$\begin{array}{c} \text{CHEM-E7225} \\ 2023 \end{array}$ 

The Lagrangia function

conditions

Constrained

problems



# Nonlinear optimisation, fundamentals (B) CHEM-E7225 (was E7195), 2023

Francesco Corona  $(\neg\_\neg)$ 

Chemical and Metallurgical Engineering School of Chemical Engineering

### The Lagrangian function

Optimality

Equality constraints

Constraine

## The Lagrangian function

Nonlinear optimisation

### The Lagrangian function

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### The Lagrangian function

Consider the nonlinear optimisation problem in the standard form

$$\min_{w \in \mathcal{R}^N} \quad f(w)$$
subject to 
$$g(w) = 0$$

$$h(w) \ge 0$$

→ Objective function

$$f: \mathcal{R}^N \to \mathcal{R}, \text{ with } f \in \mathcal{C}^2\left(\mathcal{R}^N\right)$$

→ Equality constraint function

$$g: \mathbb{R}^N \to \mathbb{R}^{N_g}$$
, with  $g \in \mathcal{C}^2\left(\mathbb{R}^N\right)$ 

→ Inequality constraint function

$$h: \mathcal{R}^N \to \mathcal{R}^{N_h}$$
, with  $h \in \mathcal{C}^2\left(\mathcal{R}^N\right)$ 

We denote a problem in this form as primal optimisation problem

### The Lagrangian function (cont.)

### The Lagrangian function

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$$\min_{w \in \mathcal{R}^{N}} \quad f(w)$$
 subject to 
$$g(w) = 0$$
 
$$h(w) \ge 0$$

The globally optimal (min) value of the objective function subjected to the constraints

$$p^* = \begin{pmatrix} \min_{w \in \mathcal{R}^N} & f(w), \text{ s.t. } g(w) = 0, h(w) \ge 0 \end{pmatrix}$$

Remember that there can be a multiplicity of points  $w^* \in \Omega$  such that  $f(w^*) = p^*$ 

- $\rightarrow$  The globally optimal value  $p^*$  of the objective function is unique
- → The globally optimal value is called the **primal optimal value**

We are interested in a lower-bound (for minimisation problems) on the optimal value  $p^{\ast}$ 

### Overview (cont.)

### The Lagrangian function

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### Example

$$\min_{x \in \mathcal{R}^2} \quad x_1^2 + x_2^2 \qquad \qquad \text{(Objective function)}$$
 subject to  $\quad x_1 - 1 = 0 \qquad \qquad \text{(Equality constraints)}$ 

$$x_2 - 1 - x_1^2 \ge 0$$
 (Inequality constraints)

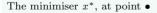
$$\rightarrow f: \mathbb{R}^2 \to \mathbb{R}, \text{ with } f \in \mathcal{C}^2(\mathbb{R}^2)$$

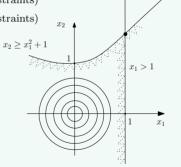
$$\rightarrow g: \mathbb{R}^2 \to \mathbb{R}, \text{ with } g \in \mathbb{C}^2(\mathbb{R}^2)$$

$$\rightarrow h: \mathcal{R}^2 \to \mathcal{R}, \text{ with } h \in \mathcal{C}^2(\mathcal{R}^2)$$

The feasible set of decision variables

$$\Omega = \{x \in \mathcal{R}^2 | h(x) \ge 0, g(x) = 0\}$$





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### The Lagrangian function

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### The Lagrangian function (cont.)

$$\min_{w \in \mathcal{R}^N} \quad f(w)$$
subject to 
$$g(w) = 0$$

$$h(w) \ge 0$$

We can define an auxiliary function and we denote it as the Lagrangian function

$$\mathcal{L}(w, \lambda, \mu) = f(w) - \lambda^{T} g(w) - \mu^{T} h(w)$$

The Lagrangian function depends on w and two sets of auxiliary variables

- → The Lagrangian multipliers, or dual variables
- The inequality multipliers,  $\mu \in \mathcal{R}^{N_h}$
- The equality multipliers,  $\lambda \in \mathcal{R}^{N_g}$

$$\mathcal{L}\left(w,\lambda,\mu\right)=f\left(w\right)-\sum_{n_{g}=1}^{N_{g}}\lambda_{n_{h}}g_{n_{g}}\left(w\right)-\sum_{n_{h}=1}^{N_{h}}\mu_{n_{g}}h_{n_{h}}\left(w\right)$$

The Lagrangian function is a scalar function,

$$\mathcal{L}: \mathcal{R}^N \times \mathcal{R}_q^N \times \mathcal{R}_{>0}^{N_h} \to \mathcal{R}$$

### The Lagrangian

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### The Lagrangian function (cont.)

$$\min_{w \in \mathcal{R}^N} f(w)$$
subject to  $g(w) = 0$ 

$$h(w) > 0$$

In expanded form, we have the Lagrangian function

$$\mathcal{L}(w,\lambda,\mu) = f(w) - \lambda^{T} g(w) - \mu^{T} h(w)$$

$$= f(w) - \begin{bmatrix} \lambda_{1} & \cdots & \lambda_{N_{g}} \end{bmatrix} \begin{bmatrix} g_{1}(w) \\ \vdots \\ g_{N_{g}}(w) \end{bmatrix} - \begin{bmatrix} \mu_{1} & \cdots & \mu_{N_{h}} \end{bmatrix} \begin{bmatrix} h_{1}(w) \\ \vdots \\ h_{N_{h}}(w) \end{bmatrix}$$

The number of multipliers must match the number of constraints

$$\rightsquigarrow$$
 (For the products  $\lambda^T g(w)$  and  $\mu^T h(w)$  to be defined)

While  $\lambda$  can take any value, we require the inequality multipliers to be positive ( $\mu > 0$ )

$$\mu \ge 0 = \begin{bmatrix} \mu_1 \ge 0 \\ \vdots \\ \mu_{N_b} \ge 0 \end{bmatrix}$$

### Overview (cont.)

### The Lagrangian function

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### Example

$$\min_{x \in \mathcal{R}^2} \quad x_1^2 + x_2^2$$
 (Objective function) subject to  $x_1 - 1 = 0$  (Equality constraints)

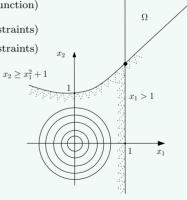
$$x_2 - 1 - x_1^2 \ge 0$$
 (Inequality constraints)

The feasible set, the set of feasible decisions

$$\Omega = \{x \in \mathcal{R}^2 | h(x) \ge 0, g(x) = 0\}$$

For point  $\widetilde{x} \in \Omega$ , the Lagrangian function

$$\mathcal{L}\left(\widetilde{x}, \lambda, \mu\right) = f\left(\widetilde{x}\right) - \lambda^{T} q\left(\widetilde{x}\right) - \mu^{T} h\left(\widetilde{x}\right)$$



### The Lagrangian function (cont.)

### The Lagrangian function

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$$\min_{x \in \mathcal{R}^2} \quad \underbrace{x_1^2 + x_2^2}_{f(x)} \qquad \qquad \text{(Objective function)}$$
 subject to 
$$\underbrace{x_1 - 1}_{g(x)} = 0 \qquad \qquad \text{(Equality constraints)}$$
 
$$\underbrace{x_2 - 1 - x_1^2}_{h(x)} \geq 0 \qquad \text{(Inequality constraints)}$$

The Lagrangian function in expanded form, for any feasible pair  $\widetilde{x}=(\widetilde{x_1},\widetilde{x_2})\in\Omega$ 

$$\mathcal{L}\left(\widetilde{x},\lambda,\mu\right) = f\left(\widetilde{x}\right) - \lambda^{T}g\left(\widetilde{x}\right) - \mu^{T}h\left(\widetilde{x}\right)$$

$$= f\left(\widetilde{x}\right) - \left[\lambda_{1}\right]^{T}\left[g_{1}\left(\widetilde{x}\right)\right] - \left[\mu_{1}\right]^{T}\left[h_{1}\left(\widetilde{x}\right)\right]$$

$$= \left(\widetilde{x}_{1}^{2} + \widetilde{x}_{2}^{2}\right) - \lambda_{1}\left(\widetilde{x}_{1} - 1\right) - \mu_{1}\left(\widetilde{x}_{2} - 1 - \widetilde{x}_{1}^{2}\right)$$

### The Lagrangian

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### The Lagrangian function (cont.)

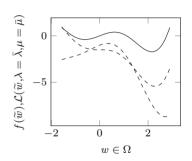
#### Lower-bound property of the Lagrangian function

For any feasible point  $\widetilde{w} \in \Omega$ , for any  $\lambda$  and for any  $\mu \geq 0$ , we have the lower-bound

$$\begin{split} \mathcal{L}\left(\widetilde{w},\lambda,\mu\right) &= f\left(\widetilde{w}\right) \underbrace{-\lambda^{T}\underbrace{g\left(\widetilde{w}\right)}_{=0} \underbrace{-\mu^{T}\underbrace{h\left(\widetilde{w}\right)}_{\geq 0}}_{\leq 0}}_{\leq f\left(\widetilde{w}\right)} \end{split}$$

Because  $w^* \in \Omega$ , thus we also have

$$\mathcal{L}\left(w^*, \lambda, \mu\right) \le f(w^*)$$



For w in the feasible set, the objective function is larger than the Lagrangian function

• (If  $\widetilde{w}$  is a primal minimiser, then the lower-bound will be retained)

### The Lagrangian function

Optimality conditions

Equality constraints Constrained

### Example

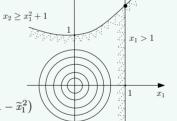
$$\min_{x \in \mathcal{R}^2} \quad x_1^2 + x_2^2 \qquad \text{(Objective function)}$$
subject to  $x_1 - 1 = 0$  (Equality constraints)
$$x_2 - 1 - x_1^2 \ge 0 \quad \text{(Inequality constraints)}$$

The feasible set

$$\Omega = \{x \in \mathcal{R}^2 | h(x) \ge 0, g(x) = 0\}$$

The Lagrangian function

$$\mathcal{L}\left(\widetilde{x},\lambda,\mu\right)=\widetilde{x}_{1}^{2}+\widetilde{x}_{2}^{2}-\lambda_{1}\left(\widetilde{x}_{1}-1\right)-\mu_{1}\left(\widetilde{x}_{2}-1-\widetilde{x}_{1}^{2}\right)$$



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For any point  $\widetilde{x} \in \Omega$  and for any  $\lambda$  and any  $\mu \geq 0$ , we have the lower-bound property

$$\mathcal{L}\left(\widetilde{x},\lambda,\mu\right) \leq f(\widetilde{x})$$

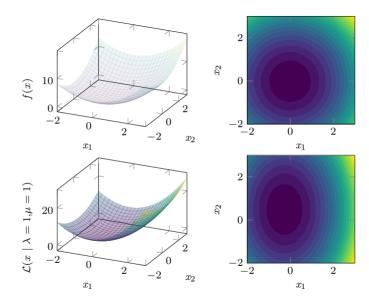
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The Lagrangian function

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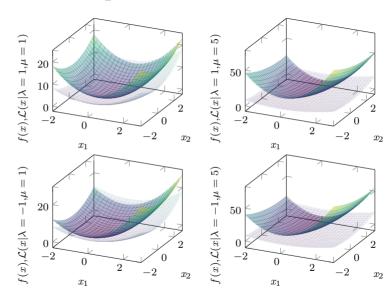


For different pairs  $(\lambda, \mu_{\geq 0})$  and for any  $\tilde{x} \in \Omega$ , we always have that  $\mathcal{L}(\tilde{x}, \lambda, \mu) \leq f(\tilde{x})$ 



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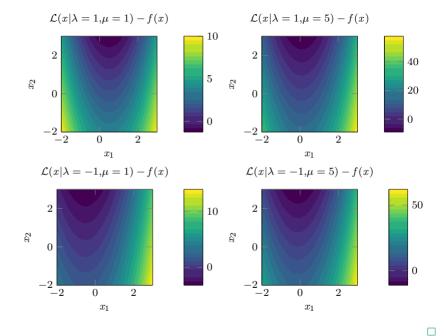


The Lagrangian function

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### The Lagrangian function | Duality

The Lagrangian function

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Consider some fixed pair of multipliers  $\bar{\lambda}$  and  $\bar{\mu} \geq 0$ , we define the Lagrange dual function

$$q\left(\bar{\lambda}, \bar{\mu}\right) = \inf_{w \in \mathcal{R}^N} \quad \mathcal{L}\left(w|\lambda = \bar{\lambda}, \mu = \bar{\mu}\right)$$

Also the Lagrange dual function is a scalar function

$$q: \mathcal{R}^{N_g} \times \mathcal{R}^{N_h}_{\geq 0} \to \mathcal{R}$$

Let  $w^*$  be the unconstrained (in  $\mathcal{R}^N$ ) minimiser of the Lagrangian function  $\mathcal{L}\left(w|\bar{\lambda},\bar{\mu}\right)$ 

$$w^* = w^* \left( \bar{\lambda}, \bar{\mu} \right)$$

Because we minimised out w, the infimum is  $\mathcal{L}\left(w^*(\bar{\lambda}, \bar{\mu})|\bar{\lambda}, \bar{\mu}\right) = q\left(\bar{\lambda}, \bar{\mu}\right)$ 

• At any feasible point  $\widetilde{w} \in \Omega$  and fixed multipliers  $(\overline{\lambda}, \overline{\mu})$ , we have

$$\mathcal{L}\left(\widetilde{w}|\bar{\lambda},\bar{\mu}\right) \geq \underbrace{\mathcal{L}\left(w^*(\bar{\lambda},\bar{\mu})|\bar{\lambda},\bar{\mu}\right)}_{=q(\bar{\lambda},\bar{\mu})}$$

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### The Lagrangian function | Duality (cont.)

Lower-bound property of the Lagrange dual function

For any pair of multipliers  $\lambda$  and  $\mu \geq 0$  and for any feasible point  $\widetilde{w} \in \Omega$ , we have that

$$\underbrace{\mathcal{L}\left(\widetilde{w},\lambda,\mu\right)\leq f\left(\widetilde{w}\right)}_{\text{lower-bound property}}$$

For some pair  $(\bar{\lambda}, \bar{\mu} \geq 0)$  and for any feasible point  $\tilde{w}$ , we have

$$\underbrace{q\left(\bar{\lambda}, \bar{\mu}\right) = \mathcal{L}\left(w^*(\bar{\lambda}, \bar{\mu}) | \bar{\lambda}, \bar{\mu}\right) \leq \mathcal{L}\left(\widetilde{w}, \bar{\lambda}, \bar{\mu}\right)}_{\text{infimum property}}$$

Combining these two inequalities, we have

$$q\left(\bar{\lambda}, \bar{\mu}\right) \leq \mathcal{L}\left(\tilde{w}, \bar{\lambda}, \bar{\mu}\right) \leq f\left(\tilde{w}\right)$$

Because  $p^* = f(w^*)$  and  $f(w^*) \le f(\widetilde{w})$ , we have  $q(\bar{\lambda}, \bar{\mu}) \le \mathcal{L}(\widetilde{w}, \bar{\lambda}, \bar{\mu}) \le f(w^*) \le f(\widetilde{w})$ 

$$q\left(\bar{\lambda},\bar{\mu}\right) \leq p^*$$

Lagrange dual functions  $q(\lambda, \mu)$  provide a lower-bound to primal values  $p^*$ 

At the global minimiser  $\widetilde{w} = w^*$ , a feasible point, we have

$$q(\lambda, \mu) \le f(w^*)$$
$$= p^*$$

## The Lagrangian function | Duality

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The Lagrange dual function  $q(\lambda, \mu)$  does not depend on primal decision variables w

• Sometimes it is possible to compute the Lagrange dual function explicitly

#### Concavity of the Lagrange dual function

The Lagrange dual function is always a concave function, also for non-convex problems  $\,$ 

• Therefore, we have that  $-q(\lambda, \mu)$  is a convex function

### The Lagrangian function

Optimality conditions

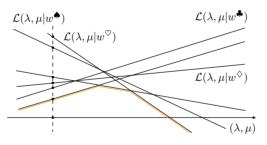
Equality constraint Constrained problems

### The Lagrangian function | Duality

For any fixed w, the Lagrangian function  $\mathcal{L}(\lambda,\mu|w)$  is an affine function of  $\lambda$  and  $\mu$ 

$$\mathcal{L}(\lambda, \mu | w) = f(w) - \lambda^{T} g(w) - \mu^{T} h(w)$$

Visually, consider a set of points  $\{w\}$  and associated Lagrangian functions  $\{\mathcal{L}(\lambda,\mu|w)\}$ 



For fixed  $\lambda, \mu$ , the dual function

$$q(\lambda, \mu) = \inf_{w \in \mathcal{R}^N} \quad \mathcal{L}(w|\lambda, \mu)$$

Or, equivalently

$$-q(\lambda, \mu) = \sup_{w \in \mathcal{R}^N} -\mathcal{L}(w|\lambda, \mu)$$

- $-q(\lambda,\mu)$  is the supremum of affine, thus convex, functions in the dual variables  $(\lambda,\mu)$ 
  - The supremum over a set of convex functions is a convex function
  - (The epigraph is the intersection of convex sets)

The Lagrangian function

Optimality conditions

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### The Lagrangian function | Duality (cont.)

The Lagrange dual function provides an understimate of the primal global minimiser

- ullet The value of the dual function that is closest is achieved when q is maximised
- It is interesting to understand how close to  $p^*$  does  $q(\lambda, \mu)$  actually get

#### Dual optimisation problem

The best lower-bound  $d^*$  is obtained by maximising the Lagrange dual function  $q\left(\lambda,\mu\right)$ 

$$\max_{\substack{\lambda \in \mathcal{R}^{N_g} \\ \mu \in \mathcal{R}^{N_h}}} q(\lambda, \mu)$$
 subject to  $\mu \ge 0$ 

The dual optimisation problem is itself a constrained optimisation problem

- It is defined as a convex (concave) maximisation problem
- The decision variables are the dual variables  $\lambda$  and  $\mu$

The convexity of the dual optimisation problem is independent of the primal problem

### The Lagrangian function

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The best lower-bound  $d^*$  is obtained by maximising the Lagrange dual function  $q\left(\lambda,\mu\right)$ 

$$d^* = \begin{pmatrix} \max_{\lambda \in \mathcal{R}^{N_g}} & q(\lambda, \mu), \text{ s.t. } \mu \ge 0 \\ \mu \in \mathcal{R}^{N_h} & \end{pmatrix}$$

For any general nonlinear programs, we have the weak-duality result

$$d^* \leq p^*$$

For any convex nonlinear programs<sup>1</sup>, we have strong-duality result

$$d^* = p^*$$

<sup>&</sup>lt;sup>1</sup>Slater's constraint qualification conditions must also be satisfied.

The Lagrangian function

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#### Example

#### Strictly convex quadratic program

Consider a strictly convex quadratic program  $(B \succ 0)$  in primal form

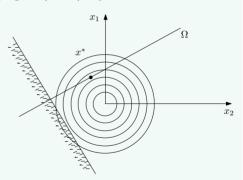
The primal optimisation problem

$$\min_{x \in \mathcal{R}^N} \quad c^T x + \frac{1}{2} x^T B x$$
subject to 
$$Ax - b = 0$$

$$Cx - d \ge 0$$

The primal global minimum

$$\rightsquigarrow p^*$$



We are interested in the Lagrange dual function  $q(\lambda, \mu)$ 

The Lagrangian function

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$$\min_{x \in \mathcal{R}^N} \quad \underbrace{c^T x + \frac{1}{2} x^T B x}_{f(w)}$$
subject to 
$$\underbrace{Ax - b}_{g(x)} = 0$$

$$\underbrace{Cx - d}_{h(x)} \ge 0$$

For the Lagrangian function, we have

$$\mathcal{L}(x,\lambda,\mu) = \underbrace{c^T x + \frac{1}{2} x^T B x}_{f(x)} - \underbrace{\lambda^T (Ax - b)}_{\lambda^T g(x)} - \underbrace{\mu^T (Cx - d)}_{\mu^T h(x)}$$

$$= c^T x + \frac{1}{2} x^T B x - \lambda^T A x + \lambda^T b - \mu^T C x + \mu^T d$$

$$= \underbrace{\lambda^T b + \mu^T d}_{\text{constant in } x} + \underbrace{(c - A^T \lambda - C^T \mu)^T x}_{\text{linear in } x} + \underbrace{\frac{1}{2} x^T B x}_{\text{quadratic in } x}$$

### The Lagrangian

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### The Lagrangian function | Duality (cont.)

$$\mathcal{L}(x, \lambda, \mu) = \lambda^{T} b + \mu^{T} d + (c - A^{T} \lambda - C^{T} \mu)^{T} x + \frac{1}{2} x^{T} B x$$

The Lagrange dual function  $q\left(\lambda,\mu\right)$  is defined as infimum of the Lagrangian function

 $\bullet$  The minimisation is with respect to the primal variables x

We have,

$$\begin{split} q\left(\lambda,\mu\right) &= \inf_{x \in \mathcal{R}^{N}} \quad \left(\lambda^{T}b + \mu^{T}d + \left(c - A^{T}\lambda - C^{T}\mu\right)^{T}x + \frac{1}{2}x^{T}Bx\right) \\ &= \lambda^{T}b + \mu^{T}d + \underbrace{\inf_{x \in \mathcal{R}^{N}} \quad \left(\left(c - A^{T}\lambda - C^{T}\mu\right)^{T}x + \frac{1}{2}x^{T}Bx\right)}_{\text{unconstrained quadratic program}} \\ &= \lambda^{T}b + \mu^{T}d - \frac{1}{2}\left(c - A^{T}\lambda - C^{T}\mu\right)^{T}B^{-1}\left(c - A^{T}\lambda - C^{T}\mu\right) \end{split}$$

We used the fact that for general unconstrained quadratic problems  $f(x^*) = \frac{1}{2}c^T B^{-1}c$ 

The Lagrangian function

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Equality constraint

$$q(\lambda, \mu) = \lambda^T b + \mu^T d - \frac{1}{2} (c - A^T \lambda - C^T \mu)^T B^{-1} (c - A^T \lambda - C^T \mu)$$

After rearranging, we formulate the dual optimisation problem

$$\max_{\substack{\lambda \in \mathcal{R}^{N_h} \\ \mu \in \mathcal{R}^{N_g}}} \quad -\frac{1}{2} c^T B^{-1} c + \begin{bmatrix} b + A B^{-1} c \\ d + C B^{-1} c \end{bmatrix}^T \begin{bmatrix} \lambda \\ \mu \end{bmatrix} - \frac{1}{2} \begin{bmatrix} \lambda \\ \mu \end{bmatrix}^T \begin{bmatrix} A \\ C \end{bmatrix} B^{-1} \begin{bmatrix} A \\ C \end{bmatrix}^T \begin{bmatrix} \lambda \\ \mu \end{bmatrix}$$
 subject to  $\mu \geq 0$ 

The objective function is concave, the dual problem is a convex quadratic program

The term  $(-1/2)c^TB^{-1}c$  is constant with respect to the dual variables

• It is retained to verify the strong duality result,  $d^* = p^*$ 

The Lagrangian function

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### Example

Linear program

The primal optimisation problem

$$\min_{w \in \mathcal{R}^N} \quad c^T w$$
subject to 
$$Aw - b = 0$$

$$Cx - d \ge 0$$

The primal global minimum

$$\leadsto p^*$$

We are interested in the Lagrange dual function  $q\left(\lambda,\mu\right)$ 

### The Lagrangian function | Duality (cont.)

The Lagrangian function

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Equality constraints

$$\min_{w \in \mathcal{R}^N} \quad c^T w$$
subject to 
$$Aw - b = 0$$

$$Cx - d \ge 0$$

For the Lagrangian function, we can write

$$\mathcal{L}(w,\lambda,\mu) = c^T w - \lambda^T (Aw - b) - \mu^T (Cw - d)$$

$$= \underbrace{\lambda^T b + \mu^T d}_{\text{constant in } x} + \underbrace{\left(c - A^T \lambda - C^T \mu\right) w}_{\text{linear in } x}$$

The Lagrange dual function, as infimum of the Lagrangian function

$$q(\lambda, \mu) = \lambda^T b + \mu^T d + \underbrace{\inf_{w \in \mathcal{R}^N} \quad \left(c - A^T \lambda - C^T \mu\right) w}_{\text{unconstrained linear program}}$$
$$= \lambda^T b + \mu^T d + \begin{cases} 0, & c - A^T \lambda - C^T \mu = 0 \\ -\infty, & \text{otherwise} \end{cases}$$

The Lagrangian function

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$$q(\lambda, \mu) = \lambda^T b + \mu^T d + \begin{cases} 0, & c - A^T \lambda - C^T \mu = 0 \\ -\infty, & \text{otherwise} \end{cases}$$

The Lagrange dual function  $q(\lambda, \mu)$  equals  $-\infty$  at all points  $(\widetilde{\lambda}, \widetilde{\mu})$  that do not satisfy the linear equality  $c - A^T \lambda - C^T \mu = 0$ , these points can be treated as infeasible points

We use this observation to formulate the dual optimisation problem,

$$\max_{\substack{\lambda \in \mathcal{R}^{N_h} \\ \mu \in \mathcal{R}^{N_g}}} \begin{bmatrix} b & d \end{bmatrix} \begin{bmatrix} \lambda \\ \mu \end{bmatrix}$$
 subject to  $c - A^T \lambda - C^T \mu = 0$   $\mu \ge 0$ 

The Lagrangian function

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## **Optimality conditions**

Nonlinear optimisation

### Optimality conditions | Unconstrained problems

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Consider the unconstrained optimisation problem with  $f: \mathcal{R}^N \to \mathcal{R}$  and  $f \in \mathcal{C}^1(\mathcal{R}^N)$ 

$$\min_{w \in \mathcal{R}^N} \quad f(w)$$

We are imprecisely assuming that the domain of definition of function f is  $\mathcal{R}^N$ 

• More precisely, the function is defined only on some set  $\mathcal{D} \subseteq \mathcal{R}^N$ 

That is, we re-write the unconstrained optimisation problem

$$\min_{w \in \mathcal{D}} f(w)$$

## 2023

## Optimality

### Optimality conditions | Unconstrained problems (cont.)

$$\min_{w \in \mathcal{D}} \quad f\left(w\right)$$

#### First-order necessary optimality conditions

If point  $w^* \in \mathcal{D}$  is a local minimiser, then the first-order necessary condition holds

$$\nabla f\left(w^*\right) = 0$$

A point  $w^*$  such that  $\nabla f(w^*) = 0$  is a stationary point

By contradiction, assume that the local minimiser  $w^*$  would be such that  $\nabla f(w^*) \neq 0$ 

• Then, there is a direction  $-\nabla f(w^*)$  that would be a descent direction  $\nabla f(w^*)^T (-\nabla f(w^*)) = -\underbrace{\|\nabla f(w^*)\|_2^2}_{>0}$ 

$$\nabla f(w) \quad (-\nabla f(w)) = -\underbrace{\|\nabla f(w)\|}_{>0}$$

In the vicinity of  $w^*$ , for a point  $\widetilde{w} = w^* + \lambda(w' - w^*)$  along such descent direction

$$f\left(w^* + \lambda(w' - w^*)\right) \approx f\left(w^*\right) + \lambda \underbrace{\nabla f\left(w^*\right)^T\left(w' - w^*\right)}_{\leq 0}$$

 $\langle f(w^*) \rangle$  (a contradiction for a local minimiser)

### The Lagrangian

### Optimality conditions

Equality const: Constrained problems

### Optimality conditions | Unconstrained problems (cont.)

$$\min_{w \in \mathcal{D}} \quad f\left(w\right)$$

#### Second-order necessary optimality conditions

If point  $w^* \in \mathcal{D}$  is a local minimiser, then the second-order necessary condition holds

$$\nabla^2 f\left(w^*\right) \succeq 0$$

Assume the existence of direction  $(w'-w^*)$  such that  $(w'-w^*)^T \nabla^2 f(w^*)(w'-w^*) < 0$ 

• Along direction  $(w' - w^*)$  the value of the objective function would diminish

In the vicinity of  $w^*$ , for a point  $\widetilde{w} = w^* + \lambda(w' - w^*)$  along such descent direction

$$\begin{split} f\left(w^* + \lambda(w' - w^*)\right) &\approx \\ f\left(w^*\right) + \lambda \underbrace{\nabla f\left(w^*\right)^T \left(w' - w^*\right)}_{=0} + \frac{1}{2} \lambda^2 \underbrace{\left(w' - w^*\right)^T \nabla^2 f\left(w^*\right) \left(w' - w^*\right)}_{<0} \\ &< f\left(w^*\right) \end{split} \quad \text{(a contradiction for a local minimiser)} \end{split}$$

### Optimality conditions | Unconstrained problems (cont.)

The Lagrangian function

conditions
Equality constraints

#### Second-order sufficient optimality conditions

The sufficient second-order condition to have a strict local minimiser

$$\nabla^2 f\left(w^*\right) \succ 0$$

### Optimality conditions | Unconstrained problems (cont.)

The Lagrangian function

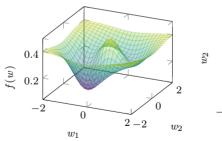
### Optimality conditions

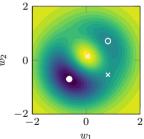
Equality constraints

### Example

#### Consider the unconstrained optimisation problem

$$\min_{w \in \mathcal{R}^2} \quad \frac{2}{5} - \frac{1}{10} \left( 5w_1^2 + 5w_2^2 + 3w_1w_2 - w_1 - 2w_2 \right) e^{\left( -\left( w_1^2 + w_2^2 \right) \right)}$$





The Lagrangian function

conditions

Equality constraints

Constrained

## **Equality constraints**

**Optimality conditions** 

### Optimality conditions | Equality constraints

The Lagrangian function

conditions

Equality constraints
Constrained

Consider the equality constrained optimisation problem in the general form

$$\min_{w \in \mathcal{R}^{N}} f(w)$$
subject to  $g(w) = 0$ 

- We assume that  $f: \mathbb{R}^N \to \mathbb{R}$  and  $g: \mathbb{R}^N \to \mathbb{R}^{N_g}$  are smooth functions
- The feasible set is  $\Omega = \{w \in \mathbb{R}^N | g(w) = 0\}$ , a differentiable manifold

We are interested in the optimality conditions for this class of optimisation problems

- To have a condition  $\nabla f\left(w\right)=0$  (or  $\nabla f\left(w\right)=0$  and  $\nabla^{2}f\left(w\right)\succeq0$ ) is not enough
- Variations in other feasible directions must not improve the objective function

Optimality conditions | Equality constraints (cont.)

The Lagrangian function

conditions

Equality constraints

problems

To formulate the optimality conditions, we need two notions from differential geometry

- The tangent vector to the feasible set  $\Omega$
- The tangent cone to the feasible set  $\Omega$

These notions will allow for a local characterisation of the feasible set

For (standard, well-behaved) equality constrained optimisation problems, the set of all the tangent vectors to the feasibility set  $\Omega$  at a feasible point  $w^*$  form a vector space

• The tangent space

### Optimality conditions | Equality constraints (cont.)

The Lagrangia function

Optimality conditions

Equality constraints
Constrained

Remember the equality constraint function, each component function need be smooth

$$g\left(w\right) = \underbrace{\begin{bmatrix}g_{1}\left(w\right)\\ \vdots\\ g_{n_{g}}\left(w\right)\\ \vdots\\ g_{N_{g}}\left(w\right)\end{bmatrix}}_{N_{g}\times 1}$$

Each function is required to be at least differentiable once, to compute the Jacobian

#### Jacobian of the equality constraints

The Jacobian of the equality constraint functions is a rectangular  $(N_g \times N)$  matrix

• It collects (transposed) gradients  $\nabla g_{n_q}(w)$  of component functions  $g_{n_q}(w)$ 

### Optimality conditions | Equality constraints (cont.)

The Lagrangian function

conditions

Equality constraints

$$g\left(w\right) = \underbrace{\begin{bmatrix}g_{1}\left(w\right)\\ \vdots\\ g_{n_{g}}\left(w\right)\\ \vdots\\ g_{N_{g}}\left(w\right)\end{bmatrix}}_{N_{g}\times 1}$$

More explicitly, the gradient vector of an equality constraint function  $g_{n_g}(w)$ 

$$\nabla g_{n_g}\left(w\right) = \underbrace{\begin{bmatrix} \partial g_{n_g}\left(w_1, \dots, w_N\right) / \partial w_1 \\ \vdots \\ \partial g_{n_g}\left(w_1, \dots, w_N\right) / \partial w_n \\ \vdots \\ \partial g_{n_g}\left(w_1, \dots, w_N\right) / \partial w_N \end{bmatrix}}_{N \times 1}$$

Each gradient  $\nabla g_{n_q}(w)$  is a column-vector of size  $(N \times 1)$ 

The Lagrangian function

Optimality

Equality constraints
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problems

### Optimality conditions | Equality constraints (cont.)

In the Jacobian of g(w), the gradients are transposed and arranged along the rows That is,

$$\nabla g\left(w\right)^{T} = \begin{bmatrix} \nabla g_{1}\left(w\right)^{T} \\ \nabla g_{2}\left(w\right)^{T} \\ \vdots \\ \nabla g_{n_{g}}\left(w\right)^{T} \\ \vdots \\ \nabla g_{N_{g}}\left(w^{*}\right)^{T} \end{bmatrix}$$

$$= \begin{bmatrix} \left[\frac{\partial g_{1}\left(w\right)}{\partial w_{1}} & \cdots & \partial g_{1}\left(w\right)}{\partial w_{1}} & \cdots & \partial g_{1}\left(w\right)}{\partial w_{n}} & \cdots & \partial g_{1}\left(w\right)}{\partial w_{N}} \right] \\ \vdots \\ \left[\frac{\partial g_{2}\left(w\right)}{\partial w_{1}} & \cdots & \partial g_{2}\left(w\right)}{\partial w_{n}} & \cdots & \partial g_{2}\left(w\right)}{\partial w_{n}} & \cdots & \partial g_{2}\left(w\right)}{\partial w_{N}} \right] \\ \vdots \\ \left[\frac{\partial g_{n_{g}}\left(w\right)}{\partial w_{1}} & \cdots & \partial g_{n_{g}}\left(w\right)}{\partial w_{n}} & \cdots & \partial g_{n_{g}}\left(w\right)}{\partial w_{n}} & \cdots & \partial g_{n_{g}}\left(w\right)}{\partial w_{N}} \right] \\ \vdots \\ \left[\frac{\partial g_{N_{g}}\left(w\right)}{\partial w_{1}} & \cdots & \partial g_{N_{g}}\left(w\right)}{\partial w_{n}} & \cdots & \partial g_{N_{g}}\left(w\right)}{\partial w_{n}} & \cdots & \partial g_{N_{g}}\left(w\right)}{\partial w_{N}} \right] \right]$$

### Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality

Equality constraints

$$\nabla g\left(w\right)^{T} = \underbrace{\begin{bmatrix} \nabla g_{1}\left(w\right)^{T} \\ \nabla g_{2}\left(w\right)^{T} \\ \vdots \\ \nabla g_{n_{g}}\left(w\right)^{T} \\ \vdots \\ \nabla g_{N_{g}}\left(w^{*}\right)^{T} \end{bmatrix}}_{N_{g} \times N}$$

We denote the Jacobian matrix of vector-valued multivariate function  $g\left(w\right)$  as  $\nabla g\left(w\right)^{T}$ 

• Alternative notation used for the Jacobian,  $J_{g}\left(w\right)$  and  $\frac{\partial g\left(w\right)}{\partial w}$ 

### Optimality conditions | Equality constraints (cont.)

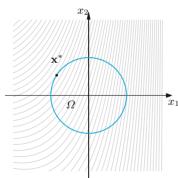
The Lagrangiar function

Optimality conditions

Equality constraints
Constrained

#### Example

Consider the minimisation of some function f(w) under some equality constraint g(w)



Let 
$$f: \mathbb{R}^2 \to \mathbb{R}$$

$$f(x) = \frac{3}{5}x_1^2 + \frac{1}{2}x_1x_2 - x_2 + 3x_1$$

Let  $g: \mathbb{R}^2 \to \mathbb{R}$ 

$$g(x) = x_1^2 + x_2^2 - 1$$

The feasible set

$$\Omega = \{ x \in \mathcal{R}^2 : g(x) = 0 \}$$

When on the constraint(s), feasibility is satisfied when moving along tangent directions

Optimality conditions must be verified along these directions

### Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality conditions

Equality constraints
Constrained
problems

#### Tangent vector

A vector  $p \in \mathbb{R}^N$  is a tangent vector to the feasible set  $\Omega$  at point  $w^* \in \Omega \subset \mathbb{R}^N$  if there exists a smooth curve  $\overline{w}(t) : [0, \varepsilon) \to \mathbb{R}^N$  such that the following is true

 $\rightarrow$  The curve for t = 0 starts at the feasible point  $w^*$ 

$$\overline{w}(0) = w^*$$

 $\rightarrow$  The curve is in feasible set for all  $t \in [0, \varepsilon)$ 

$$\overline{w}(t) \in \Omega, \quad \forall t$$

Vector p is derivative of curve  $\overline{w}$ , at t = 0

$$p = \frac{d\overline{w}(t)}{dt}\Big|_{t=}$$

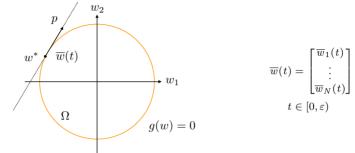
The Lagrangian function

Optimality

Equality constraints

### Optimality conditions | Equality constraints (cont.)

Curve  $\overline{w}(t)$  is parameterised by  $t,\ t$  varies over the infinitesimally small interval  $[0,\varepsilon)$ 



- $w^* \in \Omega$  is where the curve starts,  $\overline{w}(t=0) = w^*$  and  $\varepsilon$  is small enough
- Thus, the curve  $\overline{w}(t)$  remains inside  $\Omega$  (surely in the limit  $\varepsilon \to 0$ )

$$p(t) = \frac{d\overline{w}(t)}{dt} = \begin{bmatrix} d\overline{w}_1(t)/dt \\ \vdots \\ d\overline{w}_N(t)/dt \end{bmatrix} = \begin{bmatrix} p_1(t) \\ \vdots \\ p_N(t) \end{bmatrix}$$

Tangent vector p defines a direction along which it is possible move without leaving  $\Omega$ 

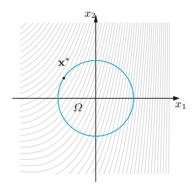
### Optimality conditions | Equality constraints (cont.)

The Lagrangia function

Optimality conditions

Equality constraints





Consider the problem with feasibility set

$$\Omega = \{x \in \mathcal{R}^2 : x_1^2 + x_2^2 - 1 = 0\}$$

The points  $x^*$  on the unit circle

$$x^* = \begin{bmatrix} x_1^* \\ x_2^* \end{bmatrix}$$

An alternative characterisation of a feasible point  $x^*$ , for some fixed  $\alpha^* \in [0, 2\pi]$ 

$$x^*(\alpha) = \begin{bmatrix} \cos(\alpha^*) \\ \sin(\alpha^*) \end{bmatrix}$$

### Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Equality constraints

For a fixed  $\alpha^*$  (fixed  $x^*$ ) and some  $\omega \in \mathcal{R}$ , we construct a feasible curve  $\overline{x}(t)$  from  $x^*$ 

Optimality

$$\overline{x}(t|\alpha^*, \omega) = \begin{bmatrix} \cos(\alpha^* + \omega t) \\ \sin(\alpha^* + \omega t) \end{bmatrix}$$

conditions

We can also determine the tangent vectors p(t) to the curve  $\overline{x}(t)$ , along the curve

$$p_{\alpha^*,\omega}(t) = \frac{d\overline{x}(t|\alpha^*,\omega)}{dt}$$
$$= \begin{bmatrix} -\omega \sin{(\alpha^* + \omega t)} \\ \omega \cos{(\alpha^* + \omega t)} \end{bmatrix}$$
$$= \omega \begin{bmatrix} -\sin{(\alpha^* + \omega t)} \\ \cos{(\alpha^* + \omega t)} \end{bmatrix}$$

Thoto

The tangent vector at t = 0 (or, at  $x^*$ ),

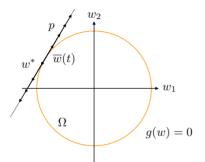
$$p_{\omega} = \frac{d\overline{x}(t)}{dt}\Big|_{t=0}$$
$$= \omega \begin{bmatrix} -\sin(\alpha^*) \\ \cos(\alpha^*) \end{bmatrix}$$

Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality conditions

Equality constraints
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#### Tangent cone

The tangent cone  $T_{\Omega}(w^*)$  of the feasible set  $\Omega$  at some feasible point  $w^* \in \Omega \subset \mathbb{R}^N$ is the set of all the tangent vectors at  $w^*$ 

• 'If p is a tangent vector, then also 2p is a tangent vector, ...'

Sometimes the set of elements of the tangent cone define a space, the tangent space

The Lagrangian function

Optimality conditions

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Constrained

### Optimality conditions | Equality constraints (cont.)

To construct a smooth curve  $\overline{w}(t)$  that satisfies the conditions needed to define tangent vectors, we can consider the equality constraint g(w) and its Taylor's expansion at  $w^*$ 

Consider the first-order Taylor's series expansion of function g at point  $w^*$ 

$$g(w) = \underbrace{g(w^*)}_{=0} + \nabla g(w^*)^T (w - w^*) + \mathcal{O}((w - w^*)^2)$$

• We know g and we can compute its gradients ( $\leadsto$  Jacobian)

Similarly, we construct the approximated curve and at t = 0 (at point  $w^*$ ) we have

$$\overline{w}(t) = \underbrace{w(0)}_{w^*} + \underbrace{\frac{d\overline{w}(t)}{dt}}_{p} \Big|_{t=0} (t-0) + \mathcal{O}\left((t-0)^2\right)$$

$$\approx w^* + tp$$

We can then construct a direction such that from  $w^*$  it is feasible, up to the first-order

$$g(w) = \underbrace{g(w^*)}_{=0} + \underbrace{\nabla g(w^*)^T (w - w^*)}_{=0} + \mathcal{O}\left((w - w^*)^2\right)$$

### Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality conditions

Equality constraints

problems

$$g(w) \approx \underbrace{g(w^*)}_{=0} + \underbrace{\nabla g(w^*)^T(w - w^*)}_{=0}$$

We consider the tangent vectors p that projected by the Jacobian  $\nabla g\left(w^{*}\right)^{T}$  are zero

$$\nabla g \left( w^* \right)^T p = 0$$

Tangent directions p that satisfy the orthogonality condition are feasible,  $g\left(\overline{w}(t)\right)=0$ 

• If the constraints at  $w^*$  are zero, along p they will remain zero (up to first-order)

The feasible tangent directions are in the null-space of the Jacobian  $J_g\left(w\right) = \nabla g(w^*)^T$ 

This suggests a criterion for building a possible tangent cone 
$$T_{\Omega}(w^*)$$

$$T_{\Omega}(w^*) = \{ p \in \mathcal{R}^N : \nabla g(w^*)^T p = 0 \}$$

## Optimality conditions | Equality constraints (cont.)

The Lagrangia function

Optimality conditions

Equality constraints
Constrained

The collection of tangent directions to  $\Omega$  that are orthogonal to the equality constraints

$$\mathcal{F}_{\Omega}(w^*) = \{ p \in \mathcal{R}^N : \nabla g_{n_g}(w^*)^T p = 0, \text{ with } n_g = 1, 2, \dots, N_g \}$$

The collection in this set is denoted as the linearised feasible cone for equality constraints

- For equality constrained problems that are smooth,  $\mathcal{F}_{\Omega}\left(w^{*}\right)$  is a space
- More generally, the set of all tangent vectors to  $\Omega$  is just a cone

In general (with inequality constraints), it is difficult to characterise the tangent cone

• The linearised feasible cone for equality constraints is a good proxy to it

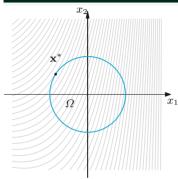
Though, in general, we have

$$\mathcal{F}_{\Omega}(w) \neq T_{\Omega}(w)$$

The Lagrangian function

Optimality conditions

Equality constraints



Consider the problem with feasibility set

$$\Omega = \{ x \in \mathcal{R}^2 | x_1^2 + x_2^2 - 1 = 0 \}$$

A possible tangent vector  $p_{\omega}(x^*)$ 

$$p_{\omega}(x^*) = \omega \begin{bmatrix} -\sin(\alpha^*) \\ \cos(\alpha^*) \end{bmatrix}$$

The vector space is mono-dimensional

The vector space corresponds to the tangent cone, it is constructed by choosing  $\omega \in \mathcal{R}$ 

$$T_{\Omega}(x^*) = \{ p \in \mathcal{R}^2 : p = \omega \begin{bmatrix} -\sin(\alpha^*) \\ \cos(\alpha^*) \end{bmatrix}, \text{ with } \omega \in \mathcal{R} \}$$

The tangent vectors are orthogonal to the gradient vector of the constraint function

$$\nabla g\left(x^{*}\right) = 2 \begin{bmatrix} \cos\left(\alpha^{*}\right) \\ \sin\left(\alpha^{*}\right) \end{bmatrix}$$

## Optimality conditions | Equality constraints (cont.)

### \_\_\_\_

Lagrangia tion

Optimality

Equality constraints

First-order necessary optimality conditions (I)

Consider the equality constrained optimisation problem

$$\min_{w \in \mathcal{R}^{N}} f(w)$$
subject to  $g(w) = 0$ 

A point  $w^*$  is a local minimiser, if  $w^* \in \Omega$  and for all tangents  $p \in T_{\Omega}(w^*)$ , we have

$$\nabla f\left(w^*\right)^T p \ge 0$$

When we consider the directions that are in the tangent cone  $T_{\Omega}(w^*)$  of point  $w^*$  in the feasible set  $\Omega$ , we must only have directions along which the objective worsens

If  $\nabla f(w^*)^T p < 0$ , then there would also exist some feasible curve  $\overline{w}(t)$  such that

$$\frac{df\left(\overline{w}\left(t\right)\right)}{dt}\Big|_{t=0} = \nabla f\left(w^{*}\right)^{T} p$$

$$< 0$$

There would exist a feasible descent direction, along which the objective improves

### Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality conditions

Equality constraints
Constrained

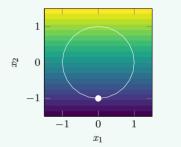
Consider the constrained optimisation

$$\min_{w \in \mathcal{R}^2} w_2$$

subject to 
$$w_1^2 + w_2^2 - 1 = 0$$

The minimiser  $w^*$ 

$$w^* = (0, -1)$$



The gradient vector of the objective function at the minimiser

$$\nabla f\left(w^*\right) = \begin{bmatrix} 0\\1 \end{bmatrix}$$

The gradient at  $w^*$  is orthogonal to the tangent space at  $w^*$ 

• Not true for (most of the) other feasible points

The Lagrangian function

Conditions

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### Optimality conditions | Equality constraints (cont.)

We are interested in the conditions under which the identity  $\mathcal{F}_{\Omega}(w^*) = T_{\Omega}(w^*)$  holds

• (When the tangent cone is also a tangent (vector) space?)

We say that the linear independence constraint qualification (LICQ) holds at point  $w^*$  if and only if the vectors  $\nabla g_{n_g}(w^*)$  are linearly independent,  $n_g = 1, \ldots, N_g$ 

•  $\{\nabla g_{n_g}(w^*)^T\}$  are the rows of the Jacobian, gradients of the equality constraints

$$\nabla g\left(w\right)^{T} = \underbrace{\begin{bmatrix} \nabla g_{1}\left(w\right)^{T} \\ \nabla g_{2}\left(w\right)^{T} \\ \vdots \\ \nabla g_{n_{g}}\left(w\right)^{T} \\ \vdots \\ \nabla g_{N_{g}}\left(w^{*}\right)^{T} \end{bmatrix}}_{N_{g} \times N}$$

The linear independence qualification is equivalent to requiring rank  $\left(\nabla g\left(w^{*}\right)^{T}\right)=N_{g}$ 

• This condition can be satisfied if and only if  $N_g \leq N$ 

### Optimality conditions | Equality constraints (cont.)

The Lagrangia function

Optimality conditions

Equality constraints

problems

It can be shown that, in general, the following holds

$$T_{\Omega}(w^*) \subseteq \mathcal{F}_{\Omega}(w^*)$$

When LICQ holds, we have

$$T_{\Omega}(w^*) = \mathcal{F}_{\Omega}(w^*)$$

We can restate the first-order optimality conditions (II)

$$\min_{w \in \mathcal{R}^{N}} f(w)$$
subject to  $g(w) = 0$ 

Point  $w^*$  is a local minimiser, if  $w^* \in \Omega$ , LICQ holds at  $w^*$ , and for all  $p \in \mathcal{F}_{\Omega}(w^*)$ 

$$\rightsquigarrow \nabla f(w^*)^T p = 0$$

The Lagrangian function

Optimality conditions

Equality constraints
Constrained

### Optimality conditions | Equality constraints (cont.)

We can further restate the first-order optimality conditions (III)

$$\min_{w \in \mathcal{R}^{N}} f(w)$$
subject to  $g(w) = 0$ 

Point  $w^*$  is a local minimiser, if  $w^* \in \Omega$ , LICQ holds at  $w^*$ , and there is a  $\lambda^* \in \mathcal{R}^{N_g}$ 

$$\leadsto$$
  $\nabla f(w^*) = \nabla g(w^*)\lambda^*$ 

Remember the Lagrangian function for equality constrained problems, we have

$$\mathcal{L}(w,\lambda) = f(w) - \lambda^{T} g(w)$$

We retrieve the optimality condition, by differentiating

$$\nabla_{w} \mathcal{L}(w^{*}, \lambda^{*}) = \nabla f(w^{*}) - \nabla g(w^{*}) \lambda^{*}$$
$$= 0$$

This result is important, because we can optimise simultaneously for both  $w^*$  and  $\lambda^*$ 

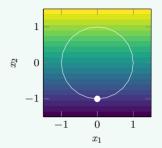
Consider the constrained optimisation

$$\min_{w \in \mathcal{R}^2} \quad w_2$$

subject to 
$$w_1^2 + w_2^2 - 1 = 0$$

The Lagrangian function

$$\mathcal{L}(w,\lambda) = w_2 - \lambda(w_1^2 + w_2^2 - 1)$$



The gradient of  $\mathcal{L}(w,\lambda) = w_2 - \lambda(w_1^2 + w_2^2 - 1)$  with respect to the primal variables w

$$abla_{w}\mathcal{L}\left(w,\lambda
ight) = egin{bmatrix} 0 \\ 1 \end{bmatrix} - \lambda egin{bmatrix} 2w_{1} \\ 2w_{2} \end{bmatrix}$$

The first-order optimality conditions,  $g(w^*)$  and  $\nabla_w \mathcal{L}(w, \lambda) = 0$ 

$$w_1^2 + w_2^2 - 1 = 0$$

$$-2\lambda w_1 = 0$$

$$-2\lambda w_2 + 1 = 0$$

### Optimality conditions | Equality constraints (cont.)

The Lagrangia function

Optimality conditions

Equality constraints

Some remarkable facts about first-order optimality conditions and Lagrangian functions

$$\mathcal{L}(w,\lambda) = f(w) - \lambda^{T} g(w)$$

The gradient of the Lagrangian function with respect to the dual  $\lambda$  equals  $-g\left(w\right)$ 

$$\nabla_{\lambda} \mathcal{L}\left(w, \lambda\right) = -g\left(w\right)$$

At a minimiser  $w^* \in \Omega$ , we have  $g(w^*) = 0$  and  $\nabla_w \mathcal{L}(w^*, \lambda^*) = 0$ , or

$$\begin{bmatrix} \nabla_{w} \mathcal{L} (w^*, \lambda^*) \\ \nabla_{\lambda} \mathcal{L} (w^*, \lambda^*) \end{bmatrix} = \nabla_{w, \lambda} \mathcal{L} (w^*, \lambda^*)$$
$$= 0$$

The LICQ condition led to define the Karhush-Kuhn-Tucker (KKT) conditions

$$\nabla_{w,\lambda} \mathcal{L} (w^*, \lambda^*) = 0$$
$$g (w^*) = 0$$

### Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality

Equality constraints
Constrained

Second-order necessary optimality conditions

$$\min_{w \in \mathcal{R}^{N}} f(w)$$
subject to  $g(w) = 0$ 

Point  $w^*$  is a local minimiser if  $w^* \in \Omega$ , LICQ holds at  $w^*$ , there exists a  $\lambda^* \in \mathcal{R}^{N_g}$  such that  $\nabla f(w^*) = \nabla g(w^*)\lambda^*$ , and for all tangent vectors  $p \in \mathcal{F}_{\Omega}(w^*)$  we also have

$$p^{T} \nabla_{w}^{2} \mathcal{L}\left(w^{*}, \lambda^{*}\right) p \geq 0$$

Second-order sufficient optimality conditions

$$p^{T} \nabla_{w}^{2} \mathcal{L}\left(w^{*}, \lambda^{*}\right) p > 0$$

The Lagrangian function

Optimality

Equality constraints

Constrained problems

# Equality and inequality constraints

**Optimality conditions** 

The Lagrangia

Conditions

Equality constraints
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problems

### Optimality conditions | Constrained problems

Consider the equality and inequality constrained optimisation problem in general form

$$\min_{x \in \mathcal{R}^{N}} \quad f(x)$$
subject to 
$$g(x) = 0$$

$$h(x) \ge 0$$

We assume smooth functions  $f: \mathbb{R}^N \to \mathbb{R}, g: \mathbb{R}^N \to \mathbb{R}^{N_g}$ , and  $h: \mathbb{R}^N \to \mathbb{R}^{N_h}$ 

$$g(w) = \begin{bmatrix} g_1(w) \\ \vdots \\ g_{N_g}(w) \end{bmatrix}$$
$$h(w) = \begin{bmatrix} h_1(w) \\ \vdots \\ h_{N_g}(w) \end{bmatrix}$$

 $\longrightarrow$  We have the set of feasible points  $\Omega = \{ w \in \mathbb{R}^N : g(w) = 0, h(w) \ge 0 \}$ 

To formulate the optimality conditions for these problems, we extend previous notions

The Lagrangian

Optimality conditions

Constrained problems

### Optimality conditions | Constrained problems (cont.)

#### Tangent vector

A vector  $p \in \mathbb{R}^N$  is a tangent vector to the feasible set  $\Omega$  at point  $w^* \in \Omega \subset \mathbb{R}^N$  if there exists a smooth curve  $\overline{w}(t) : [0, \varepsilon) \to \mathbb{R}^N$  such that the following is verified

 $\rightarrow$  The curve for t = 0 starts at the feasible point  $w^*$ 

$$\overline{w}(0) = w^*$$

 $\rightarrow$  The curve is in feasible set for all  $t \in [0, \varepsilon)$ 

$$\overline{w}(t)\in\Omega$$

 $\rightarrow$  Vector p is the derivative of  $\overline{w}$  at t=0

$$\left. \frac{d\overline{w}(t)}{dt} \right|_{t=0} = p$$

#### Tangent cone

The tangent cone  $T_{\Omega}(w^*)$  of the feasible set  $\Omega$  at point  $w^* \in \Omega \subset \mathcal{R}^N$  is the set of all the tangent vectors at  $w^*$  (same definition, now it requires a different characterisation)

### Optimality conditions | Constrained problems (cont.)

The Lagrangian function

Optimality conditions

Constrained problems

With equality constrained problems, we defined the linearised feasible cone  $\mathcal{F}_{\Omega}(w^*)$ 

• For feasible points  $w^*$ , we have first-order necessary optimality conditions

$$\nabla f(w^*)^T p \ge 0$$
, for all  $p \in \mathcal{T}_{\Omega}(w^*)$ 

• Under linear independence constraint qualification (LICQ) conditions

$$T_{\Omega}(w^*) = \mathcal{F}_{\Omega}(w^*)$$

To characterise the tangent cone with inequality constrains, we introduce new concepts

### Optimality conditions | Constrained problems (cont.)

The Lagrangian function

conditions

Constrained

We need to describe the feasibility set in the neighbourhood of a local minimiser  $w^* \in \Omega$ 

Earlier, we mentioned the notion of active constraints and active set

Consider the inequality constraint functions

$$h(w) = \begin{bmatrix} h_1(w) \\ \vdots \\ h_{N_h}(w) \end{bmatrix}$$

An inequality constraint  $h_{n_g}(w^*) \leq 0$  is said to be an active inequality constraint at  $w^* \in \Omega$  if and only if  $h_{n_g}(w^*) = 0$ , otherwise it is an inactive inequality constraint

- The index set of active inequality constraints is  $\mathcal{A}(w^*) \subset \{1, 2, \dots, N_h\}$
- The index set  $\mathcal{A}(w^*)$  of active inequality constraints is the active set
- The cardinality of the active set,  $N_{\mathcal{A}} = |\mathcal{A}(w^*)|$

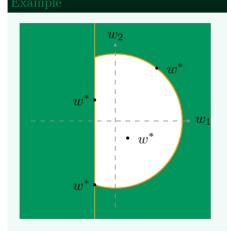
### Optimality conditions | Constrained problems (cont.)

The Lagrangian function

Optimality conditions

Equality constraints

Constrained problems



Determine the active set for the different feasible points  $w^*$ 

### Optimality conditions | Constrained problems (cont.)

The Lagrangian function

conditions
Equality constraint

Constrained

The linearised feasible cone for equality and inequality constraints

The linearised feasible cone  $\mathcal{F}_{\Omega}(w^*)$  at point  $w^* \in \Omega$  is the set of all tangent directions to  $\Omega$  that are orthogonal to the equality constraints and the active inequality constraints

$$\mathcal{F}_{\Omega}\left(w^{*}\right) = \left\{p \in \mathcal{R}^{N} : \nabla g_{n_{g}}\left(w^{*}\right)^{T}p = 0 \underbrace{\text{with } n_{g} = 1, \dots, N_{g}}_{\text{all equalities}} \right.$$

$$\nabla h_{n_{h}}\left(w^{*}\right)^{T}p \geq 0 \underbrace{\text{with } n_{h} \in \mathcal{A}(w^{*})}_{\text{active inequalities}}$$

We require that tangent directions remain inside the feasible set, up to the first order

### Optimality conditions | Constrained problems (cont.)

The Lagrangia: function

Optimality

Constrained
problems

Consider point  $w^* \in \Omega$  and the gradient vectors  $\left\{\nabla g_{n_g}\left(w^*\right)\right\}_{n_g=1}^{N_g}$  and  $\left\{\nabla h_{n_h}\left(w^*\right)\right\}_{n_h=1}^{N_h}$ 

The gradient vectors are the rows of the respective Jacobians, evaluated at point  $w^*$ 

$$\underbrace{\begin{bmatrix} \nabla g_{1}\left(w^{*}\right) \\ \vdots \\ \nabla g_{N_{g}}\left(w^{*}\right) \end{bmatrix}}_{\nabla g\left(w^{*}\right)^{T}} = \begin{bmatrix} \left[\partial g_{1}\left(w\right)/\partial w_{1} & \partial g_{1}\left(w\right)/\partial w_{2} & \cdots & \partial g_{1}\left(w\right)/\partial w_{N}\right]^{T} \\ \vdots & \vdots & & & \\ \left[\partial g_{N_{g}}\left(w\right)/\partial w_{1} & \partial g_{N_{g}}\left(w\right)/\partial w_{2} & \cdots & \partial g_{N_{g}}\left(w\right)/\partial w_{N}\right]^{T} \end{bmatrix} \\
\underbrace{\begin{bmatrix} \nabla h_{1}\left(w^{*}\right) \\ \vdots \\ \nabla h_{N_{h}}\left(w^{*}\right) \end{bmatrix}}_{\nabla h\left(w^{*}\right)^{T}} = \begin{bmatrix} \left[\partial h_{1}\left(w\right)/\partial w_{1} & \partial h_{1}\left(w\right)/\partial w_{2} & \cdots & \partial h_{1}\left(w\right)/\partial w_{N}\right]^{T} \\ \vdots & & \vdots \\ \left[\partial h_{N_{\mathcal{A}}}\left(w\right)/\partial w_{1} & \partial h_{N_{\mathcal{A}}}\left(w\right)/\partial w_{2} & \cdots & \partial h_{N_{h}}\left(w\right)/\partial w_{N}\right]^{T} \end{bmatrix} \\
\underbrace{\begin{bmatrix} \partial h_{1}\left(w\right)/\partial w_{1} & \partial h_{1}\left(w\right)/\partial w_{2} & \cdots & \partial h_{N_{h}}\left(w\right)/\partial w_{N}\right]^{T}}_{\nabla h\left(w^{*}\right)^{T}} \end{bmatrix}$$

The Lagrangian function

Optimality conditions

problems

Equality constraint Constrained Optimality conditions | Constrained problems (cont.)

At any point  $w^* \in \Omega$  in the feasible set, we have that all constraints must be satisfied

$$g(w) = 0$$
$$h(w) \ge 0$$

Moreover, at each active inequality constraint  $n_q \in \mathcal{A}(w^*)$  we have

$$\begin{bmatrix} \vdots \\ h_{n_g \in \mathcal{A}} (w^*) \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ 0 \\ \vdots \end{bmatrix}$$

For points  $w^*$  on the equality and active inequality constraint, we define

$$\overline{g}(w^*) = \begin{bmatrix} g_1(w^*) \\ \vdots \\ g_{N_g}(w^*) \\ \vdots \\ h_{n_g \in \mathcal{A}}(w^*) \\ \vdots \\ \vdots \\ (N_g + N_{\mathcal{A}}) \times 1 \end{bmatrix}$$

The Lagrangia

Conditions

Equality const

Constrained problems

### Optimality conditions | Constrained problems (cont.)

We say that the linear independence constraint qualitification (LICQ) holds at point  $w^*$  is and only if vectors  $\{\nabla g_{n_g}(w^*)\}$  and  $\{h_{n_h \in \mathcal{A}}(w^*)\}$  are linearly independent

That is, when the rank condition on the Jacobian of function  $\overline{g}$  holds

$$\operatorname{rank}\left(\frac{\partial \overline{g}\left(w^{*}\right)}{\partial w}\right) = N_{g} + N_{\mathcal{A}}$$

Importantly, note that inactive inequality constraint do not affect the LICQ coinditions

For feasible points  $w^* \in \Omega$ , we have

$$\mathcal{T}_{\Omega}(w^*) \subset \mathcal{F}_{\Omega}(w^*)$$

If LICQ holds at  $w^*$ , we also have

$$\mathcal{T}_{\Omega}(w^*) = \mathcal{F}_{\Omega}(w^*)$$

Inactive constraints do not affect the tangent cone

### Optimality conditions | Constrained problems (cont.)

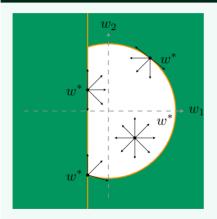
The Lagrangian function

Optimality conditions

Equality constraints

Constrained problems

### Example



Determine the tangent cone for the different feasible points  $w^*$ 

### Optimality conditions | Constrained problems (cont.)

The Lagrangian function

conditions
Equality constraints
Constrained

problems

First-order necessary optimality conditions (I)

$$\begin{aligned} \min_{w \in \mathcal{R}^N} & f\left(w\right) \\ \text{subject to} & g\left(w\right) = 0 \\ & h\left(w\right) \leq 0 \end{aligned}$$

Point  $w^*$  is a local minimiser, if  $w^* \in \Omega$ , LICQ holds at  $w^*$ , and for all  $p \in \mathcal{F}_{\Omega}(w^*)$ 

$$\rightsquigarrow \nabla f(w^*)^T p \ge 0$$

The Lagrangian function

conditions

Equality constraints

Constrained

Optimality conditions | Constrained problems (cont.)

$$\min_{w \in \mathcal{R}^{N}} \quad f(w)$$
subject to 
$$g(w) = 0$$

$$h(w) \le 0$$

The LICQ condition leads to define the Karhush-Kuhn-Tucker (KKT) conditions

Let  $w^*$  be a minimiser of objective function f, given constraint functions g and hIf LICQ holds at  $w^*$ , then there exists vectors  $\lambda^* \in \mathcal{R}^{N_g}$  and  $\mu^* \in \mathcal{R}^{N_h}$  such that

$$\nabla f(w^{*}) - \nabla g(w^{*})\lambda^{*} - \nabla h(w^{*})\mu^{*} = 0$$

$$g(w^{*}) = 0$$

$$h(w^{*}) \ge 0$$

$$\mu^{*} \ge 0$$

$$\mu_{n_{h}}^{*} h_{n_{h}}(w^{*}) = 0, \quad n_{h} = 1, \dots, N_{h}$$

First-order necessary optimality conditions (II)

### The Lagrangian

Optimality conditions

Constrained problems

## Optimality conditions | Constrained problems (cont.)

$$\frac{\nabla f\left(w^{*}\right)}{N \times 1} - \frac{\nabla g\left(w^{*}\right)}{N \times N_{g}} \underbrace{\lambda^{*}}_{N_{g} \times 1} - \underbrace{\nabla h\left(w^{*}\right)}_{N \times N_{h}} \underbrace{\mu^{*}}_{N_{h} \times 1} = 0$$

$$\underbrace{g\left(w^{*}\right)}_{N_{g} \times 1} = 0$$

$$\underbrace{h\left(w^{*}\right)}_{N_{h} \times 1} \ge 0$$

$$\underbrace{\mu^{*}}_{N_{h} \times 1} \ge 0$$

We defined the following terms,

$$\nabla f(w^*) = \left(\frac{\partial f(w^*)}{\partial w}\right)^T$$

$$\nabla g(w^*) = \left(\frac{\partial g(w^*)}{\partial w}\right)^T$$

$$\nabla h(w^*) = \left(\frac{\partial h(w^*)}{\partial w}\right)^T$$

### Optimality conditions | Constrained problems (cont.)

The Lagrangian function

conditions

Equality constraints

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problems

$$\nabla f(w^{*}) - \nabla g(w^{*})\lambda^{*} - \nabla h(w^{*})\mu^{*} = 0$$

$$g(w^{*}) = 0$$

$$h(w^{*}) \ge 0$$

$$\mu^{*} \ge 0$$

$$\mu_{n_{h}}^{*} h_{n_{h}}(w^{*}) = 0, \quad n_{h} = 1, \dots, N_{h}$$

The KKT conditions are first-order necessary optimality conditions for arbitrarily constrained problems, and thus correspond to  $\nabla f\left(w^{*}\right)=0$  for unconstrained problems

• For convex problems, the KKT conditions are sufficient for globality

The last three KKT conditions are often denoted as complementarity conditions