## OPTIMIZATION THEORY

## Reference:

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

## OPTIMALITY CONDITIONS

## THEOREM (TAYLOR'S THEOREM)

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

$$
f(x+p)=f(x)+\nabla f(x+t p)^{\prime} p \quad \nabla f=\left[\begin{array}{c}
\frac{\partial f}{\partial x_{1}} \\
\vdots \\
\frac{\partial f}{\partial x_{n}}
\end{array}\right]
$$



Brook Taylor
(1685-1731)

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

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

## OPTIMALITY CONDITIONS

## THEOREM CFIRST-ORDER NECESSARY CONDITIONSJ

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

$$
\nabla f\left(x^{*}\right)=0
$$

## Proof:

- Assume by contradiction that $p=-\nabla f\left(x^{*}\right) \neq 0$. Let $g(t)=p^{\prime} \nabla f\left(x^{*}+t p\right)$. Then $g(0)=p^{\prime} \nabla f\left(x^{*}\right)=-\left\|\nabla f\left(x^{*}\right)\right\|^{2}<0$
- $\nabla f$ 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 $t \in(0, \bar{t})$

$$
f\left(x^{*}+\bar{t} p\right)=f\left(x^{*}\right)+\bar{t} p^{\prime} \nabla f\left(x^{*}+t p\right)=f\left(x^{*}\right)+g(t) \bar{t}<f\left(x^{*}\right), \forall \bar{t} \in(0, T]
$$

- Then $x^{*}$ is not a local minimizer, which is a contradiction.


## OPTIMALITY CONDITIONS

## THEOREM [SECOND-ORDER NECESSARY CONDITIONS)

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

$$
\nabla f\left(x^{*}\right)=0, \nabla f^{2}\left(x^{*}\right) \succeq 0
$$

Proof:

- Assume by contradiction that $\nabla^{2} f\left(x^{*}\right) \nsucceq 0$. Then there exist $p$ such that $p^{\prime} \nabla^{2} f\left(x^{*}\right) p<0$.
- Since $\nabla^{2} f(x)$ is continuous around $x^{*}, \exists T>0$ such that $p^{\prime} \nabla^{2} f\left(x^{*}+t p\right) p<0$ 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

$$
f\left(x^{*}+\bar{t} p\right)=f\left(x^{*}\right)+\bar{t} p^{\prime} \nabla f\left(x^{*}\right)+\frac{1}{2} \bar{t}^{2} p^{\prime} \nabla^{2} f\left(x^{*}+t p\right) p<f\left(x^{*}\right)
$$

- Then $x^{*}$ is not a local minimizer, which is a contradiction.


## OPTIMALITY CONDITIONS

## THEOREM [SECOND-ORDER SUFFICIENT CONDITIONS]

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

## Proof:

- Since the Hessian function $\nabla^{2} f(x)$ is continuous at $x^{*}$ and $\nabla^{2} f\left(x^{*}\right) \succ 0$, $\nabla^{2} f(x) \succ 0$ for all $x$ in an open ball $B\left(x^{*}, r\right)^{1}$ for some scalar $r>0$
- For any $p$ such that $\|p\|_{2}<r$ we have that $x^{*}+p \in B\left(x^{*}, r\right)$ and hence
$f\left(x^{*}+p\right)=f\left(x^{*}\right)+p^{\prime} \nabla f\left(x^{*}\right)+\frac{1}{2} p^{\prime} \nabla^{2} f\left(x^{*}+t p\right) p=f\left(x^{*}\right)+\frac{1}{2} p^{\prime} \nabla^{2} f\left(x^{*}+t p\right) p$
for some $t \in(0,1)$.
- Since $x^{*}+t p \in B\left(x^{*}, r\right), p^{\prime} \nabla^{2} f\left(x^{*}+t p\right) p>0$, and therefore $f\left(x^{*}+p\right)>f\left(x^{*}\right), \forall p \in B(0, r)$. $\square$
${ }^{1}$ For a positive scalar $r>0$, the Euclidean ball $B\left(x_{0}, r\right)$ is the set $\left\{x:\left\|x-x_{0}\right\|_{2} \leq r\right\}$.


## OPTIMALITY CONDITIONS - CONSTRAINED CASE

- Consider the constrained optimization problem

$$
\begin{array}{rl}
\min _{x} & f(x) \\
\mathrm{s.t.} & g_{i}(x) \leq 0, i \in I \\
& g_{j}(x)=0, j \in E
\end{array}
$$

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

- A vector $x$ is feasible if $g_{i}(x) \leq 0, \forall i \in I$, 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

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

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

$$
\mathcal{F}(x)=\left\{d: d^{\prime} \nabla g_{i}(x)=0, \forall i \in E, d^{\prime} \nabla g_{i}(x) \leq 0, \forall i \in \mathcal{A}(x), i \notin E\right\}
$$

Note that $g_{i}(x+d) \approx \underbrace{g_{i}(x)}_{=0}+\nabla g_{i}(x)^{\prime} d$ for $d \rightarrow 0, \forall i \in \mathcal{A}(x)$

- Linear case example:

$$
\left\{\begin{array} { l } 
{ A _ { 1 } x \leq b _ { 1 } } \\
{ A _ { 2 } x \leq b _ { 2 } }
\end{array} \quad \longrightarrow \left\{\begin{array}{l}
A_{1} d \leq 0 \\
A_{2} d \leq 0
\end{array}\right.\right.
$$



## OPTIMALITY CONDITIONS - CONSTRAINED CASE

## THEOREM

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

$$
\nabla f\left(x^{*}\right)^{\prime} d \geq 0, \forall d \in \mathcal{F}\left(x^{*}\right)
$$

- 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, $I \cup E=\{1, \ldots, m\}$

Joseph-Louis Lagrange (1736-1813)

## KKT OPTIMALITY GONDITIONS

## THEOREM CFIRST-ORDER NECESSARY CONDITIONSJ

Let $f$ and $g_{i}, i=1, \ldots, m$, 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


William Karush
(1917-1997)


Harold W. Kuhn (1925-2014)


## KKT OPTIMALITY CONDITIONS



KKT not satisfied

$$
-\nabla f\left(x^{*}\right)=\sum_{i=1}^{m} \lambda_{i}^{*} \nabla g_{i}\left(x^{*}\right), \lambda_{i}^{*} \geq 0, E=\emptyset
$$

$$
\begin{aligned}
& f\left(x^{*}+\epsilon d\right) \approx f\left(x^{*}\right)+\epsilon \nabla f\left(x^{*}\right)^{\prime} d \\
& f \text { decreases when }-\nabla f\left(x^{*}\right)^{\prime} d>0
\end{aligned}
$$

- if $-\nabla f\left(x^{*}\right)^{\prime} d=\sum_{i=1}^{m} \lambda_{i}^{*} \nabla g_{i}\left(x^{*}\right)^{\prime} d$ were positive then $\nabla g_{i}\left(x^{*}\right)^{\prime} d>0$ for some $i \in \mathcal{A}\left(x^{*}\right)$ such that $\lambda_{i}^{*}>0$.

Hence $f$ can only decrease at $x^{*}$ if some active constraint $g_{i}$ is violated, as $g_{i}\left(x^{*}+\epsilon d\right) \approx g_{i}\left(x^{*}\right)+\epsilon \nabla g_{i}\left(x^{*}\right)^{\prime} d=\epsilon \nabla g_{i}\left(x^{*}\right)^{\prime} d>0, \epsilon>0$

- Vice versa, if $-\nabla f\left(x^{*}\right)$ does not belong to the convex cone one can move in a direction $d$ such that $d^{\prime} \nabla f\left(x^{*}\right)<0$ (that is, decrease $f$ ) while keeping $g_{i}(x) \leq 0$


## KKT CONDITIONS FOR EQUALITY-CONSTRAINED QP

- Quadratic programming problem subject to equality constraints:

$$
\left.\min \frac{1}{2} x^{\prime} Q x+c^{\prime} x \right\rvert\, \quad Q=Q^{\prime} \succ 0, A \text { full row rank }
$$

- Lagrangian function: $\mathcal{L}(x, \lambda)=\frac{1}{2} x^{\prime} Q x+c^{\prime} x+\lambda^{\prime}(A x-b)$
- KKT conditions:

$$
\begin{aligned}
& Q x+c+A^{\prime} \lambda=0 \\
& A x=b
\end{aligned} \Rightarrow \begin{aligned}
& x=-Q^{-1}\left(c+A^{\prime} \lambda\right) \\
& A Q^{-1} A^{\prime} \lambda=-\left(b+A Q^{-1} c\right)
\end{aligned}
$$

and therefore

$$
\begin{aligned}
& \lambda^{*}=-\left(A Q^{-1} A^{\prime}\right)^{-1}\left(b+A Q^{-1} c\right) \\
& x^{*}=-Q^{-1}\left(c-A^{\prime}\left(A Q^{-1} A^{\prime}\right)^{-1}\left(b+A Q^{-1} c\right)\right)
\end{aligned}
$$

- 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

$$
\begin{aligned}
\min & \frac{1}{2} x^{\prime} Q x+c^{\prime} x \\
\text { s.t. } & A x \leq b \\
& E x=f
\end{aligned}
$$

- Lagrangian function: $\mathcal{L}(x, \lambda, \nu)=\frac{1}{2} x^{\prime} Q x+c^{\prime} x+\lambda^{\prime}(A x-b)+\nu^{\prime}(E x-f)$
- KKT conditions:

$$
\begin{aligned}
& Q x+c+A^{\prime} \lambda+E^{\prime} \nu=0 \\
& E x=f \\
& A x \leq b \\
& \lambda \geq 0 \\
& \lambda^{\prime}(A x-b)=0
\end{aligned}
$$

where we replaced $\lambda_{i}\left(A_{i} x-b_{i}\right)=0, \forall i$, with $\sum_{i} \lambda_{i}\left(A_{i} x-b_{i}\right)=0$, having imposed $\lambda_{i} \geq 0, A_{i} x \leq b_{i}, \forall i$

## 2ND-ORDER NEGESSARY CONDITIONS

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

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

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

$$
w^{\prime} \nabla f\left(x^{*}\right)=\sum_{i=1}^{m} \lambda_{i}^{*} w^{\prime} \nabla g_{i}\left(x^{*}\right)=0, \forall w \in \mathcal{C}\left(x^{*}, \lambda^{*}\right)
$$

## 2ND-ORDER CONDITIONS

## THEOREM (2ND-ORDER NECESSARY CONDITIONS)

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

$$
w^{\prime} \nabla_{x x} \mathcal{L}\left(x^{*}, \lambda^{*}\right) w \geq 0, \forall w \in \mathcal{C}\left(x^{*}, \lambda^{*}\right)
$$

## THEOREM [2ND-ORDER SUFFICIENT CONDITIONS)

Assume $f, g$ be twice continuously differentiable. Let $x^{*}, \lambda^{*}$ satisfy the KKT conditions and assume that

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

Then $x^{*}$ is a strict local minimum.

## SENSITIVITY ANALYSIS

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


## SENSITIVITY ANALYSIS

- By taking the Taylor expansion of $g_{j}\left(x^{*}(\epsilon)\right)$ around $\epsilon=0$ we get

$$
g_{j}\left(x^{*}(\epsilon)\right)-g_{j}\left(x^{*}\right) \approx \nabla g_{j}\left(x^{*}\right)^{\prime}\left(x^{*}(\epsilon)-x^{*}\right), j=1, \ldots, m
$$

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

$$
\begin{aligned}
f\left(x^{*}(\epsilon)\right)-f\left(x^{*}\right) & \approx \nabla f\left(x^{*}\right)^{\prime}\left(x^{*}(\epsilon)-x^{*}\right)=\sum_{j \in \mathcal{A}\left(x^{*}\right)}-\lambda_{j}^{*} \nabla g_{j}\left(x^{*}\right)^{\prime}\left(x^{*}(\epsilon)-x^{*}\right) \\
& =\sum_{j \in \mathcal{A}\left(x^{*}\right)}-\lambda_{j}^{*}\left(g_{j}\left(x^{*}(\epsilon)\right)-g_{j}\left(x^{*}\right)\right)=\epsilon \lambda_{i}^{*}
\end{aligned}
$$

- For $\epsilon \rightarrow 0$ we get

$$
\frac{d f\left(x^{*}(\epsilon)\right)}{d \epsilon}=\lambda_{i}^{*}
$$

## SENSITIVITY ANALYSIS

## DEFINITION

Let $i \in \mathcal{A}\left(x^{*}\right)$. 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 $\frac{d f\left(x^{*}(\epsilon)\right)}{d \epsilon}=0$
- 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 $\beta_{i} g_{i}(x) \leq-\beta_{i} \in$ we get the same optimizer $x^{*}(\epsilon)$, and moreover the sensitivity at the solution is

$$
\frac{\lambda_{i}^{*}}{\beta_{i}}=\frac{d f\left(x^{*}(\epsilon)\right)}{d\left(\beta_{i} \epsilon\right)}=\frac{1}{\beta_{i}} \frac{d f\left(x^{*}(\epsilon)\right)}{d \epsilon} \quad \Rightarrow \quad \frac{d f\left(x^{*}(\epsilon)\right)}{d \epsilon}=\lambda_{i}^{*}
$$

## DUALITY

- Consider again the optimization problem

$$
\begin{array}{rl}
\min _{x} & f(x) \\
\text { s.t. } & g_{i}(x) \leq 0, i \in I \quad I \cup E=\{1, \ldots, m\} \\
& g_{j}(x)=0, j \in E
\end{array}
$$

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

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

- The domain $\mathcal{D}$ of $q$ is the set of all $\lambda$ 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 $g_{i}(x) \leq 0, \forall i \in I$ and $g_{j}(x)=0, \forall j \in E$


## DUALITY

## THEOREM (WEAK DUALITY)

For any given primal feasible $x$ and dual feasible $\lambda$

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

In particular $q(\lambda) \leq f\left(x^{*}\right)$.
Proof:

- Since $x$ and $\lambda$ 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

$$
f(x) \geq f(x)+\sum_{i=1}^{m} \lambda_{i} g_{i}(x)=\mathcal{L}(x, \lambda) \geq \inf _{x} \mathcal{L}(x, \lambda)=q(\lambda)
$$

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

$$
f\left(x^{*}\right) \geq q(\lambda), \forall \lambda \text { such that } \lambda_{i} \geq 0, i \in I
$$

## DUALITY

## 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:

$$
q\left(\alpha \lambda^{1}+(1-\alpha) \lambda^{2}\right)=\inf _{x} \mathcal{L}\left(x, \alpha \lambda^{1}+(1-\alpha) \lambda^{2}\right)
$$

$$
\begin{aligned}
& \left.=\inf _{x}\left\{f(x)+\sum_{i=1}^{m}\left(\alpha \lambda_{i}^{1}+(1-\alpha) \lambda_{i}^{2}\right)\right) g_{i}(x)\right\} \\
& =\inf _{x}\left\{(\alpha+1-\alpha) f(x)+\alpha \sum_{i=1}^{m} \lambda_{i}^{1} g_{i}(x)+(1-\alpha) \sum_{i=1}^{m} \lambda_{i}^{2} g_{i}(x)\right\}
\end{aligned}
$$

$$
=\inf _{x}\left\{\alpha\left(f(x)+\sum_{i=1}^{m} \lambda_{i}^{1} g_{i}(x)\right)+(1-\alpha)\left(f(x)+\sum_{i=1}^{m} \lambda_{i}^{2} g_{i}(x)\right)\right\}
$$

$$
\geq \inf _{x_{1}}\left\{\alpha\left(f\left(x_{1}\right)+\sum_{i=1}^{m} \lambda_{i}^{1} g_{i}\left(x_{1}\right)\right)\right\}+\inf _{x_{2}}\left\{(1-\alpha)\left(f\left(x_{2}\right)+\sum_{i=1}^{m} \lambda_{i}^{2} g_{i}\left(x_{2}\right)\right)\right\}
$$

## DUALITY

- Finally, we get

$$
q\left(\alpha \lambda^{1}+(1-\alpha) \lambda^{2}\right) \geq \alpha q\left(\lambda^{1}\right)+(1-\alpha) q\left(\lambda^{2}\right)>-\infty
$$

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 $f\left(x^{*}\right) \geq q(\lambda)$ for all dual feasible $\lambda$, we also have that the optimum of the dual problem satisfies the weak duality condition

$$
q\left(\lambda^{*}\right) \leq f\left(x^{*}\right)
$$

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


## GRADIENT OF DUAL FUNCTION AND ITS LINEAR APPROXIMATION

- Let $x^{*}(\lambda)=\arg \min _{x} \mathcal{L}(x, \lambda)$. For all $\lambda \geq 0$, the gradient

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

Proof:

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

- The first-order Taylor expansion of the dual function around $\lambda_{0}$ is

$$
q(\lambda) \approx f\left(x^{*}\left(\lambda_{0}\right)\right)+g\left(x^{*}\left(\lambda_{0}\right)\right)^{\prime} \lambda
$$

- Proof:

$$
\begin{aligned}
\overline{\bar{q}}(\lambda) \approx & q\left(\lambda_{0}\right)+\nabla_{\lambda} q\left(\lambda_{0}\right)^{\prime}\left(\lambda-\lambda_{0}\right)=q\left(\lambda_{0}\right)+g\left(x^{*}\left(\lambda_{0}\right)\right)^{\prime}\left(\lambda-\lambda_{0}\right) \\
= & \inf _{x} \mathcal{L}\left(x, \lambda_{0}\right)+g\left(x^{*}\left(\lambda_{0}\right)\right)^{\prime}\left(\lambda-\lambda_{0}\right)=f\left(x^{*}\left(\lambda_{0}\right)\right)+g\left(x^{*}\left(\lambda_{0}\right)\right)^{\prime} \lambda_{0} \\
& +g\left(x^{*}\left(\lambda_{0}\right)\right)^{\prime}\left(\lambda-\lambda_{0}\right)=f\left(x^{*}\left(\lambda_{0}\right)\right)+g\left(x^{*}\left(\lambda_{0}\right)\right)^{\prime} \lambda
\end{aligned}
$$

## STRONG DUALITY IN CONVEX PROGRAMMING

- Consider the convex programming problem

$$
\begin{array}{rl}
\min _{x} & f(x) \\
\mathrm{s.t.} & g_{i}(x) \leq 0, i \in I \quad I \cup E=\{1, \ldots, m\} \\
& A_{j} x=b_{j}, j \in E
\end{array}
$$

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 $\lambda^{*}$ satisfying the KKT conditions with $x^{*}$ solves the dual problem.

Proof:

- Assume $x^{*}, \lambda^{*}$ satisfy the KKT conditions and consider

$$
\mathcal{L}\left(x, \lambda^{*}\right)=f(x)+\sum_{i \in I} \lambda_{i}^{*} g_{i}(x)+\sum_{j \in E} \lambda_{j}^{*}\left(A_{j} x-b_{j}\right)
$$

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

$$
\mathcal{L}\left(x, \lambda^{*}\right) \geq \mathcal{L}\left(x^{*}, \lambda^{*}\right)+\overbrace{\nabla_{x} \mathcal{L}\left(x^{*}, \lambda^{*}\right)^{\prime}}^{=0 \text { because of KKT }}\left(x-x^{*}\right)=\mathcal{L}\left(x^{*}, \lambda^{*}\right)
$$

## DUALITY AND KKT CONDITIONS FOR CONVEX PROBLEMS

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

$$
\begin{aligned}
q\left(\lambda^{*}\right) & =\inf _{x} \mathcal{L}\left(x, \lambda^{*}\right)=\mathcal{L}\left(x^{*}, \lambda^{*}\right) \\
& =f\left(x^{*}\right)+\sum_{i \in I} \underbrace{\lambda_{i}^{*} g_{i}\left(x^{*}\right)}_{=0}+\sum_{j \in E} \lambda_{j}^{*}(\underbrace{A_{j} x^{*}-b_{j}}_{=0 \text { (feasplementarity) }})=f\left(x^{*}\right)
\end{aligned}
$$

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

$$
q(\lambda) \leq q\left(\lambda^{*}\right)
$$

- As $\lambda^{*}$ 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 $q\left(\lambda^{*}\right)=f\left(x^{*}\right)$
- In general, for $x_{\lambda} \in \arg \inf _{x} \mathcal{L}(x, \lambda)$ the duality gap is

$$
f\left(x_{\lambda}\right)-q(\lambda)=-\sum_{i \in I} \lambda_{i} g_{i}\left(x_{\lambda}\right)-\sum_{j \in E} \lambda_{j}\left(A_{j} x_{\lambda}-b_{j}\right)
$$

## WOLFE'S DUAL PROBLEM

- Wolfe's dual problem is defined as follows:

$$
\begin{aligned}
\max _{x, \lambda} & \mathcal{L}(x, \lambda) \\
\text { s.t. } & \nabla_{x} \mathcal{L}(x, \lambda)=0 \\
& \lambda_{i} \geq 0, \forall i \in I
\end{aligned}
$$



Philip S. Wolfe (1927-2016)

## THEOREM

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

## WOLFE'S DUAL PROBLEM

## Proof:

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

$$
\begin{aligned}
\mathcal{L}\left(x^{*}, \lambda^{*}\right) & =f\left(x^{*}\right) \geq f\left(x^{*}\right)+\sum_{i \in I} \overbrace{\lambda_{i} g_{i}\left(x^{*}\right)}^{\leq 0}+\sum_{j \in E} \lambda_{j}(\overbrace{A_{j} x^{*}-b_{j}}^{=0}) \\
& =\underbrace{\mathcal{L}\left(x^{*}, \lambda\right) \geq \mathcal{L}(x, \lambda)+\overbrace{\nabla_{x} \mathcal{L}(x, \lambda)^{\prime}}^{=0}\left(x^{*}-x\right)}_{\text {convexity of } \mathcal{L}(x, \lambda)} \\
& =\mathcal{L}(x, \lambda)
\end{aligned}
$$

- Hence $\mathcal{L}\left(x^{*}, \lambda^{*}\right)=f\left(x^{*}\right)$ is the maximum achievable value of $\mathcal{L}(x, \lambda)$ under the constraints $\nabla_{x} \mathcal{L}(x, \lambda)=0, \lambda_{i} \geq 0, \forall i \in I$.


## DUAL LINEAR PROGRAM

- Consider the linear program

$$
\begin{aligned}
\min _{x} & c^{\prime} x \\
\text { s.t. } & A x \leq b
\end{aligned}
$$

- The dual function is

$$
q(\lambda)=\inf _{x}\left\{c^{\prime} x+\lambda^{\prime}(A x-b)\right\}=\inf _{x}\left\{\left(c+A^{\prime} \lambda\right)^{\prime} x-b^{\prime} \lambda\right\}
$$

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

$$
\begin{aligned}
\max _{\lambda} & -b^{\prime} \lambda \\
\text { s.t. } & A^{\prime} \lambda=-c \\
& \lambda \geq 0
\end{aligned}
$$

$$
\begin{aligned}
\min _{\lambda} & b^{\prime} \lambda \\
\text { s.t. } & A^{\prime} \lambda=-c \\
& \lambda \geq 0
\end{aligned}
$$

- It is easy to prove that the dual of the dual LP is the original LP $\left(\min _{x, s} c^{\prime} x\right.$ s.t. $A x+s=b, s \geq 0$ ). The original $x=$ dual vector of constraint $-A^{\prime} \lambda+c=0$, and $s=$ dual vector of constraint $\lambda \geq 0$.


## THEOREM OF ALTERNATIVES

## THEOREM (THEOREM OF ALTERNATVES)

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 $A x \leq b$
2. there exists $y$ such that $y \geq 0, A^{\prime} y=0, b^{\prime} y<0$

## LEMMA [FARKAS' LEMMAJ

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

1. there exists $x$ such that $A x=b, x \geq 0$
2. there exists $y$ such that $A^{\prime} y \geq 0, b^{\prime} y<0$


Gyula Farkas (1847-1930)

## GEOMETRIC INTERPRETATION

Farkas' lemma has the following geometric interpretation.
Let $A_{i}$ be the $i$ th column of $A, i=1, \ldots, n, A=\left[A_{1} A_{2} \ldots A_{n}\right]$

- 1st alternative:

$$
b=\sum_{i=1}^{n} x_{i} A_{i}, x_{i} \geq 0, i=1, \ldots, n
$$


$b$ is in the convex cone generated by the columns of $A$

- 2nd alternative:

$$
\begin{aligned}
& y^{\prime} A_{i} \geq 0, i=1, \ldots, n \\
& y^{\prime} b<0
\end{aligned}
$$

vector $b$ cannot be in the convex cone generated by the
 columns of $A$

## DUAL LINEAR PROGRAM

## THEOREM (STRONG LP DUALITY)

1. If either the primal or the dual LP has a finite solution, so does the other and $c^{\prime} x^{*}=-b^{\prime} \lambda^{*}$ (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 $-A^{\prime}, c$

$$
-A^{\prime} \lambda=c, \lambda \geq 0 \text { infeasible } \quad \exists \exists d \in \mathbb{R}^{n}:-A d \geq 0, c^{\prime} d<0
$$

- Take a feasible $x_{0} \in \mathbb{R}^{n}$. Then $A\left(x_{0}+\sigma d\right)=A x_{0}+\sigma A d \leq b, \forall \sigma \geq 0$, and $c^{\prime}\left(x_{0}+\sigma d\right)=c^{\prime} x_{0}-\sigma\left|c^{\prime} d\right|$
- As $\sigma$ can be arbitrarily large, the infimum of the primal LP is $-\infty$.


## DUAL LP WITH NONNEGATIVE VARIABLES

- Consider the linear program
- The dual function is

$$
q(\lambda, \nu)=\inf _{x}\left\{c^{\prime} x+\lambda^{\prime}(b-A x)-\nu^{\prime} x\right\}=\inf _{x}\left\{\left(c-A^{\prime} \lambda-\nu\right)^{\prime} x+b^{\prime} \lambda\right\}=b^{\prime} \lambda
$$

for $c-A^{\prime} \lambda-\nu=0, \nu \geq 0$, or equivalently $A^{\prime} \lambda \leq c$

- The dual problem is therefore

$$
\begin{aligned}
\max _{\lambda} & b^{\prime} \lambda \\
\text { s.t. } & A^{\prime} \lambda \leq c \\
& \lambda \geq 0
\end{aligned}
$$

- At optimality $c^{\prime} x^{*}=b^{\prime} \lambda^{*}$


## DUAL LP AND LINEAR COMPLEMENTARITY PROBLEM (LCP]

- A linear complementarity problem (LCP) is a feasibility problem of the form
(Cottle, Pang, Stone, 2009)

$$
\begin{array}{r}
w=M z+q \\
w^{\prime} z=0 \\
w, z \geq 0
\end{array}
$$

- By introducing the vector $s$ of slack variables, $s=A x-b \geq 0$, the KKT conditions for the following LP are

$$
\begin{array}{rll}
\min _{x} & c^{\prime} x & c-A^{\prime} \lambda-\nu=0 \\
\mathrm{s.t.} & A x \geq b & A x-b-s=0 \\
& x \geq 0 & x, \lambda, \nu, s \geq 0 \\
x^{\prime} \nu=\lambda^{\prime} s=0
\end{array}
$$

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

$$
\underbrace{\left[\begin{array}{c}
\nu \\
s
\end{array}\right]}_{w}=\underbrace{\left[\begin{array}{cc}
0 & -A^{\prime} \\
A & 0
\end{array}\right]}_{M} \underbrace{\left[\begin{array}{c}
x \\
\lambda
\end{array}\right]}_{z}+\underbrace{\left[\begin{array}{c}
c \\
-b
\end{array}\right]}_{q}, \underbrace{\left[\begin{array}{c}
x \\
\lambda
\end{array}\right]}_{w}, \underbrace{\left[\begin{array}{c}
\nu \\
s
\end{array}\right]}_{z} \geq 0, \quad \underbrace{x^{\prime} \nu=\lambda^{\prime} s=0}_{z} \Leftrightarrow x^{\prime} \nu+\lambda^{\prime} s=w^{\prime} z=0
$$

## DUAL QUADRATIC PROGRAM

- Consider the quadratic program

$$
\begin{aligned}
\min _{x} & \frac{1}{2} x^{\prime} Q x+c^{\prime} x \\
\text { s.t. } & A x \leq b
\end{aligned}
$$

$$
Q=Q^{\prime} \succ 0
$$

- The dual function is $q(\lambda)=\inf _{x}\left\{\frac{1}{2} x^{\prime} Q x+c^{\prime} x+\lambda^{\prime}(A x-b)\right\}$
- Since $Q \succ 0$ the infimum is achieved when $0=\nabla_{x} \mathcal{L}\left(x_{\lambda}, \lambda\right)=Q x_{\lambda}+c+A^{\prime} \lambda$, i.e., for $x_{\lambda}=-Q^{-1}\left(c+A^{\prime} \lambda\right)$.
- By substitution, Lagrange's dual QP problem is therefore

$$
\max _{\lambda \geq 0}-\left(\frac{1}{2} \lambda^{\prime}\left(A Q^{-1} A^{\prime}\right) \lambda+\left(b+A Q^{-1} c\right)^{\prime} \lambda+\frac{1}{2} c^{\prime} Q^{-1} c\right)
$$

## DUAL QP AND LCP

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

$$
\begin{aligned}
\min _{\lambda} & \frac{1}{2} \lambda^{\prime}\left(A Q^{-1} A^{\prime}\right) \lambda+\left(b+A Q^{-1} c\right)^{\prime} \lambda \\
\text { s.t. } & \lambda \geq 0
\end{aligned}
$$

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

$$
\begin{aligned}
& H \lambda+d=s \\
& s^{\prime} \lambda=0 \\
& s, \lambda \geq 0
\end{aligned}
$$

where $H=A Q^{-1} A^{\prime}$ is the dual Hessian and $d=b+A Q^{-1} c$

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


## LCP AND DUAL QP

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

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

- Consider the QP problem

$$
\begin{array}{cl}
\min & \frac{1}{2} y^{\prime} M y+d^{\prime} y \\
\text { s.t. } & y \geq 0
\end{array}
$$

- The corresponding KKT optimality conditions are

$$
\begin{aligned}
M y+d-x & =0 \\
y & \geq 0 \\
x & \geq 0 \\
x_{i} y_{i} & =0, \quad i=1, \ldots, n
\end{aligned}
$$

that are exactly the given LCP

## WOLFE'S DUAL QP

- Consider now Wolfe's dual problem

$$
\begin{aligned}
\max _{x, \lambda} & \frac{1}{2} x^{\prime} Q x+c^{\prime} x+\lambda^{\prime}(A x-b) \\
\text { s.t. } & Q x+c+A^{\prime} \lambda=0, \lambda \geq 0
\end{aligned}
$$

- We can subtract $0=\left(Q x+c+A^{\prime} \lambda\right)^{\prime} x$ without changing the function and get the convex programming problem

$$
\begin{aligned}
\max _{x, \lambda} & -\frac{1}{2} x^{\prime} Q x-\lambda^{\prime} b \\
\text { s.t. } & Q x+c+A^{\prime} \lambda=0 \\
& \lambda \geq 0
\end{aligned}
$$

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


## DUAL OF QP REFORMULATION OF LASSO

- Consider again the LASSO problem

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

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

$$
\min _{y, z \geq 0} \frac{1}{2}\|A(y-z)-b\|_{2}^{2}+\gamma \mathbb{I}^{\prime}(y+z)
$$

where $\mathbb{I}^{\prime}=\left[\begin{array}{lll}1 \ldots\end{array}\right]$ (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)

$$
\begin{aligned}
\min _{v} & \frac{1}{2}\|v-b\|_{2}^{2}-b^{\prime} b \\
\text { s.t. } & \left\|A^{\prime} v\right\|_{\infty} \leq \gamma
\end{aligned}
$$

## DUAL OF QP REFORMULATION OF LASSO

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

$$
\begin{aligned}
\min _{v} & \frac{1}{2} v^{\prime} v-b^{\prime} v-\frac{1}{2} b^{\prime} b \\
\text { s.t. } & -\gamma \mathbb{I} \leq A^{\prime} v \leq \gamma \mathbb{I}
\end{aligned}
$$

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

$$
\min _{y, z \geq 0} \frac{1}{2}\left[\begin{array}{c}
y \\
z
\end{array}\right]\left[\begin{array}{c}
A^{\prime} \\
-A^{\prime}
\end{array}\right] I^{-1}[A-A]\left[\begin{array}{l}
y \\
z
\end{array}\right]+\left(\gamma\left[\begin{array}{l}
\mathbb{I} \\
\mathbb{I}
\end{array}\right]-\left[\begin{array}{c}
A^{\prime} \\
-A^{\prime}
\end{array}\right] I^{-1} b\right)^{\prime}\left[\begin{array}{l}
y \\
z
\end{array}\right]+\frac{1}{2} b^{\prime} b-\frac{1}{2} b^{\prime} b
$$

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


## SUPPORT VECTOR REGRESSION

- We have a training set $\left(x_{1}, y_{1}\right), \ldots,\left(x_{N}, y_{N}\right), x_{i} \in \mathbb{R}^{n}, y \in \mathbb{R}$ and want to fit a linear function

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

such that each $\left|y_{i}-f\left(x_{i}\right)\right| \leq \epsilon$

- Since such a function $f$ may not exist, we want to penalize $\left|y_{i}-f\left(x_{i}\right)\right|>\epsilon$

$$
\begin{aligned}
\min _{w, b, v, s} & \frac{1}{2}\|w\|_{2}^{2}+C \sum_{i=1}^{N}\left(v_{i}+s_{i}\right) \\
\text { s.t. } & y_{i}-w^{\prime} x_{i}-b \leq \epsilon+v_{i} \\
& y_{i}-w^{\prime} x_{i}-b \geq-\epsilon-s_{i} \\
& v_{i}, s_{i} \geq 0, \quad i=1, \ldots, N
\end{aligned}
$$




## SUPPORT VECTOR REGRESSION

- By setting $X=\left[\begin{array}{lll}x_{1} & \ldots & x_{N}\end{array}\right], Y=\left[\begin{array}{lll}y_{1} & \ldots & y_{N}\end{array}\right]^{\prime}$, we can rewrite in vector form

$$
\begin{aligned}
\min _{w, b, v, s} & \frac{1}{2} w^{\prime} w+C \mathbb{I}^{\prime}(v+s) \\
\text { s.t. } & Y-X^{\prime} w-b \mathbb{I} \leq \epsilon \mathbb{I}+v \\
& Y-X^{\prime} w-b \mathbb{I} \geq-\epsilon \mathbb{I}-s \\
& v, s \geq 0
\end{aligned}
$$

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

$$
\begin{aligned}
\mathcal{L}\left(\left[\begin{array}{l}
w \\
b \\
v \\
s
\end{array}\right],\left[\begin{array}{c}
\alpha \\
\beta \\
\gamma \\
\delta
\end{array}\right]\right)= & \frac{1}{2} w^{\prime} w+C \mathbb{I}^{\prime}(v+s)+\alpha^{\prime}\left(Y-X^{\prime} w-(b+\epsilon) \mathbb{I}-v\right) \\
& +\beta^{\prime}\left(-Y+X^{\prime} w+(b-\epsilon) \mathbb{I}-s\right)-\gamma^{\prime} v-\delta^{\prime} s
\end{aligned}
$$

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


## SUPPORT VECTOR REGRESSION

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

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

- By substituting the above expressions in the Lagrangian we get

$$
\begin{aligned}
q(\alpha, \beta, \gamma, \delta) & =\frac{1}{2} w^{\prime} w+\left(Y-X^{\prime} w\right)^{\prime}(\alpha-\beta)-\epsilon \mathbb{I}^{\prime}(\alpha+\beta) \\
& =-\frac{1}{2}(\alpha-\beta)^{\prime} X^{\prime} X(\alpha-\beta)+Y^{\prime}(\alpha-\beta)-\epsilon \mathbb{I}^{\prime}(\alpha+\beta)
\end{aligned}
$$

- The dual problem is therefore the following QP

$$
\begin{aligned}
\min _{\alpha, \beta} & \frac{1}{2}(\alpha-\beta)^{\prime} X^{\prime} X(\alpha-\beta)-Y^{\prime}(\alpha-\beta)+\epsilon \mathbb{I}^{\prime}(\alpha+\beta) \\
\text { s.t. } & 0 \leq \alpha \leq C \mathbb{I}, \quad 0 \leq \beta \leq C \mathbb{I}, \quad \mathbb{I}^{\prime}(\alpha-\beta)=0
\end{aligned}
$$

## SUPPORT VECTOR REGRESSION

- After solving the dual QP problem we can retrieve

$$
\begin{gathered}
w=X\left(\alpha^{*}-\beta^{*}\right)=\sum_{i=1}^{N}\left(\alpha_{i}^{*}-\beta_{i}^{*}\right) x_{i} \\
f(x)=w^{\prime} x+b=\left(\alpha^{*}-\beta^{*}\right)^{\prime} X^{\prime} x+b=\sum_{i=1}^{N}\left(\alpha_{i}^{*}-\beta_{i}^{*}\right) x_{i}^{\prime} x+b \\
f(x)=\sum_{i=1}^{N}\left(\alpha_{i}^{*}-\beta_{i}^{*}\right) x_{i}^{\prime} x+b
\end{gathered}
$$

(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 $\ell_{1}$-regularized problem

$$
\begin{aligned}
\min _{z} & \frac{1}{2} z^{\prime} X^{\prime} X z-Y^{\prime} z+\epsilon\|z\|_{1} \\
\text { s.t. } & \left|z_{i}\right| \leq C, \quad \sum_{i=1}^{N} z_{i}=0
\end{aligned}
$$

## SUPPORT VECTOR REGRESSION

- The scalar $b$ can be retrieved from the complementarity slackness conditions

$$
\begin{aligned}
0 & =\alpha_{i}\left(y_{i}-x_{i}^{\prime} w-(b+\epsilon)-v_{i}\right), \quad i=1, \ldots, N \\
0 & =\beta_{i}\left(-y_{i}+x_{i}^{\prime} w+(b-\epsilon)-s_{i}\right) \\
0 & =\gamma_{i} v_{i}=\left(C-\alpha_{i}\right) v_{i} \\
0 & =\delta_{i} s_{i}=\left(C-\beta_{i}\right) s_{i}
\end{aligned}
$$

- if any $\alpha_{i}^{*} \in(0, C)$ then $v_{i}^{*}=0 \Rightarrow b^{*}=y_{i}-x_{i}^{\prime} w^{*}-\epsilon$
- if any $\beta_{i}^{*} \in(0, C)$ then $s_{i}^{*}=0 \Rightarrow b^{*}=y_{i}-x_{i}^{\prime} w^{*}+\epsilon$


## SUPPORT VECTOR REGRESSION

- Otherwise, consider the case all $\alpha_{i}^{*}, \beta_{i}^{*} \in\{0, C\}$
- $\alpha_{i}^{*}, \beta_{i}^{*}$ cannot be positive at the same time, as they refer to bilateral constraints ( $y_{i}-w^{\prime} x_{i}-b$ cannot be both positive and negative)

$$
\begin{array}{rlll}
\alpha_{i}=0 & \Rightarrow & v_{i}=0 & \Rightarrow \\
\beta_{i}=0 & \Rightarrow & y_{i}-x_{i}^{\prime} w-(b+\epsilon) \leq 0 \\
\alpha_{i}=C & \Rightarrow & \Rightarrow & -y_{i}+x_{i}^{\prime} w+(b-\epsilon) \leq 0 \\
\beta_{i}=0 & \Rightarrow & s_{i}=0, & -y_{i}+x_{i}^{\prime} w+(b-\epsilon) \leq 0 \\
\beta_{i}=0 & \Rightarrow & v_{i}=0, & y_{i}-x_{i}^{\prime} w-(b+\epsilon) \leq 0
\end{array}
$$

- Let $\mathcal{I}=\left\{i: \alpha_{i}^{*}=0\right.$ or $\left.\beta_{i}^{*}=C\right\}$ and $\mathcal{J}=\left\{i: \alpha_{i}^{*}=C\right.$ or $\left.\beta_{i}^{*}=0\right\}$. Then

$$
\begin{aligned}
b^{*} & \geq y_{i}-x_{i}^{\prime} w^{*}-\epsilon, \quad \forall i \in \mathcal{I} \\
b^{*} & \leq y_{i}-x_{i}^{\prime} w^{*}+\epsilon, \quad \forall i \in \mathcal{J}
\end{aligned}
$$

- Therefore, any $b^{*} \in\left[\max _{i \in \mathcal{I}}\left\{y_{i}-x_{i}^{\prime} w^{*}-\epsilon\right\}, \min _{i \in \mathcal{J}}\left\{y_{i}-x_{i}^{\prime} w^{*}+\epsilon\right\}\right]$ is optimal


## SUPPORT VECTOR REGRESSION

- Kernel trick: if we generalize $x_{i}$ to an arbitrary nonlinear basis $\phi\left(x_{i}\right)$ we get

$$
f(x)=\sum_{i=1}^{N}\left(\alpha_{i}^{*}-\beta_{i}^{*}\right) k\left(x_{i}, x\right)+b
$$

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

- Example: $x \in \mathbb{R}^{2}, \phi(x)=\left[\begin{array}{lll}x_{1}^{2} & \sqrt{2} x_{1} x_{2} & x_{2}^{2}\end{array}\right]^{\prime}, k(x, y)=\left(x^{\prime} y\right)^{2}$
- The $(i, j)$ th term $x_{i}^{\prime} x_{j}$ of the dual Hessian gets replaced by $k\left(x_{i}, x_{j}\right)$
- $b$ depends on $x_{i}^{\prime} w=x_{i}^{\prime} X(\alpha-\beta)$ that gets replaced by $k\left(x_{i}, X\right)\left(\alpha^{*}-\beta^{*}\right)$
- Therefore $\phi, w$ 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 $\phi$ is infinite dimensional


## EXAMPLE OF SUPPORT VECTOR REGRESSION

- Generate $N=100$ random samples of the course-logo function

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

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


