

## Higher derivatives & multivariate extrema

Lemma Let  $f: \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $x \in \text{int Dom}(f)$ .

Assume  $x$  loc. extremum of  $f$ . Then

$$\forall w \in \mathbb{R}^n: \frac{\partial f}{\partial w}(x) \text{ exists} \Rightarrow \frac{\partial f}{\partial w}(x) \geq 0$$

$$\forall i=1..n: \frac{\partial f}{\partial x_i}(x) \text{ exists} \Rightarrow \frac{\partial f}{\partial x_i}(x) = 0$$

In particular, if  $f$  diff. at  $x$ , then

$$Df(x) = \nabla f(x) = 0$$

PF  $x$  loc. min  $\Rightarrow \exists \delta > 0 \forall z \in B(x, \delta): f(z) \geq f(x)$   
 So if  $v \in \mathbb{R}^n$ , then  
 $f(x+tv) \geq f(x)$

for  $h > 0$  small ( $h \|v\| < \delta$ )

So  $\frac{\partial f}{\partial n}(x) = \lim_{h \rightarrow 0^+} \frac{f(x+tv) - f(x)}{h} \geq 0.$

If  $\frac{\partial f}{\partial x_i} \neq 0$ , then

$\frac{\partial f}{\partial x_i}(x) = \frac{\partial f}{\partial e_i}(x) = \underbrace{\frac{\partial f}{\partial (-e_i)}(x)}_{\leq 0} \geq 0 \quad \square$

Ex  $f(x,y) = x^2 + y^2$   
 $\nabla f(x,y) = (2x, 2y) \stackrel{(x,y)=0}{=} (0,0)$

Ex  $f(x,y) = \sqrt{x^2 + y^2}$   
 $\frac{\partial f}{\partial x}(0,0) = \|v\| \geq 0.$

Further analysis requires higher derivatives

Def We say  $f$  is twice differentiable at  $x$  if  $Df$  is differentiable at  $x$ .  
 We write  $D^2f(x) := D(Df)(x)$

Def The  $k$ -th is defined  
 Given  $x, \dots$   
 $\frac{\partial^2 f}{\partial x_i \partial x_j}$   
 This the  $k$ -th wrt. variables

Ex:  $f(x,y) = \dots$   
 $\begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix}$

$\exists \delta > 0 \forall \epsilon \in B(x, \delta), f(z) \geq f(x)$   
 , then  
 $f(x) \geq f(x)$   
 $(\|h\| < \delta)$   
 $\lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} = 0$   
 , then  
 $\frac{\partial f}{\partial x_i}(x) = \frac{\partial f}{\partial x_i}(x) = 0$   
 $\Rightarrow \square$

Ex  $f(x,y) = x^2 + y^2$   
 $\nabla f(x,y) = (2x, 2y)$   $(x,y) = (0,0)$   
 $\frac{\partial f}{\partial x}(0,0) = \| \nabla f \| \geq 0$

Further analysis requires higher derivatives

Def We say  $f$  is twice differentiable at  $x$  if  $Df$  is differentiable at  $x$ .  
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Def The  $k$ -th-partial derivative of  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  is defined recursively as:

Given  $i_1, \dots, i_k \in \{1, \dots, n\}$ ,

$$\frac{\partial^k f}{\partial x_{i_1} \dots \partial x_{i_k}} = \frac{\partial}{\partial x_{i_1}} \left( \frac{\partial^{k-1} f}{\partial x_{i_2} \dots \partial x_{i_k}} \right)$$

This is the  $k$ -th partial derivative of  $f$  w.r.t. variables  $x_{i_1}, \dots, x_{i_k}$ .

Ex:  $f(x,y) = x^4 + y^3 x$ ,  $\frac{\partial f}{\partial x} = 4x^3 + y^3$ ,  $\frac{\partial f}{\partial y} = 3y^2 x$

$$\begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix} = \begin{pmatrix} 12x^2 & 3y^2 \\ 3y^2 & 6yx \end{pmatrix}$$

Thm (Clairaut's thm, proved by KH Schwarz 1873)

Let  $f: \mathbb{R}^2 \rightarrow \mathbb{R}$  and  $x \in \text{int Dom}(f)$  be s.t.  
for some  $\delta > 0$ :

- $f$  cont. on  $B(x, \delta)$
- $\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}$  exist and are cont. on  $B(x, \delta)$
- $\frac{\partial^2 f}{\partial x_1 \partial x_2}, \frac{\partial^2 f}{\partial x_2 \partial x_1}$  exist on  $B(x, \delta)$

Then  $\frac{\partial^2 f}{\partial x_1 \partial x_2}, \frac{\partial^2 f}{\partial x_2 \partial x_1}$  cont at  $x \Rightarrow \frac{\partial^2 f}{\partial x_1 \partial x_2}(x) = \frac{\partial^2 f}{\partial x_2 \partial x_1}(x)$

Pf  $h(t,s) = f(x+te_1+se_2) - f(x+te_1) - f(x+se_2) + f(x)$

MVT:  $(t,s \geq 0)$ :  $h(t,0) = 0$

$\exists s' \in (0,s)$ :  $h(t,s) = \left( \frac{\partial f}{\partial x_2}(x+te_1+s'e_2) - \frac{\partial f}{\partial x_2}(x+s'e_2) \right) s$

$\exists t' \in (0,t)$ :  $\stackrel{\text{MVT}}{=} \frac{\partial^2 f}{\partial x_1 \partial x_2}(x+t'e_1+s'e_2) st$

By symmetry:

$\exists s'' \in (0,s) \exists t'' \in (0,t)$ :  $h(t,s) = \frac{\partial^2 f}{\partial x_2 \partial x_1}(x+t''e_1+s''e_2) st$

As  $t \rightarrow 0^+$ ,  $s \rightarrow 0^+$ , both derivations converge to their value at  $x$ .

The matrix

$$\text{Hess}(f)(x) := \left\{ \frac{\partial^2 f}{\partial x_i \partial x_j} \right\}_{i,j=1}^n$$

is called the Hessian of  $f$  at  $x$

Lemma Suppose  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  is twice continuously differentiable on an open neighborhood of  $x$

Then  $x$  is local extremum implies

$$\forall v \in \mathbb{R}^n, \quad v^T \text{Hess}(f)(x) v \geq 0,$$

i.e.,  $\text{Hess}(f)(x)$  is positive semidefinite.

Pf  $h(t) = f(x+tv) - f(x)$   
 $\frac{\nabla f(x)=0}{=} f(x+tv) - f(x) - t \nabla f(x)$

$$\lim_{t \rightarrow 0} \frac{h(t)}{t^2} = \lim_{t \rightarrow 0} \frac{v^T \nabla f(x+tv) - v^T \nabla f(x)}{t}$$

$$= \lim_{t \rightarrow 0} \sum_{i=1}^n v_i \frac{\frac{\partial f}{\partial x_i}(x+tv) - \frac{\partial f}{\partial x_i}(x)}{t}$$

$$= \sum_{i,j=1}^n v_i v_j \lim_{t \rightarrow 0} \frac{\partial^2 f}{\partial x_j \partial x_i}(x+tv)$$

$$= v^T \text{Hess}(f)(x) v \stackrel{\geq 0}{\leftarrow} \quad \square$$

$x$  loc. min  $\Rightarrow h(t) \geq 0$  for  $t$  small  $\Rightarrow \square$

Lemma Let  $f: \mathbb{R}^n$   
be s.d.  $\exists \delta > 0$ .  $f$   
ad.  $\nabla f(x) = 0$

and  $\forall z \in B(x, \delta)$ ;

Then  $x$  is local min

Pf. Use  $h$  above:  $\forall t$   
(Assuming  $t > 0$ )  $\exists t$

$\left. \begin{matrix} \dots \\ \dots \\ \dots \end{matrix} \right\}_{i,j=1}^n$   
 $f$  at  $x$   
 $\mathbb{R}$  is twice continuously  
 neighborhood of  $x$   
 implies  
 $\mathbf{A} \succeq 0$ ,  
 is semidefinite.

Pf  $h(t) = f(x+tv) - f(x)$   
 $\stackrel{v \neq 0}{=} f(x+tv) - f(x) - t v \cdot \nabla f(x)$   
 $\lim_{t \rightarrow 0} \frac{h(t)}{t^2} = \lim_{t \rightarrow 0} \frac{v \cdot \nabla f(x+tv) - v \cdot \nabla f(x)}{t}$   
 $= \lim_{t \rightarrow 0} \sum_{i=1}^n v_i \frac{\frac{\partial f}{\partial x_i}(x+tv) - \frac{\partial f}{\partial x_i}(x)}{t}$   
 $= \sum_{i,j=1}^n v_i v_j \lim_{t \rightarrow 0} \frac{\partial^2 f}{\partial x_j \partial x_i}(x+tv)$   
 $= v \cdot \text{Hess}(f)(x) v \succeq 0$   
 $x \text{ loc. min} \Rightarrow h(t) \geq 0 \text{ for } t \text{ small} \Rightarrow \square$

Lemma Let  $f: \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $x \in \text{Int Dom}(f)$   
 be s.t.  $\exists \delta > 0$ :  $f$  twice cont. d. diff on  $B(x, \delta)$

and  $\nabla f(x) = 0$

and  $\forall z \in B(x, \delta)$ ;  $\text{Hess}(f)(z)$  is pos. semi-def.

Then  $x$  is local minimum of  $f$ .

Pf; Use  $h$  above; Taylor's theorem:

(Assuming  $t > 0$ )  $\exists t' \in (0, t)$ ;  $h(t) = \frac{1}{2} t^2 h''(t')$   
 $= \frac{1}{2} t^2 v \cdot \text{Hess}(x+tv) v$   
 $\geq 0 \quad \square$

Ex  $f(x, y) = x^2 + y^2$

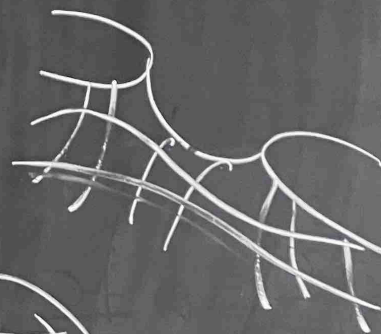
$$\text{Hess}(f)(0,0) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$



Ex  $f(x, y) = x^2 + y^2 - 8xy$

$$\text{Hess}(f)(0,0) = \begin{pmatrix} 2 & -8 \\ -8 & 2 \end{pmatrix}$$

Not pos. semidef.



Ex  $f(x, y) = -(x^2 + y^2)$

