OPTIMIZATION THEORY

Reference:

J. Nocedal and S.J. Wright, "Numerical Optimization," 2006. Chapter 2

THEOREM (TAYLOR'S THEOREM)

Let $f: \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable and $p \in \mathbb{R}^n$. Then for some $t \in (0,1)$ we have that

$$f(x+p) = f(x) + \nabla f(x+tp)'p \qquad \nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$



Brook Taylor (1685–1731)

Moreover, if f is twice continuously differentiable, for some $t \in (0, 1)$ we have that

$$f(x+p) = f(x) + \nabla f(x)'p + \frac{1}{2}p'\nabla^2 f(x+tp)p$$

THEOREM (FIRST-ORDER NECESSARY CONDITIONS)

Let $f:\mathbb{R}^n\to\mathbb{R}$ be continuously differentiable and x^* a local optimizer. Then

$$\nabla f(x^*) = 0$$

Proof:

- Assume by contradiction that $p=-\nabla f(x^*)\neq 0.$ Let $g(t)=p'\nabla f(x^*+tp).$ Then $g(0)=p'\nabla f(x^*)=-\|\nabla f(x^*)\|^2<0$
- ∇f is continuous around x^* , so g is also continuous wrt t in t = 0, and therefore $\exists T > 0$ such that g(t) < 0 for all $t \in [0, T]$
- For any $\bar{t} \in (0,T]$ by Taylor's theorem we have that for some $t \in (0,\bar{t})$

 $f(x^* + \bar{t}p) = f(x^*) + \bar{t}p' \nabla f(x^* + tp) = f(x^*) + g(t)\bar{t} < f(x^*), \, \forall \bar{t} \in (0,T]$

• Then x^* is not a local minimizer, which is a contradiction.

OPTIMALITY CONDITIONS

THEOREM (SECOND-ORDER NECESSARY CONDITIONS)

Let the Hessian matrix function $\nabla^2 f : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ exist and be continuous in an open neighborhood of a local optimizer x^* . Then

$$\nabla f(x^*) = 0, \nabla f^2(x^*) \succeq 0$$

Proof:

- Assume by contradiction that $\nabla^2 f(x^*) \not\succeq 0$. Then there exist p such that $p' \nabla^2 f(x^*) p < 0$.
- Since $\nabla^2 f(x)$ is continuous around x^* , $\exists T > 0$ such that $p' \nabla^2 f(x^* + tp) p < 0$ for all $t \in [0, T]$.
- By doing a Taylor expansion around $x^*, \forall \bar{t} \in (0,T]$ there exists $t \in (0,\bar{t})$ such that

$$f(x^* + \bar{t}p) = f(x^*) + \bar{t}p'\nabla f(x^*) + \frac{1}{2}\bar{t}^2p'\nabla^2 f(x^* + tp)p < f(x^*)$$

• Then x^* is not a local minimizer, which is a contradiction.

THEOREM (SECOND-ORDER SUFFICIENT CONDITIONS)

Let $\nabla^2 f: \mathbb{R}^n \to \mathbb{R}^{n \times n}$ exist and be continuous in an open neighborhood of x^* . Let $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \succ 0$. Then x^* is a strict local minimizer of f.

Proof:

- Since the Hessian function $\nabla^2 f(x)$ is continuous at x^* and $\nabla^2 f(x^*) \succ 0$, $\nabla^2 f(x) \succ 0$ for all x in an open ball $B(x^*, r)^1$ for some scalar r > 0
- For any p such that $\|p\|_2 < r$ we have that $x^* + p \in B(x^*,r)$ and hence

$$f(x^*+p) = f(x^*) + p'\nabla f(x^*) + \frac{1}{2}p'\nabla^2 f(x^*+tp)p = f(x^*) + \frac{1}{2}p'\nabla^2 f(x^*+tp)p$$

for some $t \in (0, 1)$.

• Since $x^* + tp \in B(x^*, r)$, $p' \nabla^2 f(x^* + tp)p > 0$, and therefore $f(x^* + p) > f(x^*)$, $\forall p \in B(0, r)$.

¹For a positive scalar r > 0, the Euclidean ball $B(x_0, r)$ is the set $\{x : ||x - x_0||_2 \le r\}$.

OPTIMALITY CONDITIONS - CONSTRAINED CASE

• Consider the constrained optimization problem

$$\begin{aligned} \min_x & f(x) \\ \text{s.t.} & g_i(x) \leq 0, \ i \in I \\ & g_j(x) = 0, \ j \in E \end{aligned}$$

with $I \cup E = \{1, ..., m\}.$

- A vector x is feasible if $g_i(x) \le 0, \forall i \in I$, and $g_j(x) = 0, \forall j \in E$
- We say that the inequality constraint $i \in I$ is active if $g_i(x) = 0$, inactive if $g_i(x) < 0$ (equality constraints $g_j(x), j \in E$, are always active).

OPTIMALITY CONDITIONS - CONSTRAINED CASE

• The active set $\mathcal{A}(x)$ at any feasible vector x is the set of indexes

 $\mathcal{A}(x) = \{i \in I : g_i(x) = 0\} \cup E$

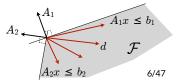
- We say that the linear independence constraint qualification (LICQ) condition holds at x if the vectors $\{\nabla g_i(x)\}_{i\in \mathcal{A}(x)}$ are linearly independent
- The set $\mathcal{F}(x)$ of linearized feasible directions at a feasible x is the cone

$$\mathcal{F}(x) = \{ d: d' \nabla g_i(x) = 0, \, \forall i \in E, \, d' \nabla g_i(x) \le 0, \, \forall i \in \mathcal{A}(x), \, i \notin E \}$$

Note that
$$g_i(x+d) \approx \underbrace{g_i(x)}_{=0} + \nabla g_i(x)' d$$
 for $d \to 0, \forall i \in \mathcal{A}(x)$

• Linear case example:

$$\left\{\begin{array}{rrrr} A_1x &\leq b_1 \\ A_2x &\leq b_2 \end{array}\right\} \longrightarrow \left\{\begin{array}{rrrr} A_1d &\leq 0 \\ A_2d &\leq 0 \end{array}\right.$$



OPTIMALITY CONDITIONS - CONSTRAINED CASE

THEOREM

If x^* is a local minimum and the LICQ condition is satisfied then

 $\nabla f(x^*)'d \ge 0, \, \forall d \in \mathcal{F}(x^*)$

• Define the Lagrangian function

$$\mathcal{L}(x,\lambda) = f(x) + \sum_{i=1}^{m} \lambda_i g_i(x)$$

where $\lambda \in \mathbb{R}^m$ are the Lagrange multipliers, $I \cup E = \{1, \dots, m\}$



Joseph-Louis Lagrange (1736–1813)

KKT OPTIMALITY CONDITIONS

THEOREM (FIRST-ORDER NECESSARY CONDITIONS)

Let f and g_i , i = 1, ..., m, be continuously differentiable and x^* a local optimizer. Let the LICQ condition hold at x^* . Then $\exists \lambda^* \in \mathbb{R}^m$ such that

Karush Kuhn Tucker (KKT) conditions

$\nabla_x \mathcal{L}(x^*, \lambda^*)$	=	0	
$g_i(x^*)$	\leq	0	$\forall i \in I$
$g_i(x^*)$	=	0	$\forall i \in E$
λ_i^*	\geq	0	$\forall i \in I$
$\lambda_i^* g_i(x^*)$	=	0	$\forall i = 1, \dots, m$



William Karush (1917–1997)



Harold W. Kuhn (1925–2014)

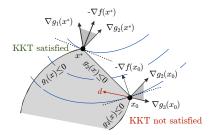


Albert W. Tucker (1905–1995) 8/47

• $\lambda_i^* g_i(x^*) = 0$ is a complementary slackness condition

- strict complementarity holds if $\lambda_i^* > 0$ for all $i \in \mathcal{A}(x^*)$
- λ^* is unique if the LICQ condition holds

KKT OPTIMALITY CONDITIONS



$$\begin{split} -\nabla f(x^*) &= \sum_{i=1}^m \lambda_i^* \nabla g_i(x^*), \, \lambda_i^* \geq 0, \\ E &= \emptyset \\ f(x^* + \epsilon d) \approx f(x^*) + \epsilon \nabla f(x^*)' d \\ f \text{ decreases when } -\nabla f(x^*)' d > 0 \end{split}$$

• if $-\nabla f(x^*)'d = \sum_{i=1}^m \lambda_i^* \nabla g_i(x^*)'d$ were positive then $\nabla g_i(x^*)'d > 0$ for some $i \in \mathcal{A}(x^*)$ such that $\lambda_i^* > 0$.

Hence f can only decrease at x^* if some active constraint g_i is violated, as $g_i(x^* + \epsilon d) \approx g_i(x^*) + \epsilon \nabla g_i(x^*)' d = \epsilon \nabla g_i(x^*)' d > 0, \epsilon > 0$

• Vice versa, if $-\nabla f(x^*)$ does not belong to the convex cone one can move in a direction d such that $d'\nabla f(x^*) < 0$ (that is, decrease f) while keeping $g_i(x) \leq 0$

KKT CONDITIONS FOR EQUALITY-CONSTRAINED QP

• Quadratic programming problem subject to equality constraints:

- Lagrangian function: $\mathcal{L}(x,\lambda) = \frac{1}{2}x'Qx + c'x + \lambda'(Ax b)$
- KKT conditions:

$$\begin{array}{l} Qx+c+A'\lambda=0\\ Ax=b \end{array} \Rightarrow \begin{array}{l} x=-Q^{-1}(c+A'\lambda)\\ AQ^{-1}A'\lambda=-(b+AQ^{-1}c) \end{array}$$

and therefore

$$\begin{split} \lambda^* &= -(AQ^{-1}A')^{-1}(b + AQ^{-1}c) \\ x^* &= -Q^{-1}(c - A'(AQ^{-1}A')^{-1}(b + AQ^{-1}c)) \end{split}$$

• In this case, the KKT conditions are also **sufficient** for optimality (this is a convex optimization problem, see later ...)

KKT CONDITIONS FOR QP

Quadratic programming problem

$$\begin{array}{ll} \min & \frac{1}{2}x'Qx + c'x \\ \text{s.t.} & Ax \leq b \\ & Ex = f \end{array}$$

- Lagrangian function: $\mathcal{L}(x,\lambda,\nu) = \frac{1}{2}x'Qx + c'x + \lambda'(Ax b) + \nu'(Ex f)$
- KKT conditions:

$$Qx + c + A'\lambda + E'\nu = 0$$

$$Ex = f$$

$$Ax \le b$$

$$\lambda \ge 0$$

$$\lambda'(Ax - b) = 0$$

where we replaced $\lambda_i(A_ix - b_i) = 0$, $\forall i$, with $\sum_i \lambda_i(A_ix - b_i) = 0$, having imposed $\lambda_i \ge 0$, $A_ix \le b_i$, $\forall i$

• Let x^*, λ^* satisfy the KKT conditions. The critical cone $\mathcal{C}(x^*, \lambda^*)$ is defined as

$$\mathcal{C}(x^*,\lambda^*) = \left\{ \begin{array}{ll} \nabla g_i(x^*)'w = 0, & \forall i \in E \\ w: & \nabla g_i(x^*)'w = 0, & \forall i \in \mathcal{A}(x^*) \cap I \text{ with } \lambda_i^* > 0 \\ & \nabla g_i(x^*)'w \le 0, & \forall i \in \mathcal{A}(x^*) \cap I \text{ with } \lambda_i^* = 0 \end{array} \right\}$$

• The critical cone $C(x^*, \lambda^*)$ contains directions in $\mathcal{F}(x^*)$ for which it is not clear from gradient information only whether f will increase or decrease, as from the KKT conditions we have

$$w'\nabla f(x^*) = \sum_{i=1}^{m} \lambda_i^* w' \nabla g_i(x^*) = 0, \, \forall w \in \mathcal{C}(x^*, \lambda^*)$$

^{``}Numerical Optimization'' - ©2023 A. Bemporad. All rights reserved.

SUPPLEMENTARY MATERIAL

THEOREM (2ND-ORDER NECESSARY CONDITIONS)

Assume f, g be twice continuously differentiable. Let x^* be a local minimum and the LICQ condition satisfied and λ^* such that the KKT conditions are satisfied. Then

$$w' \nabla_{xx} \mathcal{L}(x^*, \lambda^*) w \ge 0, \ \forall w \in \mathcal{C}(x^*, \lambda^*)$$

THEOREM (2ND-ORDER SUFFICIENT CONDITIONS)

Assume f,g be twice continuously differentiable. Let x^*,λ^* satisfy the KKT conditions and assume that

$$w' \nabla_{xx} \mathcal{L}(x^*, \lambda^*) w > 0, \ \forall w \in \mathcal{C}(x^*, \lambda^*), \ w \neq 0$$

Then x^* is a strict local minimum.

SENSITIVITY ANALYSIS

- <u>Question</u>: if we slightly perturb a constraint g_i how much $f(x^*)$ will change?
- The Lagrange multipliers λ^* answer such a sensitivity analysis question
- If $g_i(x^*) < 0 \iff \lambda_i^* = 0$, perturbing $g_i(x) \le 0$ to $g_i(x) \le -\epsilon$ does not change the solution, $\forall \epsilon < -g_i(x^*)$, as the same x^* , λ^* satisfy the KKT
- Let us change one of the active constraints $g_i(x) \leq 0$ to $g_i(x) \leq -\epsilon$, $i \in \mathcal{A}(x^*)$
- Let $x^*(\epsilon)$ be the perturbed optimal solution and assume $|\epsilon|$ small enough so that $\mathcal{A}(x^*(\epsilon))=\mathcal{A}(x^*)$

[`]Numerical Optimization'' - ©2023 A. Bemporad. All rights reserved.

SENSITIVITY ANALYSIS

• By taking the Taylor expansion of $g_j(x^*(\epsilon))$ around $\epsilon = 0$ we get

$$g_j(x^*(\epsilon)) - g_j(x^*) \approx \nabla g_j(x^*)'(x^*(\epsilon) - x^*), \ j = 1, \dots, m$$

- Since we assumed $\mathcal{A}(x^*(\epsilon)) = \mathcal{A}(x^*)$, then $g_i(x^*(\epsilon)) = -\epsilon$ and $g_j(x^*(\epsilon)) = 0$, $\forall j \in \mathcal{A}(x^*) \setminus \{i\}$, in addition to $g_j(x^*) = 0$, $\forall j \in \mathcal{A}(x^*)$
- By expanding $f(x^*(\epsilon))$ around $\epsilon = 0$ and using the KKT conditions

$$f(x^*(\epsilon)) - f(x^*) \approx \nabla f(x^*)'(x^*(\epsilon) - x^*) = \sum_{j \in \mathcal{A}(x^*)} -\lambda_j^* \nabla g_j(x^*)'(x^*(\epsilon) - x^*)$$
$$= \sum_{j \in \mathcal{A}(x^*)} -\lambda_j^*(g_j(x^*(\epsilon)) - g_j(x^*)) = \epsilon \lambda_i^*$$

- For $\epsilon \to 0$ we get

$$\frac{df(x^*(\epsilon))}{d\epsilon} = \lambda_i^*$$

SENSITIVITY ANALYSIS

DEFINITION

Let $i \in \mathcal{A}(x^*)$. An inequality constraint g_i is strongly active if $\lambda_i^* > 0$, weakly active if $\lambda_i^* = 0$

- If a constraint is weakly active, modifying it slightly does not change the optimal value since $\frac{df(x^*(\epsilon))}{d\epsilon} = 0$
- Let us scale the constraints to $\beta_i g_i(x) \leq 0, \beta_i > 0$. The KKT conditions are satisfied for x^* and $\frac{\lambda_i^*}{\beta_i}$
- For the consistent perturbation of the constraint $\beta_i g_i(x) \leq -\beta_i \epsilon$ we get the same optimizer $x^*(\epsilon)$, and moreover the sensitivity at the solution is

DUALITY

• Consider again the optimization problem

$$\min_{x} \quad f(x) \\ \text{s.t.} \quad g_{i}(x) \leq 0, \ i \in I \qquad I \cup E = \{1, \dots, m\} \\ \quad g_{j}(x) = 0, \ j \in E$$

• Define the dual function $q: \mathbb{R}^m \to \mathbb{R} \cup \{-\infty\}$

$$q(\lambda) = \inf_{x} \mathcal{L}(x, \lambda) = \inf_{x} \left\{ f(x) + \sum_{i=1}^{m} \lambda_{i} g_{i}(x) \right\}$$

- The domain $\mathcal D$ of q is the set of all λ for which $q(\lambda)>-\infty$
- A vector $\lambda \in \mathcal{D}$ is dual feasible if $\lambda_i \geq 0, \forall i \in I$
- A vector is $x \in \mathbb{R}^n$ primal feasible if $g_i(x) \le 0, \forall i \in I$ and $g_j(x) = 0, \forall j \in E$

DUALITY

THEOREM (WEAK DUALITY)

For any given primal feasible x and dual feasible λ

$$q(\lambda) \le f(x)$$

In particular $q(\lambda) \leq f(x^*)$.

Proof:

- Since x and λ are feasible, $\lambda_i g_i(x) \leq 0$, $\forall i \in I$ and $\lambda_j g_j(x) = 0$, $\forall j \in E$
- Therefore

$$f(x) \ge f(x) + \sum_{i=1}^{m} \lambda_i g_i(x) = \mathcal{L}(x, \lambda) \ge \inf_x \mathcal{L}(x, \lambda) = q(\lambda)$$

- Since the above relation holds for all feasible x, in particular it holds for x^*

 $f(x^*) \ge q(\lambda), \, \forall \lambda \text{ such that } \lambda_i \ge 0, \, i \in I$

THEOREM

The dual function $q(\lambda)$ is concave and its domain \mathcal{D} is convex.

Proof:

• Take any $\lambda^1, \lambda^2 \in \mathcal{D}$, and $\alpha \in [0, 1]$. We want to verify that $\alpha\lambda^1 + (1-\alpha)\lambda^2 \in \mathcal{D}$ and that Jensen's inequality holds: $q(\alpha\lambda^{1} + (1-\alpha)\lambda^{2}) = \inf \mathcal{L}(x, \alpha\lambda^{1} + (1-\alpha)\lambda^{2})$ $= \inf_{x} \left\{ f(x) + \sum_{i=1}^{m} (\alpha \lambda_{i}^{1} + (1-\alpha)\lambda_{i}^{2}))g_{i}(x) \right\}$ $= \inf_{x} \left\{ (\alpha + 1 - \alpha)f(x) + \alpha \sum_{i=1}^{m} \lambda_{i}^{1}g_{i}(x) + (1 - \alpha) \sum_{i=1}^{m} \lambda_{i}^{2}g_{i}(x) \right\}$ $= \inf_{x} \left\{ \alpha(f(x) + \sum_{i=1}^{m} \lambda_i^1 g_i(x)) + (1 - \alpha)(f(x) + \sum_{i=1}^{m} \lambda_i^2 g_i(x)) \right\}$ $\geq \inf_{x_1} \left\{ \alpha(f(x_1) + \sum_{i=1}^m \lambda_i^1 g_i(x_1)) \right\} + \inf_{x_2} \left\{ (1-\alpha)(f(x_2) + \sum_{i=1}^m \lambda_i^2 g_i(x_2)) \right\}$ 19/47



• Finally, we get

$$q(\alpha\lambda^1 + (1-\alpha)\lambda^2) \ge \alpha q(\lambda^1) + (1-\alpha)q(\lambda^2) > -\infty$$

which proves that q is concave and that $\alpha \lambda^1 + (1-\alpha)\lambda^2 \in \mathcal{D}$

• Recall that the minimum of a finite number of affine functions is concave. $q(\lambda)$ is the minimum of infinitely many affine functions (one for each x).

DUAL PROBLEM

• We define dual problem of a given optimization problem the new problem

$$\begin{aligned} \max_{\lambda} & q(\lambda) \\ \text{s.t.} & \lambda_i \geq 0, \, \forall i \in I \\ & \lambda \in \mathcal{D} \end{aligned}$$

- The dual problem is always a convex programming problem, even if the primal problem is not convex
- Since $f(x^*) \ge q(\lambda)$ for all dual feasible λ , we also have that the optimum of the dual problem satisfies the weak duality condition

$$q(\lambda^*) \leq f(x^*)$$

- Strong duality holds when $q(\lambda^*) = f(x^*)$
- The difference $f(x^*) q(\lambda^*)$ is called $\operatorname{\textbf{duality gap}}$

GRADIENT OF DUAL FUNCTION AND ITS LINEAR APPROXIMATION

• Let $x^*(\lambda) = \arg \min_x \mathcal{L}(x, \lambda)$. For all $\lambda \ge 0$, the gradient

$$\nabla_{\lambda}q(\lambda) = g(x^*(\lambda))$$

Proof:

$$\begin{aligned} \nabla_{\lambda} q(\lambda) &= \nabla_{\lambda} (\inf_{x} \mathcal{L}(x,\lambda)) = \nabla_{\lambda} \mathcal{L}(x^{*}(\lambda),\lambda) \\ &= \nabla_{\lambda} x^{*}(\lambda) \qquad \underbrace{\frac{\partial \mathcal{L}(x^{*}(\lambda),\lambda)}{\partial x}}_{= 0 \text{ by optimality of } x^{*}(\lambda)} + \underbrace{\frac{\partial \mathcal{L}(x^{*}(\lambda),\lambda)}{\partial \lambda}}_{= g(x^{*}(\lambda))} \end{aligned}$$

• The first-order Taylor expansion of the dual function around λ_0 is

$$q(\lambda) \approx f(x^*(\lambda_0)) + g(x^*(\lambda_0))'\lambda$$

<u>Proof:</u>

$$\begin{split} \overline{q}(\lambda) &\approx q(\lambda_0) + \nabla_{\lambda} q(\lambda_0)'(\lambda - \lambda_0) = q(\lambda_0) + g(x^*(\lambda_0))'(\lambda - \lambda_0) \\ &= \inf_x \mathcal{L}(x, \lambda_0) + g(x^*(\lambda_0))'(\lambda - \lambda_0) = f(x^*(\lambda_0)) + g(x^*(\lambda_0))'\lambda_0 \\ &+ g(x^*(\lambda_0))'(\lambda - \lambda_0) = f(x^*(\lambda_0)) + g(x^*(\lambda_0))'\lambda \end{split}$$

STRONG DUALITY IN CONVEX PROGRAMMING

• Consider the convex programming problem

$$\min_{x} \quad f(x) \\ \text{s.t.} \quad g_{i}(x) \leq 0, \ i \in I \qquad I \cup E = \{1, \dots, m\} \\ A_{j}x = b_{j}, \ j \in E$$

where are f, g_i are convex functions.

• We say that **Slater's constraint qualification** is verified if the problem is strictly feasible:

$$\exists x: g_i(x) < 0, \, \forall i \in I, \, A_j x = b_j, \, \forall j \in E$$

- Strong duality always holds if Slater's constraint qualification is satisfied
- Other types of constraint qualifications exist

DUALITY AND KKT CONDITIONS FOR CONVEX PROBLEMS

THEOREM

Let x^* be the solution of a convex programming problem and f, g_i differentiable at x^* . Any λ^* satisfying the KKT conditions with x^* solves the dual problem.

Proof:

- Assume x^*, λ^* satisfy the KKT conditions and consider

$$\mathcal{L}(x,\lambda^*) = f(x) + \sum_{i \in I} \lambda_i^* g_i(x) + \sum_{j \in E} \lambda_j^* (A_j x - b_j)$$

- $\mathcal{L}(x, \lambda^*)$ is differentiable w.r.t. x at x^* , and is also a convex function of x, as $\lambda_i^* \ge 0$ for all $i \in I$
- By convexity of $\mathcal{L}(x,\lambda^*)$ we obtain

$$\mathcal{L}(x,\lambda^*) \geq \mathcal{L}(x^*,\lambda^*) + \overbrace{\nabla_x \mathcal{L}(x^*,\lambda^*)'}^{\text{so because of KKT}} (x-x^*) = \mathcal{L}(x^*,\lambda^*)$$

DUALITY AND KKT CONDITIONS FOR CONVEX PROBLEMS

- Since $\mathcal{L}(x,\lambda^*) \geq \mathcal{L}(x^*,\lambda^*)$ for all x we get

$$\begin{split} q(\lambda^*) &= \inf_x \mathcal{L}(x,\lambda^*) = \mathcal{L}(x^*,\lambda^*) \\ &= f(x^*) + \sum_{i \in I} \underbrace{\lambda_i^* g_i(x^*)}_{=0} + \sum_{j \in E} \lambda_j^* (\underbrace{A_j x^* - b_j}_{=0}) = f(x^*) \end{split}$$

- Since $q(\lambda) \leq f(x^*)$ for all dual feasible $\lambda,$ it follows that

 $q(\lambda) \le q(\lambda^*)$

- As λ^* is dual feasible, it is therefore an optimizer of the dual problem.
- Note that we have also proved that the duality gap is zero, as $q(\lambda^*)=f(x^*)$
- In general, for $x_{\lambda} \in rginf_x \mathcal{L}(x,\lambda)$ the duality gap is

$$f(x_{\lambda}) - q(\lambda) = -\sum_{i \in I} \lambda_i g_i(x_{\lambda}) - \sum_{j \in E} \lambda_j (A_j x_{\lambda} - b_j)$$

• Wolfe's dual problem is defined as follows:

 $\max_{x,\lambda} \quad \mathcal{L}(x,\lambda) \\ \text{s.t.} \quad \nabla_x \mathcal{L}(x,\lambda) = 0 \\ \lambda_i \ge 0, \, \forall i \in I$



Philip S. Wolfe (1927-2016)

THEOREM

Consider a convex programming problem with f, g_i differentiable on \mathbb{R}^n . Let x^*, λ^* satisfy the KKT conditions and LICQ hold. Then x^*, λ^* is an optimizer of Wolfe's dual problem.

WOLFE'S DUAL PROBLEM

Proof:

- Since (x^*, λ^*) satisfies the KKT conditions it is a feasible point of Wolfe's dual problem, and moreover $\mathcal{L}(x^*, \lambda^*) = f(x^*)$
- For any (x,λ) satisfying $abla_x \mathcal{L}(x,\lambda) = 0$, $\lambda_i \geq 0$, $\forall i \in I$, we get

$$\begin{split} \mathcal{L}(x^*,\lambda^*) &= f(x^*) \geq f(x^*) + \sum_{i \in I} \overbrace{\lambda_i g_i(x^*)}^{\leq 0} + \sum_{j \in E} \lambda_j (\overrightarrow{A_j x^* - b_j}) \\ &= \underbrace{\mathcal{L}(x^*,\lambda) \geq \mathcal{L}(x,\lambda) + \overbrace{\nabla_x \mathcal{L}(x,\lambda)'(x^* - x)}^{= 0}}_{\text{convexity of } \mathcal{L}(x,\lambda)} \\ &= \mathcal{L}(x,\lambda) \end{split}$$

• Hence $\mathcal{L}(x^*, \lambda^*) = f(x^*)$ is the maximum achievable value of $\mathcal{L}(x, \lambda)$ under the constraints $\nabla_x \mathcal{L}(x, \lambda) = 0, \lambda_i \ge 0, \forall i \in I.$

П

DUAL LINEAR PROGRAM

• Consider the linear program

$$\begin{array}{ll} \min_x & c'x \\ \text{s.t.} & Ax \leq b \end{array}$$

• The dual function is

$$q(\lambda) = \inf_x \{c'x + \lambda'(Ax - b)\} = \inf_x \{(c + A'\lambda)'x - b'\lambda\}$$

- $\bullet \ \ q(\lambda) > -\infty \ {\rm only} \ {\rm when} \ c + A'\lambda = 0, {\rm and} \ q(\lambda) = -b'\lambda$
- The dual problem is therefore



• It is easy to prove that the dual of the dual LP is the original LP ($\min_{x,s} c'x$ s.t. $Ax + s = b, s \ge 0$). The original x = dual vector of constraint $-A'\lambda + c = 0$, and s = dual vector of constraint $\lambda \ge 0$.

THEOREM (THEOREM OF ALTERNATIVES)

For given $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, exactly one of the following two alternatives is true:

- 1. there exists x such that $Ax \leq b$
- 2. there exists y such that $y \ge 0$, A'y = 0, b'y < 0

LEMMA (FARKAS' LEMMA)

For a given matrix A and vector b, exactly one of the following two alternatives is true:

- 1. there exists x such that Ax = b, $x \ge 0$
- 2. there exists y such that $A'y \ge 0, b'y < 0$



Gyula Farkas (1847–1930)

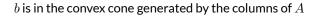
GEOMETRIC INTERPRETATION

Farkas' lemma has the following geometric interpretation. Let A_i be the *i*th column of $A, i = 1, ..., n, A = [A_1 A_2 ... A_n]$

SUPPI FM

• 1st alternative:

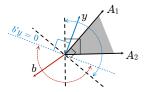
$$b = \sum_{i=1}^{n} x_i A_i, \ x_i \ge 0, \ i = 1, \dots, n$$



• 2nd alternative:

$$y'A_i \ge 0, \ i = 1, \dots, n$$

 $y'b < 0$



vector \boldsymbol{b} cannot be in the convex cone generated by the columns of \boldsymbol{A}

THEOREM (STRONG LP DUALITY)

- 1. If either the primal or the dual LP has a finite solution, so does the other and $c'x^* = -b'\lambda^*$ (strong duality)
- 2. If one of the two is unbounded the other is infeasible
- To see that infeasibility of dual LP implies unboundedness of a feasible primal LP, apply Farkas' Lemma with matrices -A', c

 $-A'\lambda = c, \ \lambda \ge 0$ infeasible $\exists d \in \mathbb{R}^n: \ -Ad \ge 0, \ c'd < 0$

- Take a feasible $x_0 \in \mathbb{R}^n$. Then $A(x_0 + \sigma d) = Ax_0 + \sigma Ad \le b, \forall \sigma \ge 0$, and $c'(x_0 + \sigma d) = c'x_0 \sigma |c'd|$
- As σ can be arbitrarily large, the infimum of the primal LP is $-\infty$.

DUAL LP WITH NONNEGATIVE VARIABLES

SUPPLEMENTARY MATERIAL

• Consider the linear program

$$\begin{array}{ll} \min_x & c'x \\ \text{s.t.} & Ax \ge b \\ & x \ge 0 \end{array}$$

• The dual function is

$$q(\lambda,\nu) = \inf_x \{c'x + \lambda'(b - Ax) - \nu'x\} = \inf_x \{(c - A'\lambda - \nu)'x + b'\lambda\} = b'\lambda$$

for $c-A'\lambda-\nu=0,\nu\geq 0,$ or equivalently $A'\lambda\leq c$

• The dual problem is therefore

$$\begin{array}{ll} \max_{\lambda} & b'\lambda \\ \text{s.t.} & A'\lambda \leq c \\ & \lambda \geq 0 \end{array}$$

• At optimality $c'x^* = b'\lambda^*$

DUAL LP AND LINEAR COMPLEMENTARITY PROBLEM (LCP)

• A linear complementarity problem (LCP) is a feasibility problem of the form

(Cottle, Pang, Stone, 2009)

$$w = Mz + q$$
$$w'z = 0$$
$$w, z \ge 0$$

• By introducing the vector s of slack variables, $s = Ax - b \ge 0$, the KKT conditions for the following LP are

$$\min_{x} \quad c'x \\ \text{s.t.} \quad Ax \ge b \\ x \ge 0 \\ x'\nu = \lambda's = 0 \\ c - A'\lambda - \nu = 0 \\ Ax - b - s = 0 \\ x, \lambda, \nu, s \ge 0 \\ x'\nu = \lambda's = 0$$

. . .

• Therefore, the original LP can be solved by solving the LCP

$$\underbrace{\begin{bmatrix} \nu \\ s \end{bmatrix}}_{w} = \underbrace{\begin{bmatrix} 0 & -A' \\ A & 0 \end{bmatrix}}_{M} \underbrace{\begin{bmatrix} x \\ \lambda \end{bmatrix}}_{z} + \underbrace{\begin{bmatrix} c \\ -b \end{bmatrix}}_{q}, \underbrace{\begin{bmatrix} x \\ \lambda \end{bmatrix}}_{w}, \underbrace{\begin{bmatrix} \nu \\ s \end{bmatrix}}_{z} \ge 0, \qquad \underbrace{x'\nu = \lambda's = 0}_{w'\nu + \lambda's = w'z = 0}$$
Numerical Optimization" - ©2023 A. Bemporad. All rights reserved. 33/47

DUAL QUADRATIC PROGRAM

• Consider the quadratic program

• The dual function is
$$q(\lambda) = \inf_{x} \left\{ \frac{1}{2}x'Qx + c'x + \lambda'(Ax - b) \right\}$$

- Since $Q \succ 0$ the infimum is achieved when $0 = \nabla_x \mathcal{L}(x_\lambda, \lambda) = Qx_\lambda + c + A'\lambda$, i.e., for $x_\lambda = -Q^{-1}(c + A'\lambda)$.
- By substitution, Lagrange's dual QP problem is therefore

$$\max_{\lambda \geq 0} - \left(\frac{1}{2}\lambda'(AQ^{-1}A')\lambda + (b + AQ^{-1}c)'\lambda + \frac{1}{2}c'Q^{-1}c\right)$$

• Let $Q \succ 0$ and consider the dual QP problem

$$\begin{split} \min_{\lambda} & \frac{1}{2}\lambda'(AQ^{-1}A')\lambda + (b + AQ^{-1}c)'\lambda \\ \text{s.t.} & \lambda \geq 0 \end{split}$$

• The KKT conditions for the dual QP are the LCP problem

$$H\lambda + d = s$$
$$s'\lambda = 0$$
$$s, \lambda \ge 0$$

where $H = AQ^{-1}A'$ is the dual Hessian and $d = b + AQ^{-1}c$

• We can therefore solve the QP problem as an LCP to get the dual solution λ^* and then reconstruct the primal solution $x^*=-Q^{-1}(c+A'\lambda^*)$

LCP AND DUAL QP

• Vice versa, let $M = M' \succ 0, M \in \mathbb{R}^{n \times n}$, and consider the LCP

```
\begin{aligned} x &= My + d\\ 0 &\leq x \perp y \geq 0 \end{aligned}
```

• Consider the QP problem

$$\min_{\substack{1 \\ y \neq 0}} \frac{1}{2}y'My + d'y$$
 s.t. $y \ge 0$

• The corresponding KKT optimality conditions are

$$\begin{array}{rclrcl} My + d - x & = & 0 \\ & y & \geq & 0 \\ & x & \geq & 0 \\ & x_i y_i & = & 0, \quad i = 1, \dots, n \end{array}$$

that are exactly the given LCP

SUPPLEMENTARY MATERIAL

• Consider now Wolfe's dual problem

1

$$\max_{x,\lambda} \quad \frac{1}{2}x'Qx + c'x + \lambda'(Ax - b)$$

s.t.
$$Qx + c + A'\lambda = 0, \ \lambda \ge 0$$

• We can subtract $0 = (Qx + c + A'\lambda)'x$ without changing the function and get the convex programming problem

$$\max_{x,\lambda} \quad -\frac{1}{2}x'Qx - \lambda'b$$

s.t.
$$Qx + c + A'\lambda = 0$$

$$\lambda \ge 0$$

• Note that Wolfe's dual QP only requires $Q \succeq 0$.

DUAL OF QP REFORMULATION OF LASSO

• Consider again the LASSO problem

$$\min_{x} \frac{1}{2} \|Ax - b\|_{2}^{2} + \gamma \|x\|_{1} \qquad A \in \mathbb{R}^{m \times n}, \ b \in \mathbb{R}^{m}, \ \gamma > 0$$

• With x = y - z and $y, z \ge 0$, LASSO becomes the positive semidefinite QP

$$\min_{y,z \ge 0} \frac{1}{2} \|A(y-z) - b\|_2^2 + \gamma \, \mathbb{I}'(y+z)$$

where ${\mathbb I}'=[1\ \dots\ 1]$ (as $\gamma>0$ at least one of y_i^*, z_i^* will be zero at optimality)

• The above QP is the dual of the following least distance programming (LDP) (constrained LS) problem (see next slide)

$$\min_{v} \quad \frac{1}{2} \|v - b\|_{2}^{2} - b'b$$
s.t.
$$\|A'v\|_{\infty} \leq \gamma$$

DUAL OF QP REFORMULATION OF LASSO

• Proof: The constrained LS problem is equivalent to the following QP

$$\begin{array}{ll} \min_{v} & \frac{1}{2}v'v - b'v - \frac{1}{2}b'b \\ \text{s.t.} & -\gamma \, \mathrm{I\hspace{-.1em}I} \leq A'v \leq \gamma \, \mathrm{I\hspace{-.1em}I} \end{array}$$

whose dual QP problem is exactly the original LASSO's QP reformulation

$$\min_{y,z\geq 0}\frac{1}{2}\begin{bmatrix}y\\z\end{bmatrix}\begin{bmatrix}A'\\-A'\end{bmatrix}I^{-1}\begin{bmatrix}A-A\end{bmatrix}\begin{bmatrix}y\\z\end{bmatrix}+(\gamma\begin{bmatrix}1\\1\end{bmatrix}-\begin{bmatrix}A'\\-A'\end{bmatrix}I^{-1}b)'\begin{bmatrix}y\\z\end{bmatrix}+\frac{1}{2}b'b-\frac{1}{2}b'b$$

- The LDP reformulation of LASSO is always a strictly convex QP with m variables, 2n constraints, and Hessian = identity matrix
- The original QP formulation is only convex with 2n variables and 2n constraints

• We have a training set $(x_1, y_1), \ldots, (x_N, y_N), x_i \in \mathbb{R}^n, y \in \mathbb{R}$ and want to fit a linear function

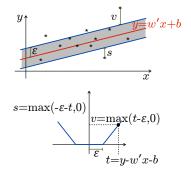
$$f(x) = w'x + b \quad w \in \mathbb{R}^n, b \in \mathbb{R}$$

such that each $|y_i - f(x_i)| \le \epsilon$

 Since such a function f may not exist, we want to penalize |y_i - f(x_i)| > ε

$$\min_{w,b,v,s} \quad \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^N (v_i + s_i)$$

s.t. $y_i - w' x_i - b \le \epsilon + v_i$
 $y_i - w' x_i - b \ge -\epsilon - s_i$
 $v_i, s_i \ge 0, \quad i = 1, \dots, N$



SUPPLEMENTARY MATERIAL

• By setting $X = [x_1 \ \dots \ x_N], Y = [y_1 \ \dots \ y_N]'$, we can rewrite in vector form

$$\min_{\substack{w,b,v,s \\ \text{s.t.}}} \quad \frac{1}{2}w'w + C \, \mathbb{I}'(v+s) \\ \text{s.t.} \quad Y - X'w - b \, \mathbb{I} \le \epsilon \, \mathbb{I} + v \\ Y - X'w - b \, \mathbb{I} \ge -\epsilon \, \mathbb{I} - s \\ v,s \ge 0$$

- Introduce the vectors of \mathbb{R}^N of Lagrange multipliers $\alpha,\beta,\gamma,\delta\geq 0$
- The Lagrangian function is

$$\mathcal{L}\left(\begin{bmatrix} w\\b\\v\\s\end{bmatrix},\begin{bmatrix} \alpha\\\beta\\\gamma\\\delta\end{bmatrix}\right) = \frac{1}{2}w'w + C\,\mathbb{1}'(v+s) + \alpha'(Y - X'w - (b+\epsilon)\,\mathbb{1}-v) \\ + \beta'(-Y + X'w + (b-\epsilon)\,\mathbb{1}-s) - \gamma'v - \delta's$$

- The dual function $q(\alpha,\beta,\gamma,\delta) = \inf_{w,b,v,s} \mathcal{L}(w,b,v,s,\alpha,\beta,\gamma,\delta)$

[`]Numerical Optimization'' - ©2023 A. Bemporad. All rights reserved.

• Let us zero the partial derivatives of \mathcal{L} with respect to w, b, v, s:

$$\begin{array}{rcl} 0 = \frac{\partial \mathcal{L}}{\partial w} &=& w - X\alpha + X\beta \quad \Rightarrow \quad w = X(\alpha - \beta) \\ 0 = \frac{\partial \mathcal{L}}{\partial b} &=& -\alpha' \, \mathbb{I} + \beta' \, \mathbb{I} \quad \Rightarrow \quad \mathbb{I}'(\alpha - \beta) = 0 \\ 0 = \frac{\partial \mathcal{L}}{\partial v} &=& C \, \mathbb{I} - \alpha - \gamma \quad \Rightarrow \quad \gamma = C \, \mathbb{I} - \alpha \geq 0 \\ 0 = \frac{\partial \mathcal{L}}{\partial s} &=& C \, \mathbb{I} - \beta - \delta \quad \Rightarrow \quad \delta = C \, \mathbb{I} - \beta \geq 0 \end{array}$$

SUPPLEMENTARY MATER

• By substituting the above expressions in the Lagrangian we get

$$q(\alpha, \beta, \gamma, \delta) = \frac{1}{2}w'w + (Y - X'w)'(\alpha - \beta) - \epsilon \mathbf{I}'(\alpha + \beta)$$
$$= -\frac{1}{2}(\alpha - \beta)'X'X(\alpha - \beta) + Y'(\alpha - \beta) - \epsilon \mathbf{I}'(\alpha + \beta)$$

• The dual problem is therefore the following QP

$$\min_{\alpha,\beta} \quad \frac{1}{2}(\alpha-\beta)'X'X(\alpha-\beta) - Y'(\alpha-\beta) + \epsilon \, \mathbb{I}'(\alpha+\beta)$$

s.t. $0 \le \alpha \le C \, \mathbb{I}, \quad 0 \le \beta \le C \, \mathbb{I}, \quad \mathbb{I}'(\alpha-\beta) = 0$

After solving the dual QP problem we can retrieve

$$w = X(\alpha^* - \beta^*) = \sum_{i=1}^{N} (\alpha_i^* - \beta_i^*) x_i$$

$$f(x) = w'x + b = (\alpha^* - \beta^*)' X'x + b = \sum_{i=1}^{N} (\alpha_i^* - \beta_i^*) x_i'x + b$$

$$\left| f(x) = \sum_{i=1}^{N} (\alpha_i^* - \beta_i^*) x_i'x + b \right|$$

SUPPLEMENTARY

(see next slide for how to reconstruct b)

- f(x) is defined by a linear combination of the training vectors x_i
- The vectors x_i for which $\alpha_i^* \beta_i^* \neq 0$ are called support vectors
- Note that the QP is also equivalent to the ℓ_1 -regularized problem

$$\min_{z} \quad \frac{1}{2} z' X' X z - Y' z + \epsilon \|z\|_{1} \\ \text{s.t.} \quad |z_{i}| \le C, \quad \sum_{i=1}^{N} z_{i} = 0$$

SUPPLEMENTARY MATERIAL

• The scalar b can be retrieved from the complementarity slackness conditions

$$\begin{array}{rcl}
0 &=& \alpha_i (y_i - x'_i w - (b + \epsilon) - v_i), & i = 1, \dots, N \\
0 &=& \beta_i (-y_i + x'_i w + (b - \epsilon) - s_i) \\
0 &=& \gamma_i v_i = (C - \alpha_i) v_i \\
0 &=& \delta_i s_i = (C - \beta_i) s_i
\end{array}$$

- if any $\alpha^*_i \in (0,C)$ then $v^*_i = 0 \Rightarrow b^* = y_i x'_i w^* \epsilon$
- if any $\beta_i^* \in (0,C)$ then $s_i^* = 0 \,{\Rightarrow}\, b^* = y_i x_i' w^* + \epsilon$

- Otherwise, consider the case all $\alpha^*_i, \beta^*_i \in \{0, C\}$
- α_i^*, β_i^* cannot be positive at the same time, as they refer to bilateral constraints $(y_i w'x_i b \text{ cannot be both positive and negative})$

• Let $\mathcal{I} = \{i : \alpha_i^* = 0 \text{ or } \beta_i^* = C\}$ and $\mathcal{J} = \{i : \alpha_i^* = C \text{ or } \beta_i^* = 0\}$. Then

$$b^* \ge y_i - x'_i w^* - \epsilon, \quad \forall i \in \mathcal{I}$$
$$b^* \le y_i - x'_i w^* + \epsilon, \quad \forall i \in \mathcal{J}$$

• Therefore, any $b^* \in [\max_{i \in \mathcal{I}} \{y_i - x'_i w^* - \epsilon\}, \min_{i \in \mathcal{J}} \{y_i - x'_i w^* + \epsilon\}]$ is optimal

SUPPLEMENTARY MATERIAL

• Kernel trick: if we generalize x_i to an arbitrary nonlinear basis $\phi(x_i)$ we get

$$f(x) = \sum_{i=1}^{N} (\alpha_i^* - \beta_i^*) k(x_i, x) + b$$

where $k(x,y)=\phi'(x)\phi(y)$ is a kernel function, $k:\mathbb{R}^n\times\mathbb{R}^n\to\mathbb{R}$

- Example: $x\in \mathbb{R}^2, \phi(x)=[x_1^2\quad \sqrt{2}x_1x_2\quad x_2^2]', k(x,y)=(x'y)^2$
- The (i, j)th term $x'_i x_j$ of the dual Hessian gets replaced by $k(x_i, x_j)$
- b depends on $x_i'w=x_i'X(\alpha-\beta)$ that gets replaced by $k(x_i,X)(\alpha^*-\beta^*)$
- Therefore ϕ , w are not required, and can have arbitrary dimensions !
- Example: Gaussian radial basis function kernel $k(x, y) = e^{-\frac{1}{2}||x-y||^2/\sigma^2}$ (RBF) the corresponding ϕ is infinite dimensional

EXAMPLE OF SUPPORT VECTOR REGRESSION

- Generate ${\cal N}=100$ random samples of the course-logo function

$$f(x_1, x_2) = -e^{-(x_1^2 + x_2^2)} + 0.3\sin\left(\frac{1}{10}x_1^3 + x_2^2\right) + 1.2$$

• Solve SVR problem with $C=100, \epsilon=0.01,$ Gaussian kernel with $\sigma=1$

