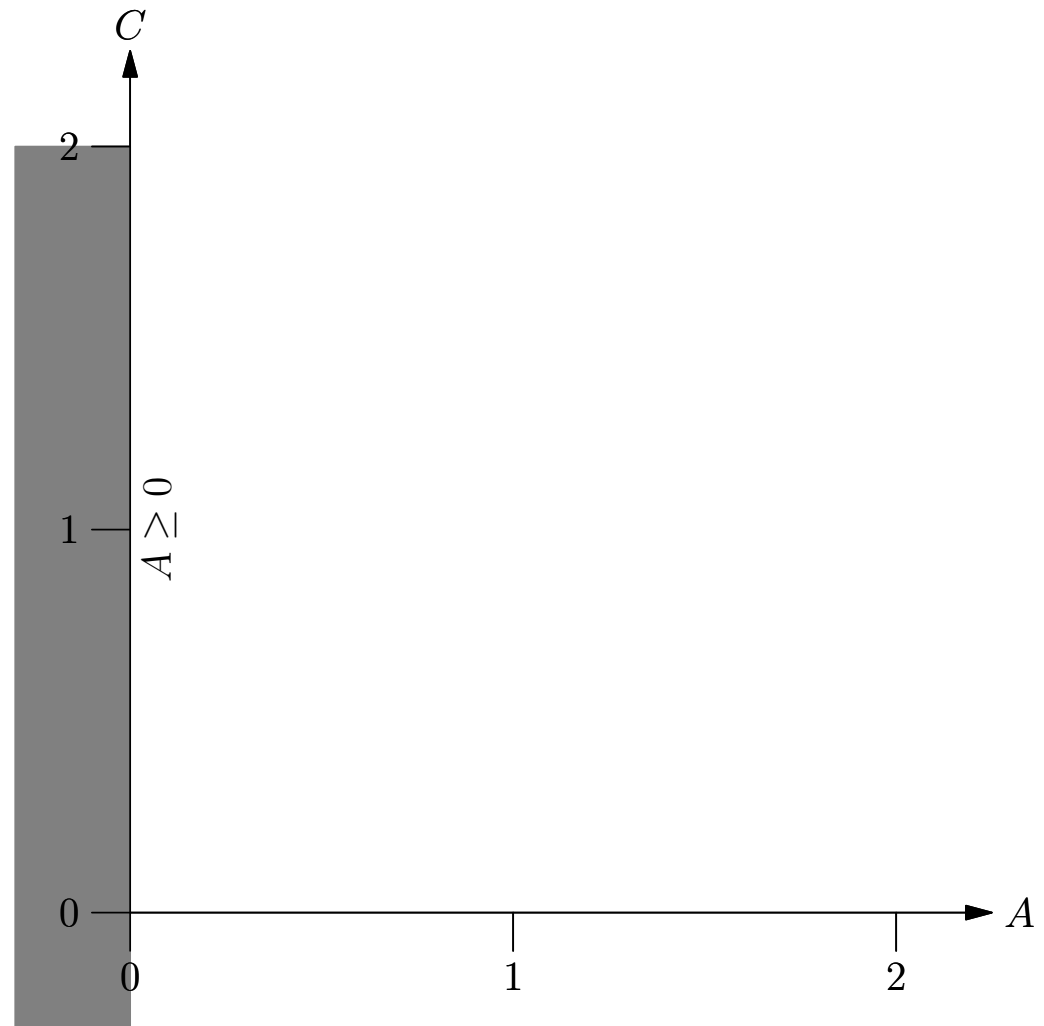
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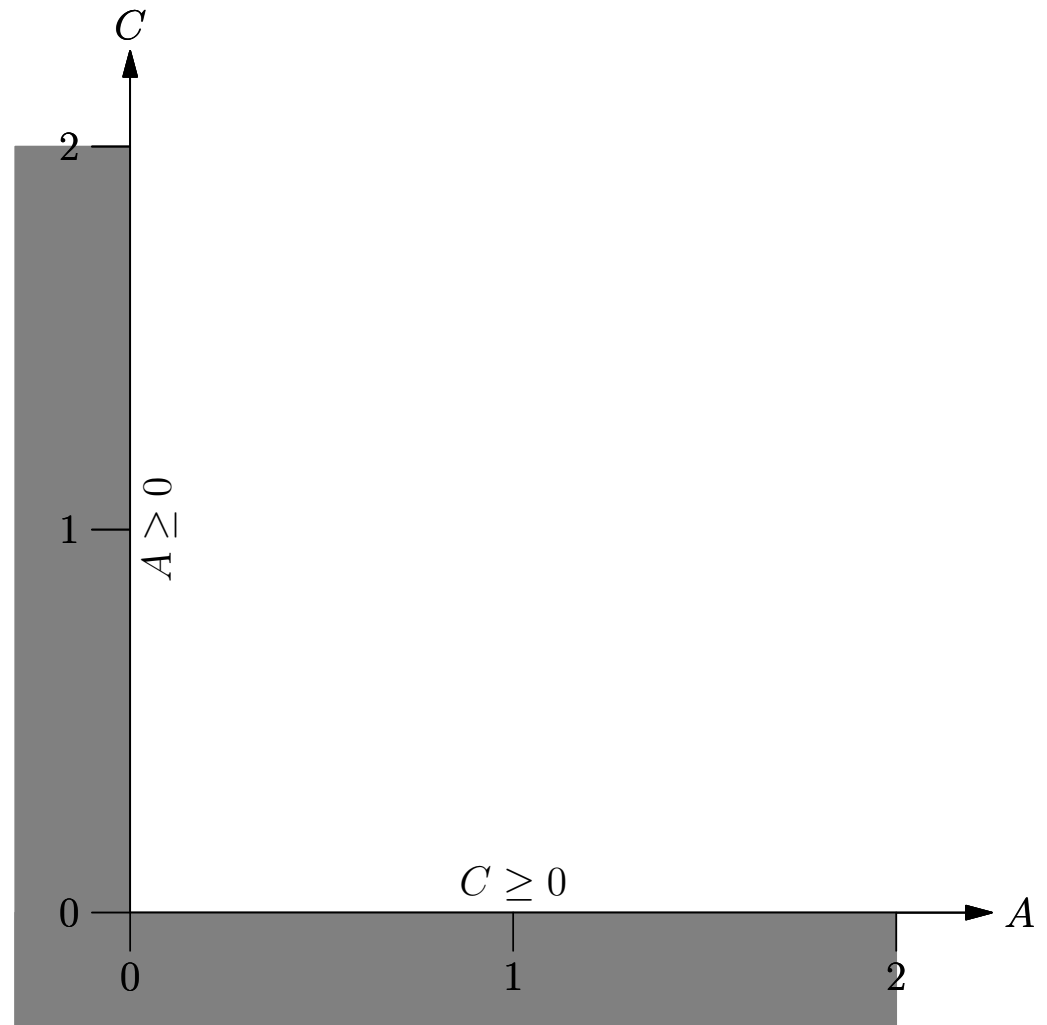
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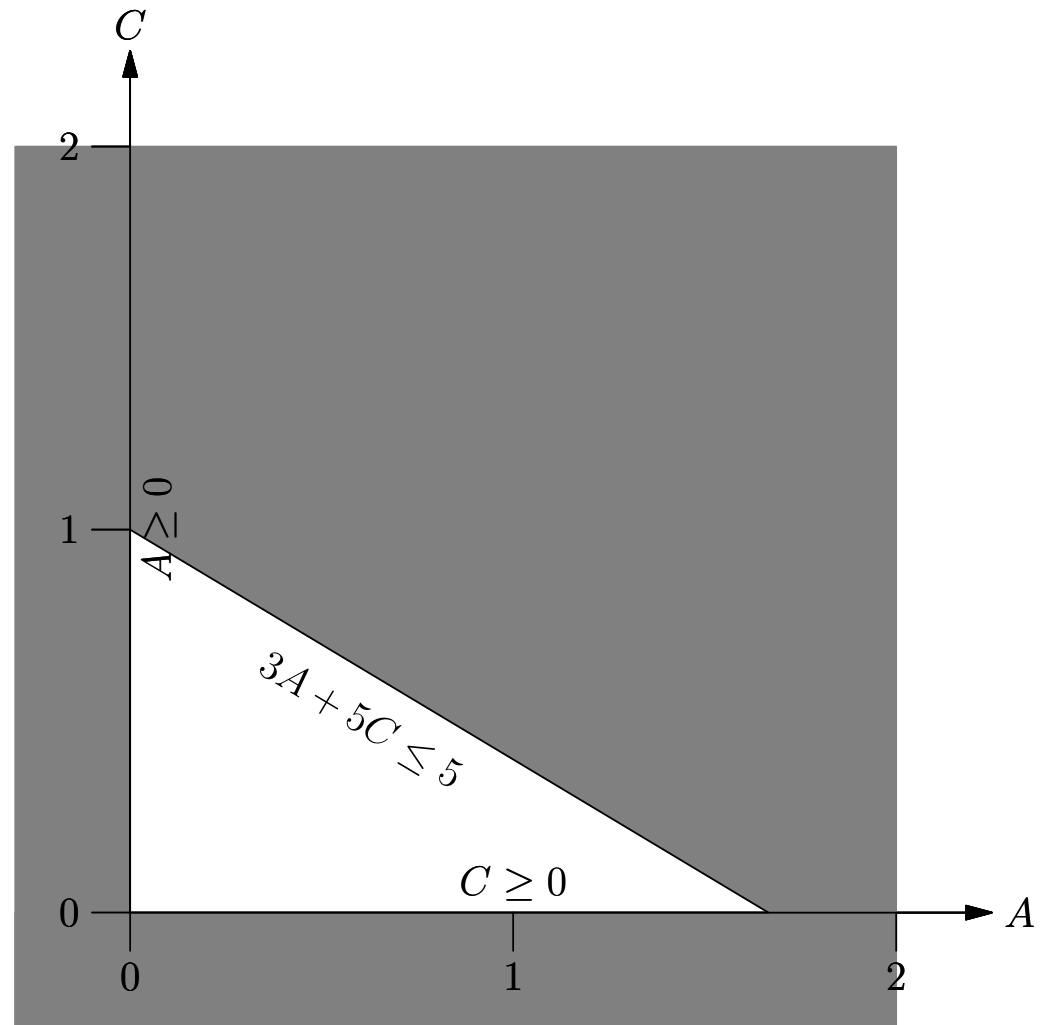
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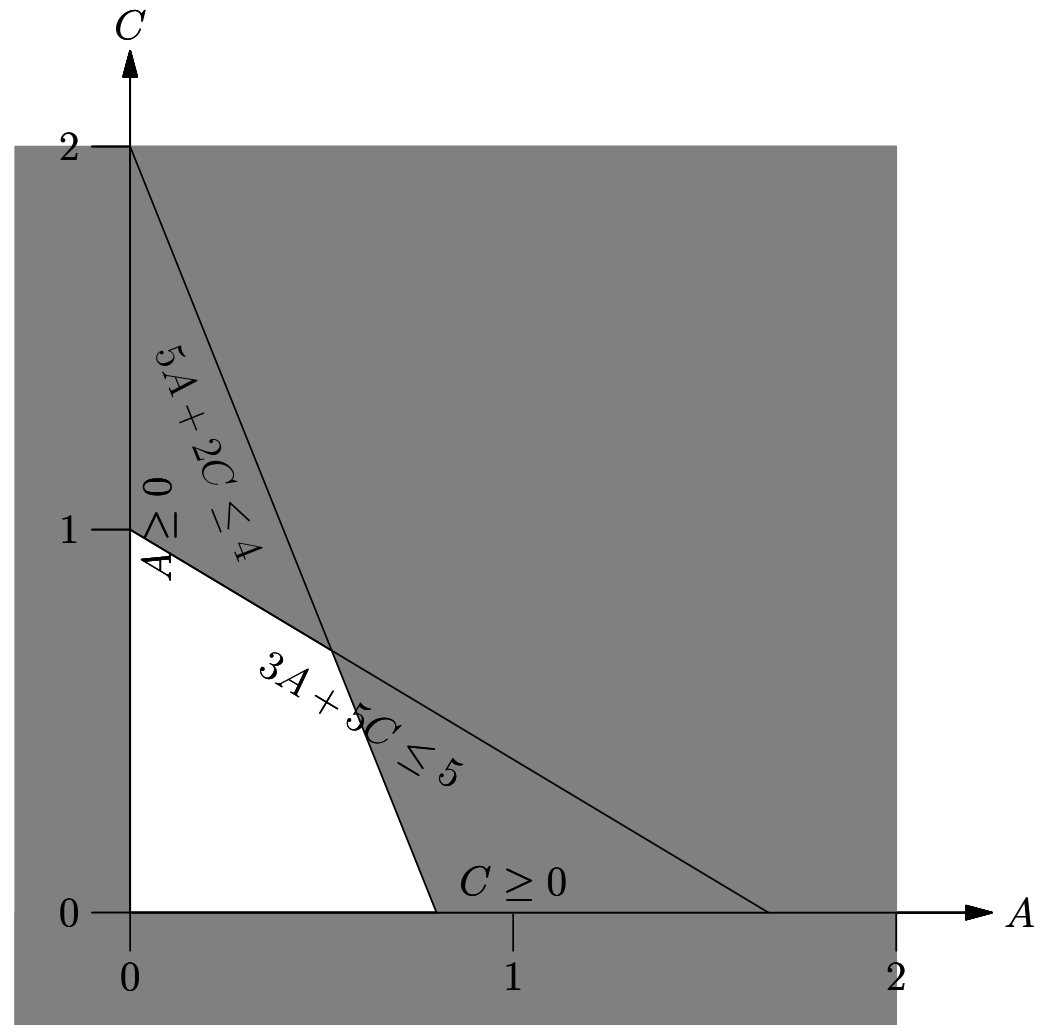
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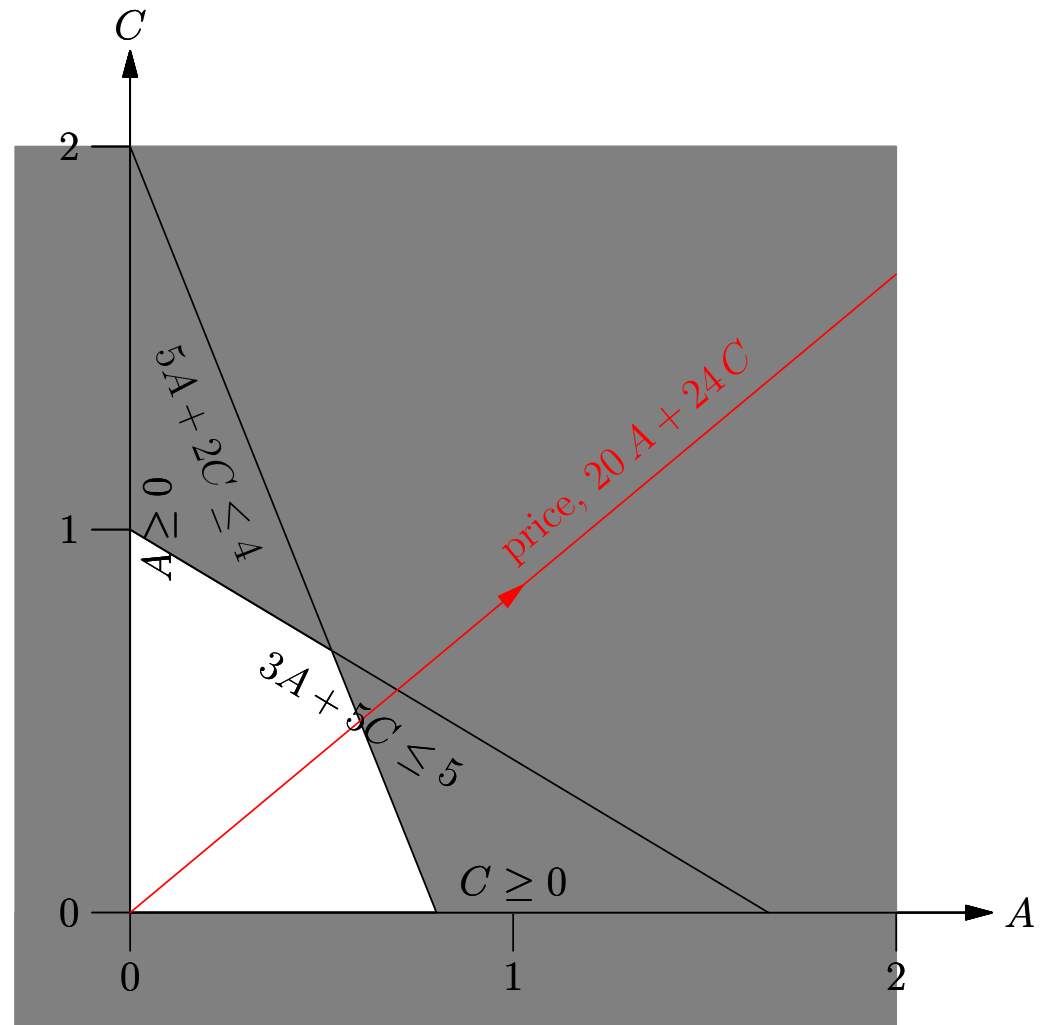
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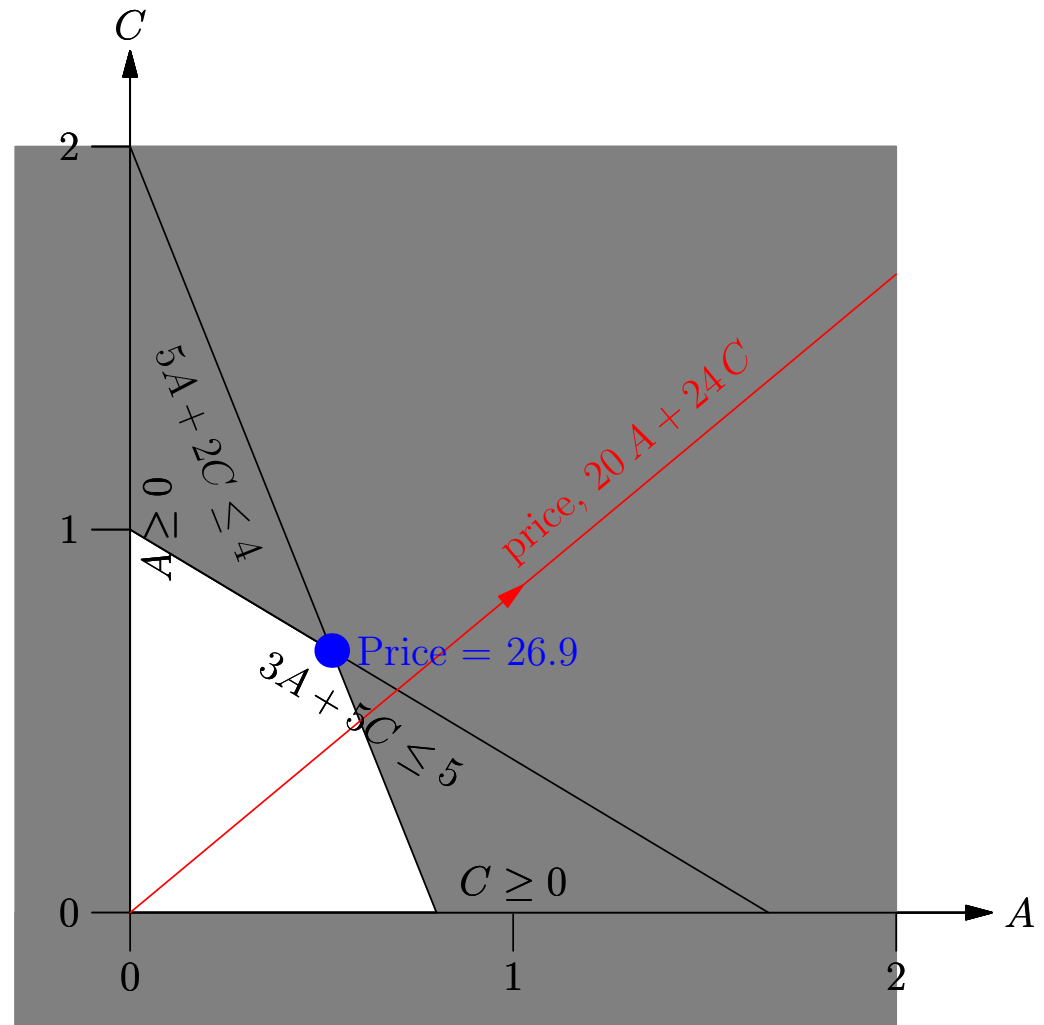
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Why?

- 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 x while the second linear programme depends on the number of constraints (or dimensionality of α)
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Quadratic Programming

- A quadratic programme involves minimising a quadratic function $x^\top Qx$ (with $Q \succ 0$) subject to linear constraints $Mx = b$ (or $Mx \leq b$)
- We can define the Lagrangian

$$\mathcal{L}(x, \alpha) = x^\top Qx - \alpha^\top (Mx - b)$$

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Solution to Quadratic Programming Problem

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- Then

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Dual Quadratic Programming Problem

- Substituting $x^* = \frac{1}{2}\mathbf{Q}^{-1}\mathbf{M}^\top\alpha$ into

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

- We get the dual problem

$$\max_{\alpha} -\frac{1}{4}\alpha^\top \mathbf{M}\mathbf{Q}^{-1}\mathbf{M}^\top\alpha + \alpha^\top b$$

- If the constraints were inequality constraints then we have $\alpha_i \geq 0$
- We have exchanged one quadratic programme for another, but sometimes that very useful (e.g. SVMs)

Dual Quadratic Programming Problem

- Substituting $x^* = \frac{1}{2}\mathbf{Q}^{-1}\mathbf{M}^\top\alpha$ into

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

- We get the dual problem

$$\max_{\alpha} -\frac{1}{4}\alpha^\top \mathbf{M} \mathbf{Q}^{-1} \mathbf{M}^\top \alpha + \alpha^\top b$$

- If the constraints were inequality constraints then we have $\alpha_i \geq 0$
- We have exchanged one quadratic programme for another, but sometimes that very useful (e.g. SVMs)

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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)
- For inequality constraints we need to satisfy KKT conditions
- For simple situations (linear and quadratic programming) we can eliminate the original variables to obtain the dual problem

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