$\begin{array}{c} \text{CHEM-E7225} \\ 2022 \end{array}$

The Lagrangia function

conditions

Constrained

problems



Nonlinear optimisation, fundamentals (B) CHEM-E7225 (was E7195), 2022

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The Lagrangian function

Optimality

Equality constraints

Constraine

The Lagrangian function

Nonlinear optimisation

The Lagrangian

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Constrained problems

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

$$h\left(w
ight)\geq0$$

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

→ Equality constraint function

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

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

$$h(w) \ge 0$$

The globally optimal value of the objective function subjected to the constraints

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

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

- \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 on the optimal value p^*

Overview (cont.)

The Lagrangian

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

$$x_2$$
 :

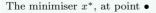
$$\rightarrow f: \mathbb{R}^2 \to \mathbb{R}, \text{ with } f \in \mathbb{C}^2(\mathbb{R}^2)$$

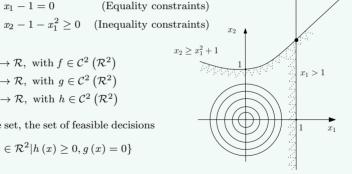
$$\rightarrow g: \mathbb{R}^2 \to \mathbb{R}, \text{ with } g \in \mathbb{C}^2(\mathbb{R}^2)$$

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

The feasible set, the set of feasible decisions

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





Ω

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 denoted as the Lagrangian function

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

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, $\lambda \in \mathcal{R}^{N_g}$

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

The Lagrangian function,

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

The Lagrangian function

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The Lagrangian function (cont.)

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

$$h(w) \ge 0$$

In expanded form, we have

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

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

The number of multipliers must match the number of constraints

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

We require the inequality multipliers to be positive $(\mu \geq 0)$

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

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)

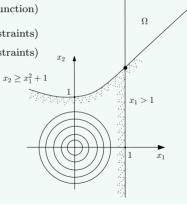
$$x_2 - 1 - x_1^2 \ge 0$$
 (Inequality constraints)

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

$$\underbrace{x_2 - 1 - x_1^2}_{h(x)} \geq 0 \qquad \text{(Inequality constraints)}$$

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

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

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

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

The Lagrangian function

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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 λ and for any $\mu \geq 0$, we have the lower-bound

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

Clearly, we also have that

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

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

• (That is, 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

$$\mathcal{L}\left(\widetilde{x},\lambda,\mu\right) = \widetilde{x}_1^2 + \widetilde{x}_2^2 - \lambda_1\left(\widetilde{x}_1 - 1\right) - \mu_1\left(\widetilde{x}_2 - 1 - \widetilde{x}_1^2\right)$$

 $x_2 \ge x_1^2 + 1$ $x_1 > 1$ $-\widetilde{x}_1^2$

Ω

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

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

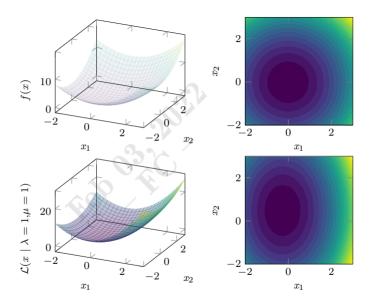
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The Lagrangian function

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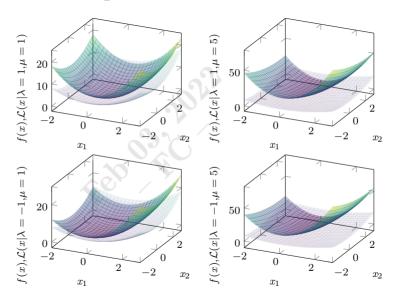


For different pairs $(\lambda, \mu_{\geq 0})$ and for any $\tilde{x} \in \Omega$, we always have that $\mathcal{L}(\tilde{x}, \lambda, \mu) \leq f(\tilde{x})$

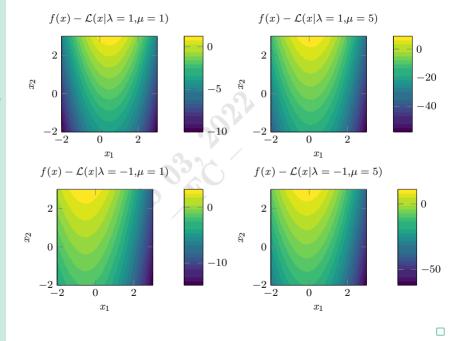


Optimality conditions

Equality constrains Constrained problems



The Lagrangian



The Lagrangian function | Duality

The Lagrangian function

Optimality conditions

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

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

Thus, the Lagrange dual function is a scalar function

$$q:\mathcal{R}^{N_g} imes\mathcal{R}^{N_h}_{\geq 0} o\mathcal{R}$$

Let w^* be the unconstrained 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 other feasible point \widetilde{w} and with fixed (λ, μ) , we have

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

2022

The Lagrangian

The Lagrangian function | Duality (cont.)

Lower-bound property of the Lagrange dual function

For any multipliers λ and $\mu \geq 0$, we have that for any feasible point \widetilde{w}

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

Moreover, at that feasible point \widetilde{w}

$$q(\lambda, \mu) \leq \mathcal{L}(\widetilde{w}, \lambda, \mu)$$

Thus, we have the following

$$q(\lambda, \mu) \le \mathcal{L}(\widetilde{w}, \lambda, \mu) \le f(\widetilde{w})$$

Because $p^* \leq f(\widetilde{w})$, we have $q(\lambda, \mu) \leq p^*$

$$q(\lambda,\mu) \leq p^{\gamma}$$

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

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

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

The Lagrangian

Optimality

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The Lagrangian function | Duality

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

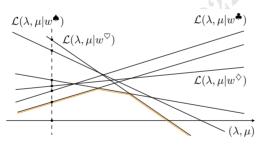
Equality constraint Constrained problems

The Lagrangian function | Duality

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

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

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



For fixed λ, μ , the dual function

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

Or, equivalently

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

- $-q\left(\lambda,\mu\right)$ is the supremum of affine, thus convex, functions in the dual variables (λ,μ)
 - 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 $q(\lambda, \mu)$

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

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 λ and μ

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

The Lagrangian function | Duality (cont.)

 $\begin{array}{c} {\rm The\ Lagrangian} \\ {\rm function} \end{array}$

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

$$d^{*} = \left(\max_{\substack{\lambda \in \mathcal{R}^{N_g} \\ \mu \in \mathcal{R}^{N_h}}} \quad q\left(\lambda, \mu\right), \text{ s.t. } \mu \geq 0 \right)$$

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

$$d^* \le p^*$$

For any convex nonlinear programs¹, we have strong-duality result

$$d^* = p^*$$

¹Slater's constraint qualification conditions must also be satisfied.

The Lagrangian function | Duality (cont.)

The Lagrangian function

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Example

Strictly convex quadratic program

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

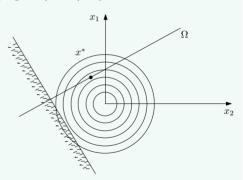
The primal optimisation problem

$$\min_{x \in \mathcal{R}^N} \quad c^T x + \frac{1}{2} x^T B x$$
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 | Duality (cont.)

The Lagrangian function

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$$\min_{x \in \mathcal{R}^N} \underbrace{c^T x + \frac{1}{2} x^T B x}_{f(w)}$$
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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Equality constraints Constrained 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 $q(\lambda, \mu)$ is defined as infimum of the Lagrangian function

• The minimisation is with respect to the primal variables x

We have,

$$q(\lambda, \mu) = \inf_{x \in \mathcal{R}^N} \left(\lambda^T b + \mu^T d + (c - A^T \lambda - C^T \mu)^T x + \frac{1}{2} x^T B x \right)$$

$$= \lambda^T b + \mu^T d + \inf_{x \in \mathcal{R}^N} \left((c - A^T \lambda - C^T \mu)^T x + \frac{1}{2} x^T B x \right)$$

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

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

The Lagrangian function | Duality (cont.)

The Lagrangian function

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

After rearranging, we formulate the dual optimisation problem

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

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 | Duality (cont.)

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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$$\begin{aligned} & \min_{w \in \mathcal{R}^N} & c^T w \\ \text{subject to} & Aw - b = 0 \\ & Cx - d \geq 0 \end{aligned}$$

For the Lagrangian function, we can write

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

The Lagrange dual, as infimum of the Lagrangian

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

The Lagrangian function | Duality (cont.)

The Lagrangian function

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

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 $c - A^T \lambda - C^T \mu = 0$

$$\mu \ge 0$$

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

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

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

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

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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 would be such that $\nabla f(w^*) \neq 0$

• Then, there is a direction $-\nabla f(w^*)$ that would be a descent direction

$$\nabla f(w^*)^T (-\nabla f(w^*)) = -\|\nabla f(w^*)\|_2^2 < 0$$

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

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

 $< f(w^*)$ (a contradiction for a local minimiser)

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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 objective function would diminish

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

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

Optimality conditions | Unconstrained problems (cont.)

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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

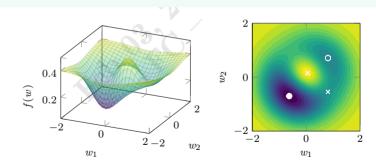
Equality constraints

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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

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Equality constraints

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 $\Omega = \{w \in \mathcal{R}^N | g(w) = 0\}$, 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

Optimality

Equality constraints

problems

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

- The tangent vector to the feasible set Ω
- The tangent cone to the feasible set Ω

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 Ω at a feasible point w^* form a vector space

• The tangent space

Optimality conditions | Equality constraints (cont.)

The Lagrangia function

Optimality conditions

Equality constraints

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

$$g\left(w\right) = \underbrace{\begin{bmatrix}g_{1}\left(w\right)\\ \vdots\\ g_{n_{g}}\left(w\right)\\ \vdots\\ g_{N_{g}}\left(w\right)\end{bmatrix}}_{N_{g}\times1}$$

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 $\nabla g_{n_q}\left(w\right)$ of component functions $g_{n_q}\left(w\right)$

Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality

Equality constraints

$$g\left(w\right) = \underbrace{\begin{bmatrix}g_{1}\left(w\right)\\ \vdots\\ g_{n_{g}}\left(w\right)\\ \vdots\\ g_{N_{g}}\left(w\right)\end{bmatrix}}_{N_{g}\times1}$$

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

$$abla g_{n_g}\left(w
ight) = egin{bmatrix} \partial g_{n_g}\left(w_1,\ldots,w_N
ight)/\partial w_1 \ dots \ \partial g_{n_g}\left(w_1,\ldots,w_N
ight)/\partial w_n \ dots \ \partial g_{n_g}\left(w_1,\ldots,w_N
ight)/\partial w_N \end{bmatrix} \ egin{bmatrix} \partial g_{n_g}\left(w_1,\ldots,w_N
ight)/\partial w_N \ \partial g_{n_g}\left(w_1,\ldots,w_N
ight)/\partial w_N \end{bmatrix} \ egin{bmatrix} \partial g_{n_g}\left(w_1,\ldots,w_N
ight)/\partial w_N \ \partial g_{n_g}\left(w_1,\ldots,w_N
ight)/\partial$$

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

The Lagrangian function

Optimality

Equality constraints
Constrained

Optimality conditions | Equality constraints (cont.)

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

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

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

$$= \underbrace{\begin{bmatrix} \left[\partial g_{1}\left(w\right) / \partial w_{1} & \cdots & \partial g_{1}\left(w\right) / \partial w_{n} & \cdots & \partial g_{1}\left(w\right) / \partial w_{N} \right]}_{\left[\partial g_{n_{g}}\left(w\right) / \partial w_{1} & \cdots & \partial g_{n_{g}}\left(w\right) / \partial w_{n} & \cdots & \partial g_{n_{g}}\left(w\right) / \partial w_{N} \end{bmatrix}}_{N_{g} \times N}$$

Optimality conditions | Equality constraints (cont.)

Equality constraints

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

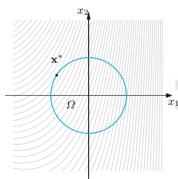
We denote the Jacobian matrix of vector-valued multivariate function $g\left(w\right)$ as $\nabla g\left(w\right)^{T}$

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

Optimality conditions | Equality constraints (cont.)

Equality constraints

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



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

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

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

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

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

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 Lagrangia function

Optimality conditions

Equality constraints

Constrained

problems

Tangent vector

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

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

Then, vector p is the derivative of \overline{w} at t = 0

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

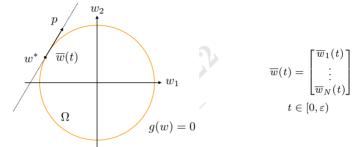
The Lagrangian function

Optimality

Equality constraints
Constrained

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 ε is small enough
- Thus, the curve $\overline{w}(t)$ remains inside Ω (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 Ω

Optimality conditions | Equality constraints (cont.)

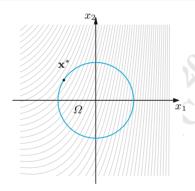
The Lagrangia function

Optimality conditions

Equality constraints

Constrained problems

Example



Consider the usual feasibility set

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

The points x^* on the unit circle

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

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

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

Optimality conditions | Equality constraints (cont.)

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

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

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

We can also determine the tangent vectors along the curve,

$$p_{\omega}(t) = \frac{d\overline{x}(t)}{dt}$$

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

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

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

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

The Lagrangian function

Conditions

Equality constraints

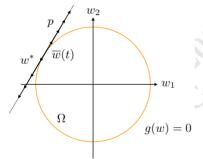
Constrain problems

Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality conditions

Equality constraints
Constrained
problems



Tangent cone

The tangent cone $T_{\Omega}(w^*)$ of the feasible set Ω at point $w^* \in \Omega \subset \mathcal{R}^N$ 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 Lagrangia function

conditions

Equality constraints
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, at t = 0 (that is, at point w^*), we have the approximated curve

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

$$\approx w^* + tp$$

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

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

Optimality conditions | Equality constraints (cont.)

The Lagrangian function

Optimality conditions

Equality constraints

problems

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

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 $J_g(w)$

This suggests a criterior 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 Ω 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 Ω is just a cone

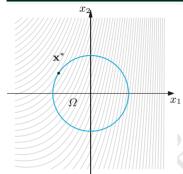
In general (with inequality constraints), it is difficult to characterise the tangent cone

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

Though, in general, we have

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

Equality constraints



Consider the usual 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.)

The Lagrangia

function

Equality constraints

Constrained problems 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 Ω , 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

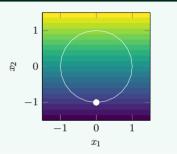
Example

Consider the constrained optimisation

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

Optimality

Equality constraints
Constrained

Optimality conditions | Equality constraints (cont.)

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

We say that the linear independence constraint qualification (LICQ) holds at point w^* if and only if the vectors $\nabla g_{n_q}(w^*)$ 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

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 $g(w) =$

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

Optimality

Equality constraints

Optimality conditions | Equality constraints (cont.)

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

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

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

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

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

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

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

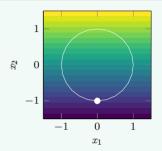
Equality constraints

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 $\nabla_w \mathcal{L}(w,\lambda) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} - \lambda \begin{bmatrix} 2w_1 \\ 2w_2 \end{bmatrix}$

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

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

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

The Lagrangia

Optimality

Equality constraints

Optimality conditions | Equality constraints (cont.)

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

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

The gradient of the Lagrangian function with respect to the dual λ 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 $g\left(w^*\right) = 0$ and $\nabla_w \mathcal{L}\left(w^*, \lambda^*\right) = 0$, or

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

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

conditions

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 Lagrangian function

Optimality conditions

Equality constraints

Constrained 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 $g(x) = 0$

$$h(x) \ge 0$$

 $h\left(x\right)\geq0$ • We assume a smooth functions $f:\mathcal{R}^{N}\to\mathcal{R},\ g:\mathcal{R}^{N}\to\mathcal{R}^{N_{g}},\ \mathrm{and}\ h:\mathcal{R}^{N}\to\mathcal{R}^{N_{h}}$

$$g\left(w\right) = \begin{bmatrix} g_{1}\left(w\right) \\ \vdots \\ g_{N_{g}}\left(w\right) \end{bmatrix}$$
$$h\left(w\right) = \begin{bmatrix} h_{1}\left(w\right) \\ \vdots \\ h_{N_{b}}\left(w\right) \end{bmatrix}$$

• 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 Ω 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^*

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

 \leadsto 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

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

Tangent cone

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

Optimality conditions | Constrained problems (cont.)

The Lagrangian function

Conditions

Constrained

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

problems

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

The active constraints and the active set

Consider the inequality constraint functions

$$h\left(w\right) = \begin{bmatrix} h_{1}\left(w\right) \\ \vdots \\ h_{N_{h}}\left(w\right) \end{bmatrix}$$

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 $A(w^*)$ is denoted as the active set
- The cardinality of the active set, $N_{\mathcal{A}} = |\mathcal{A}(w^*)|$

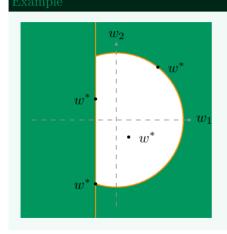
Optimality conditions | Constrained problems (cont.)

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

Optimality conditions

problems

Equality constraints
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 Ω that are orthogonal to the equality constraints and the active inequality constraints

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

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

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

Optimality conditions | Constrained problems (cont.)

The Lagrangian function

Optimality conditions

problems

Equality constraints

Constrained

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 Jacobians evaluated at point w^* ,

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

Constrained problems

Optimality conditions | Constrained problems (cont.)

At a feasible point $w^* \in \Omega$, we have

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

Moreover, at the active inequality constraints 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 constraints and the active inequality constraint, we define

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

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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 $\{\nabla g_{n_q}(w^*)\}$ and $\{h_{n_h \in \mathcal{A}}(w^*)\}$ are linearly independent

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

$$\operatorname{rank}\!\left(rac{\partial\overline{g}\left(w^{*}
ight)}{\partial w}
ight)=N_{g}+\mathcal{N}_{\mathcal{A}}$$

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

For feasible points $w^*\in\Omega,$ we have $\mathcal{T}_\Omega(w^*)\subset\mathcal{F}_\Omega(w^*)$

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

If LICQ holds at w^* , we also have

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

Inactive constraints do not affect the tangent cone

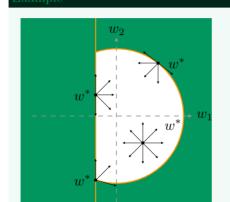
Optimality conditions | Constrained problems (cont.)

The Lagrangian function

Optimality conditions

Equality constraints

Constrained



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

Optimality conditions | Constrained problems (cont.)

Constrained problems

First-order necessary optimality conditions (I

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

$$h(w) \le 0$$

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

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

The Lagrangian

conditions

Constrained

problems

Optimality conditions | Constrained problems (cont.)

$$\min_{w \in \mathcal{R}^{N}} f(w)$$
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 $\lambda \in \mathbb{R}^{N_g}$ and $\mu \in \mathbb{R}^{N_h}$ 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

Equality constrain

Constrained problems

Optimality conditions | Constrained problems (cont.)

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

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

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

$$\underbrace{\mu^{*}_{N_{h}} \cdot h_{n_{h}}\left(w^{*}\right)}_{N_{h} \times 1} = 0, \quad n_{h} = 1, \dots, N_{h}$$

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

Constrained 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