

Background

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Computational Mathematics for Learning and Data Analysis
Master in Computer Science – University of Pisa

Outline

Motivation

Sets and sequences

Vector spaces and topology

Functions

Derivatives, Gradients and Hessians

A walkthrough on simple functions

Wrap up & References

- ▶ X any set, $f : X \rightarrow \mathbb{R}$ any function: optimization problem

$$(P) \quad f_* = \min\{f(x) : x \in X\}$$

- ▶ X feasible region, f objective function, $\nu(P) = f_*$ optimal value
- ▶ “min” w.l.o.g.: $\min\{f(x) : x \in X\} = -\max\{-f(x) : x \in X\}$,
(but $\min\{f(x)\} \neq \max\{f(x)\}$, often rather different problems)
- ▶ $x \in X$ feasible solution; often $X \subset F$, $x \in F \setminus X$ unfeasible solution
- ▶ $f_* \leq f(x) \forall x \in X$, $\forall v > f_* \exists x \in X$ s.t. $f(x) < v$
- ▶ We want any optimal solution: $x_* \in X$ such that $f(x_*) = f_*$
- ▶ Impossible (X inaccessible cardinal, f non computable function, ...)
- ▶ Even with very simple f / X , x_* may just not exist

- ▶ “Bad case” I: $X = \emptyset$ (“empty”)

1. $\min\{x : x \in \mathbb{R} \wedge x \leq -1 \wedge x \geq 1\}$

There just is **no solution** (which may be important to know)

- ▶ “Bad case” II: $\forall M \exists x_M \in X \text{ s.t. } f(x_M) \leq M$ (“unbounded [below]”)

2. $\min\{x : x \in \mathbb{R} \wedge x \leq 0\}$

There are **solutions as good as you like** (which may be important to know)

- ▶ **Not really bad cases**, just things that can happen
- ▶ **Solving an optimization problem** actually three different things:
 - ▶ Finding x_* and **proving it is optimal** (how??)
 - ▶ **Proving $X = \emptyset$** (how??)
 - ▶ **Constructively proving f unbounded below on X** (how??)

- Things can be worse: not empty, not unbounded, but no x_* either:

3. $\min\{x : x \in \mathbb{R} \wedge x > 0\}$ (“bad” X)

4. $\min\{1/x : x \in \mathbb{R} \wedge x > 0\}$ (“bad” f and X)

5. $\min\left\{f(x) = \begin{cases} x & \text{if } x > 0 \\ 1 & \text{if } x = 0 \end{cases} : x \in [0, 1]\right\}$ (“bad” f)

- Assumptions needed on f and X to ensure “things work”

- Something of an hair-splitting exercise: typically

“ $x \in \mathbb{R}$ ” actually mean “ $x \in \mathbb{Q}$ ” with up to k digits precision

- Many (but not all) problems go away if goal is “just” to find approximately optimal \bar{x} and prove it (how??)

$$f(\bar{x}) - f_* \leq \varepsilon \text{ (absolute) or } (f(\bar{x}) - f_*) / |f_*| \leq \varepsilon \text{ (relative) error}$$

and some ε is required anyway in most cases

- ▶ Already “ $f : X \rightarrow \mathbb{R}$ ” a rather strong assumption:
can “condense the value of x with a single number”

- ▶ Often you need more than one, say

$$(P) \quad \min \{ [f_1(x), f_2(x)] : x \in X \}$$

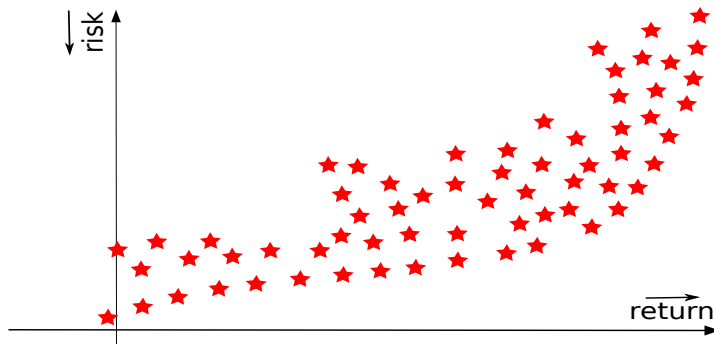
with f_1, f_2 contrasting and/or with incomparable units (apples vs. oranges)

- ▶ Textbook example: portfolio selection problem

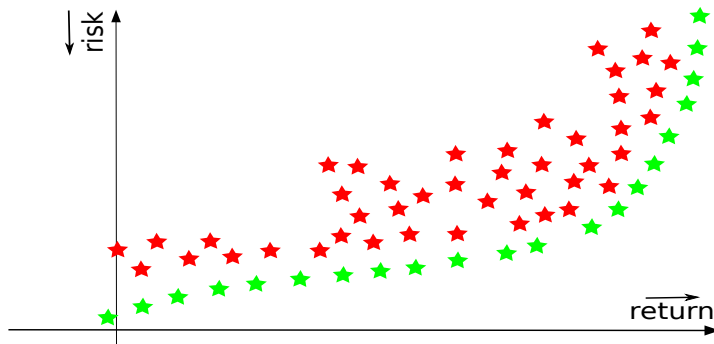
- ▶ X = set of financial instruments portfolios I can buy
- ▶ $f_1(x)$ = expected return of portfolio x (€)
- ▶ $f_2(x)$ = risk of portfolio x not achieving the expected return (% , CVAR, ...)

- ▶ Countless many others:

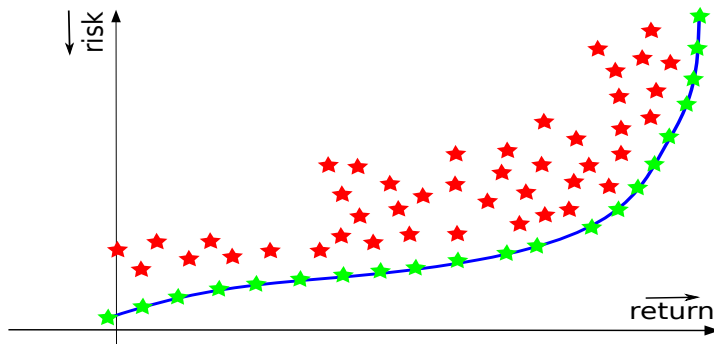
- ▶ car cost vs. flashiness vs. km/l vs. # seats vs. trunk space ...
- ▶ # separated points vs. margin in SVM
- ▶ ...



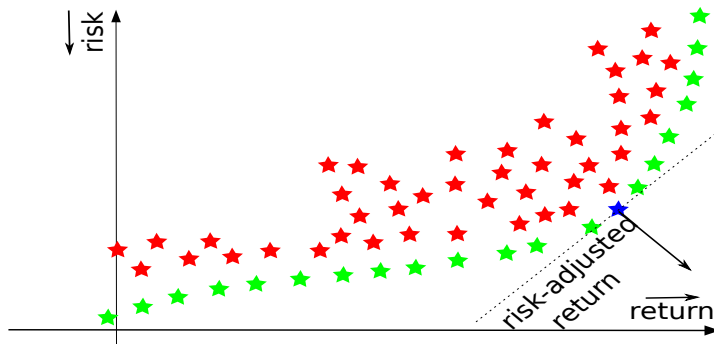
- No “best” solution, only



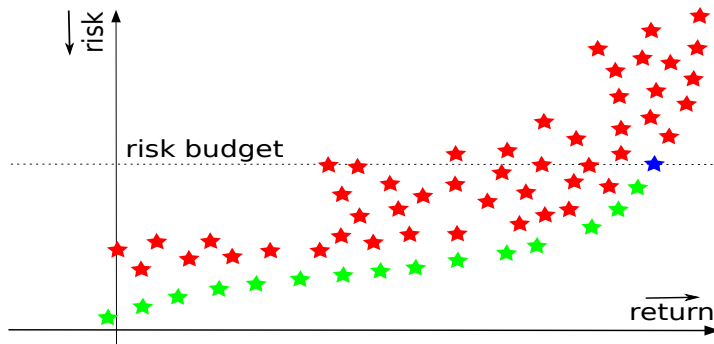
- No “best” solution, only non-dominated ones on the



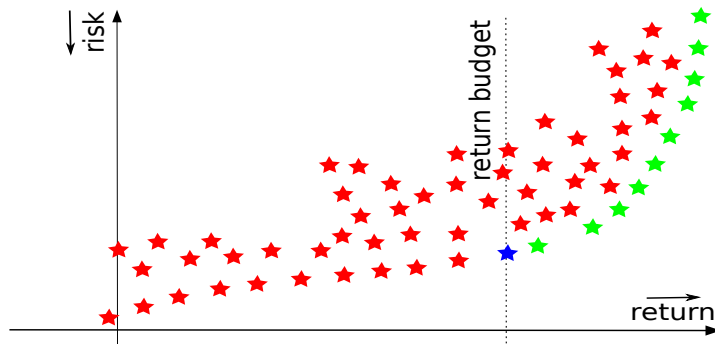
- ▶ No “best” solution, only non-dominated ones on the Pareto frontier
- ▶ Two practical solutions:



- ▶ No “best” solution, only non-dominated ones on the Pareto frontier
- ▶ Two practical solutions: maximize risk-adjusted return,
a.k.a. scalarization $\min \{ f_1(x) + \alpha f_2(x) : x \in X \}$ (which α ??)



- ▶ No “best” solution, only **non-dominated ones** on the **Pareto frontier**
- ▶ Two practical solutions: maximize return with **budget on maximum risk**,
a.k.a. **budgeting** $\min \{ f_1(x) : f_2(x) \leq \beta_2, x \in X \}$ (**which β_2 ??**)



- ▶ No “best” solution, only **non-dominated ones** on the **Pareto frontier**
- ▶ Two practical solutions: minimize risk with **budget on minimum return**, a.k.a. **budgeting** $\min \{ f_2(x) : f_1(x) \leq \beta_1, x \in X \}$ (which $\beta_1??$)
- ▶ All **a bit fuzzy**, but it's the nature of the beast
- ▶ We always **assume this done** if necessary at **modelling stage** (cf. SVM)

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► Since we minimize/maximize stuff, infima/suprema are important

► “ $f : X \rightarrow \mathbb{R}$ ” precisely because \mathbb{R} totally ordered:

$$\forall x, y \in X, \text{ either } f(x) \leq f(y) \text{ or } f(y) \leq f(x)$$

(\mathbb{R}^k is not such for $k > 1$, cf. multi-objective)

$$\text{► } S \subseteq \mathbb{R}, \underline{s} = \inf S \iff \underline{s} \leq s \ \forall s \in S \ \wedge \ \forall t > \underline{s} \exists s \in S \text{ s.t. } s \leq t$$

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► Issue: $\inf S / \sup S$ may not exist in \mathbb{R}

► Set of extended reals: $\overline{\mathbb{R}} = \{-\infty\} \cup \mathbb{R} \cup \{+\infty\}$ (usually just \mathbb{R})

► For all $S \subseteq \mathbb{R}, \sup / \inf S \in \overline{\mathbb{R}}$

► $\inf S = -\infty$ just a convenient notation for “there is no (finite) inf”

► $\inf \emptyset = \infty, \sup \emptyset = -\infty$

► Should write “ $\inf\{f(x) \dots\}$ ”, but we want optimal solutions (if any)

- ▶ We often do **iterations**, hence produce **sequences** v_1, v_2, \dots
(think **sequence of iterates** $\{x_i\} \subset X$ and $v_i = f(x_i)$)
- ▶ Typically we **can't get f_* in finite time** ($\exists i \ v_i = f_*$), but we can
“get as close as we want”: **there in the limit**
- ▶ $\lim_{i \rightarrow \infty} v_i = v \iff \forall \varepsilon > 0 \exists h \text{ s.t. } |v_i - v| \leq \varepsilon \ \forall i \geq h$
- ▶ A sequence **may not have limit**: are we “not converging”?
- ▶ **Any monotone sequence has a limit** (monotone algorithms are good)
- ▶ The **obvious** way to **make $\{v_i\}$ monotone**: **keep aside the best**
 $v_i^* = \min\{v_h : h \leq i\}$ (best value at iteration i)
- ▶ $v_1^* \geq v_2^* \geq v_3^* \geq \dots \implies v_\infty^* = \lim_{i \rightarrow \infty} v_i^* \geq f_*$ (asymptotic estimate)
- ▶ $\lim_{i \rightarrow \infty} v_i^* = v_\infty^* = f_* \implies \{v_i\}$ **minimizing sequence** (of values)

- ▶ Extract monotone sequences from $\{v_i\}$ “the hard way”:

$$\underline{v}_i = \inf\{v_h : h \geq i\} \quad , \quad \bar{v}_i = \sup\{v_h : h \geq i\}$$

- ▶ $\underline{v}_1 \leq \underline{v}_2 \leq \underline{v}_3 \leq \dots, \bar{v}_1 \geq \bar{v}_2 \geq \bar{v}_3 \geq \dots \implies$ they still have a limit

- ▶ $\liminf_{i \rightarrow \infty} v_i := \lim_{i \rightarrow \infty} \underline{v}_i = \sup_i \underline{v}_i$

- ▶ $\limsup_{i \rightarrow \infty} v_i := \lim_{i \rightarrow \infty} \bar{v}_i = \inf_i \bar{v}_i$

- ▶ $\bar{v}_i \geq \underline{v}_i \implies \limsup_{i \rightarrow \infty} v_i \geq \liminf_{i \rightarrow \infty} v_i$

- ▶ $\lim_{i \rightarrow \infty} v_i = v \iff \limsup_{i \rightarrow \infty} v_i = v = \liminf_{i \rightarrow \infty} v_i$

- ▶ $\liminf_{i \rightarrow \infty} v_i = f_* \implies \{v_i\}$ minimizing sequence (of values)

- ▶ A stronger definition: $\liminf_{i \rightarrow \infty} v_i = f_* \implies \lim_{i \rightarrow \infty} v_i^* = f_*$

Exercise: Prove the result

Exercise: Prove that \Leftarrow does not hold. Discuss the significance if v_i is the sequence of values of iterates of a minimization algorithm

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- ▶ Single numbers are not enough (except for objective function values)
- ▶ Euclidean space $\mathbb{R}^n := \{ [x_1, x_2, \dots, x_n] : x_i \in \mathbb{R} \quad i = 1, \dots, n \}$
- ▶ $\mathbb{R}^n = \mathbb{R} \times \mathbb{R} \times \dots \mathbb{R}$, Cartesian product of \mathbb{R} n times
- ▶ $x \in \mathbb{R}^n$ usually considered “column vector” $\in \mathbb{R}^{n \times 1}$ (a “ T ” needed)
- ▶ Closed under sum and scalar multiplication

$$x + y := [x_1 + y_1, \dots, x_n + y_n] \quad , \quad \alpha x := [\alpha x_1, \dots, \alpha x_n]$$

- ▶ **Finite** vector space: each $x \in \mathbb{R}^n$ can be obtained from a **finite basis** (canonical base is u_i having 1 in position i and 0 elsewhere)
- ▶ Not all vector spaces are finite
- ▶ **Not** a totally ordered set
- ▶ Concept of “limit” requires **topology**: “what is close to what”

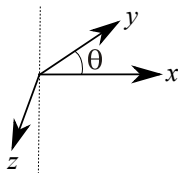
- scalar product of $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$:

$$\langle x, y \rangle := y^T x = \sum_{i=1}^n x_i y_i = x_1 y_1 + \cdots + x_n y_n$$

(will often succumb to temptation to write it just “ yx ” or “ $y \cdot x$ ”)

- Properties \equiv definition of scalar product:

1. $\langle x, y \rangle = \langle y, x \rangle \quad \forall x, y \in \mathbb{R}^n$ (symmetry)
2. $\langle x, x \rangle \geq 0 \quad \forall x \in \mathbb{R}^n, \quad \langle x, x \rangle = 0 \iff x = 0$
3. $\langle \alpha x, y \rangle = \alpha \langle x, y \rangle \quad \forall x \in \mathbb{R}^n, \alpha \in \mathbb{R}$
4. $\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle \quad \forall x, y, z \in \mathbb{R}^n$



- Geometric interpretation: $\langle x, y \rangle = \|x\| \cdot \|y\| \cdot \cos(\theta)$

1. $x \perp y \iff \langle x, y \rangle = 0$
2. $\langle x, y \rangle > 0 \equiv$ “ x and y point in the same direction”

- More general: $\langle x, y \rangle_M := y^T M x$ with $M \succ 0$ ($x \mapsto M^{-1/2} x$)
- Other spaces (matrices, integrable functions, random variables, ...)
- Not just theoretical stuff (recall SVM)

- ▶ Euclidean norm: $\|x\| := \sqrt{x_1^2 + \cdots + x_n^2} = \sqrt{\langle x, x \rangle}$ (induced by $\langle \cdot, \cdot \rangle$)
- ▶ Properties \equiv definition of norm:
 1. $\|x\| \geq 0 \quad \forall x \in \mathbb{R}^n, \|x\| = 0 \iff x = 0$
 2. $\|\alpha x\| = |\alpha| \|x\| \quad \forall x \in \mathbb{R}^n, \alpha \in \mathbb{R}$
 3. $\|x + y\| \leq \|x\| + \|y\| \quad \forall x, y \in \mathbb{R}^n$ (triangle inequality)
- ▶ $|\langle x, y \rangle|^2 \leq \|x\| \|y\| \quad \forall x, y \in \mathbb{R}^n$ (Cauchy-Schwarz inequality)
- ▶ $\|x + y\|^2 = \|x\|^2 + \|y\|^2 + 2\langle x, y \rangle$
- ▶ $2\|x\|^2 + 2\|y\|^2 = \|x + y\|^2 + \|x - y\|^2$ (Parallelogram Law)

- ▶ Just the “most natural” among many:

- ▶ $\|x\|_1 := \sum_{i=1}^n |x_i|$
- ▶ $\|x\|_\infty := \max\{|x_i| : i = 1, \dots, n\}$
- ▶ $\|x\|_0 := |\{i : |x_i| > 0\}|$
- ▶ Other ones (e.g. for matrices ...)

- ▶ Many (but **not all**) derive from p -norm:

$$\|x\|_p := \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}$$

- ▶ Convex for $p \geq 1$, **nonconvex** for $p < 1$

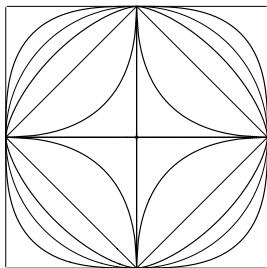
- ▶ $\|\cdot\|_1$ “best convex approximation” of $\|\cdot\|_0$ (compressed sensing, ...)

- ▶ $\langle x, y \rangle^2 \leq \|x\|_p \|y\|_q \quad 1/p + 1/q = 1$ (Hölder's inequality)

- ▶ Hereafter “ $\|\cdot\| = \|\cdot\|_2$ ”, but **all norms are topologically equivalent**:

$$\exists 0 < \alpha < \beta \text{ s.t. } \alpha \|x\|' \leq \|x\| \leq \beta \|x\|' \quad \forall x$$

(because \mathbb{R}^n is a **finite** vector space)



- Euclidean distance between x and y

$$d(x, y) := \|x - y\| = \sqrt{(x_1 - y_1)^2 + \cdots + (x_n - y_n)^2}$$

(“norm of x when y is the origin”)

- Properties \equiv definition of distance:

1. $d(x, y) \geq 0 \quad \forall x, y \in \mathbb{R}^n$, $d(x, y) = 0 \iff x = y$
2. $d(\alpha x, 0) = |\alpha|d(x, 0) \quad \forall x \in \mathbb{R}^n, \alpha \in \mathbb{R}$
3. $d(x, y) \leq d(x, z) + d(z, y) \quad \forall x, y, z \in \mathbb{R}^n$ (triangle inequality)

- Ball, center $x \in \mathbb{R}^n$, radius $r > 0$: $\mathcal{B}(x, r) := \{y \in \mathbb{R}^n : \|y - x\| \leq r\}$
(the points “close” to x in the chosen norm)

- The distance/norm defines the topology of the vector space, but doesn't really matter: all is “ \exists ball”, “ \forall small ball”, and all norms are equivalent

- Finally, **limit** of sequence $\{x_i\} \subset \mathbb{R}^n$:

$$\lim_{i \rightarrow \infty} x_i = x \equiv \{x_i\} \rightarrow x$$

$$\iff \forall \varepsilon > 0 \exists h \text{ s.t. } d(x_i, x) \leq \varepsilon \forall i \geq h$$

$$\iff \forall \varepsilon > 0 \exists h \text{ s.t. } x_i \in \mathcal{B}(x, \varepsilon) \forall i \geq h$$

$$\iff \lim_{i \rightarrow \infty} d(x_i, x) = 0$$

- Points of $\{x_i\}$ **eventually all** come arbitrarily close to x
- **No obvious** \liminf / \limsup (\mathbb{R}^n is **not** totally ordered)

Exercise: Would $\liminf_{i \rightarrow \infty} d(x_i, x) = 0$ and/or $\limsup_{i \rightarrow \infty} d(x_i, x) = 0$ make sense? Which?

► We want to solve $(P) \ f_* = \min\{f(x) : x \in X\}$ with $X \subseteq \mathbb{R}^n$

► Construct a **minimizing sequence**: $\{x_i\}$ s.t. $\{f(x_i)\} \rightarrow f_*$

► We know it is **not** enough for having “solved” (P) , recall

$$3. \min\{x : x \in \mathbb{R} \wedge x > 0\} \quad \{x_i = 1/i\} \quad \{f(x_i)\} \rightarrow 0$$

$$4. \min\{1/x : x \in \mathbb{R} \wedge x > 0\} \quad \{x_i = i\} \quad \{f(x_i)\} \rightarrow 0$$

► Minimizing sequences, but **no optimal solution**

► Want **conditions** that ensure

$$\{f(x_i)\} \rightarrow f_* \implies \{x_i\} \rightarrow x_* \in X \text{ optimal solution}$$

► **Two** different problems

► There are more (remember the other cases)

- ▶ Given $S \subseteq \mathbb{R}^n$, interior/boundary points of S :
 - ▶ $x \in \text{int}(S) \equiv \text{interior of } S := \exists r > 0 \text{ s.t. } \mathcal{B}(x, r) \subseteq S$
 - ▶ $x \in \partial(S) \equiv \text{boundary of } S := \forall r > 0 \exists y, z \in \mathcal{B}(x, r) \text{ s.t. } y \in S \wedge z \notin S$
- note: $x \in \text{int}(S) \implies x \in S$, but $x \in \partial S \not\implies x \in S$
- ▶ S open if $S = \text{int}(S)$: “I have no points on the boundary”
- ▶ $\text{cl}(S) \equiv \text{closure of } S := \text{int}(S) \cup \partial S$: “me and my boundary”
- ▶ $S \subseteq \mathbb{R}^n$ closed if $S = \text{cl}(S) \equiv \mathbb{R}^n \setminus S$ (the complement) open:
“all points on my boundary are mine”
- ▶ $\text{int}(S) \neq \emptyset \implies S$ full dimensional
- ▶ Sometimes, relative interior useful

- ▶ S closed $\iff \forall S \supset \{x_i\} \rightarrow x \implies x \in S$
 \equiv all limit points of sequences in S are in S
- ▶ Algebra of open/closed sets:
 - ▶ $\{S_i\}$ (infinitely many) open sets $\implies \bigcup_i S_i$ open
 - ▶ S_1 and S_2 are open $\implies S_1 \cap S_2$ is open
 - ▶ $\{S_i\}$ (infinitely many) closed sets $\implies \bigcap_i S_i$ closed
 - ▶ S_1 and S_2 are closed $\implies S_1 \cup S_2$ is closed

Exercise: prove \mathbb{R}^n and \emptyset are **both** closed and open (hint: what boundary?)

Exercise: exhibit a set that is **neither** open nor closed

Exercise: $\{S_i\}$ (infinitely many) open sets $\implies \bigcap_i S_i$ open: true?

Exercise: $\{S_i\}$ (infinitely many) closed sets $\implies \bigcup_i S_i$ closed: true?

- ▶ $S \subseteq \mathbb{R}^n$ is **bounded** $:= \exists r > 0$ s.t. $S \subseteq \mathcal{B}(0, r)$
- ▶ Closed + bounded = **compact**
- ▶ Sequences $\{x_i\} \subset \mathbb{R}^n$ and $\{n_i\} \subseteq \mathbb{N}$, **subsequence** $\{x_{n_i}\} \subseteq \{x_i\}$
- ▶ Sequence $\{x_i\}$: x is an **accumulation point** if $\exists \{x_{n_i}\} \rightarrow x \equiv \liminf_{i \rightarrow \infty} d(x_i, x) = 0$
- ▶ Bolzano-Weierstrass Theorem: if $S \subseteq \mathbb{R}^n$ is **compact**, then **any** sequence $\{x_i\} \subseteq S$ has an **accumulation point** $x \in S$
- ▶ X compact \implies any minimizing sequence has one accumulation point (candidate to be an optimal solution)

- ▶ Somewhat surprising: $|\{x_i\}| = \aleph_0 \ll \aleph_1 = |\mathbb{R}^n|$
- ▶ In hindsight, not: it is very hard to keep all points far from each other
- ▶ Unitary hypercube $[0, 1]^n$, divide each side equally: $(h + 1)^n$ points give a regular mesh of h^n hypercubes, each of volume $(1/h)^n$
- ▶ Again, thanks to \mathbb{R}^n being a finite vector space
- ▶ “Closed” and “bounded” each solve a separate issue, recall
 3. $\min\{x : x \in \mathbb{R} \wedge x > 0\} \quad \{x_i = 1/i\} \quad \{f(x_i)\} \rightarrow 0$
 4. $\min\{1/x : x \in \mathbb{R} \wedge x > 0\} \quad \{x_i = i\} \quad \{f(x_i)\} \rightarrow 0$
- ▶ But not all issues solved yet, recall

$$5. \min\{f(x) : x \in [0, 1]\} \text{ with } f(x) = \begin{cases} x & \text{if } x > 0 \\ 1 & \text{if } x = 0 \end{cases}$$

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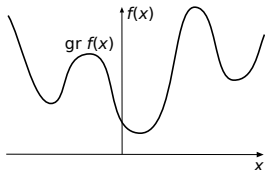
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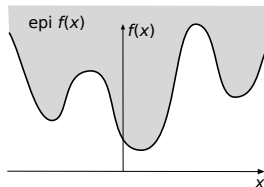
- ▶ $f : D \rightarrow \mathbb{R}$, domain $D = \text{dom}(f)$ may not be all \mathbb{R}^n
- ▶ Equivalent for minimization: $f : \mathbb{R}^n \rightarrow \bar{\mathbb{R}}$, $f(x) = \infty$ for $x \notin D$
(usually OK to ignore $\text{dom}(f)$ if f extended-real-valued)

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- ▶ f “lives” in \mathbb{R}^{n+1}
- ▶ $\text{gr}(f) = \{ (f(x), x) : x \in \text{dom}(f) \}$ (graph)

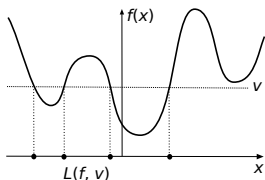
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- ▶ f “lives” in \mathbb{R}^{n+1}
- ▶ $\text{gr}(f) = \{ (f(x), x) : x \in \text{dom}(f) \}$ (graph)
- ▶ $\text{epi}(f) = \{ (v, x) : x \in \text{dom}(f) \wedge v \geq f(x) \}$
(epigraph, we are minimizing)

- ▶ Looking at f in \mathbb{R}^n requires projection:

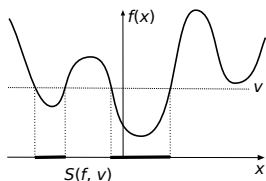
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- ▶ Equivalent for minimization: $f : \mathbb{R}^n \rightarrow \bar{\mathbb{R}}$, $f(x) = \infty$ for $x \notin D$
(usually OK to ignore $\text{dom}(f)$ if f extended-real-valued)



- ▶ f “lives” in \mathbb{R}^{n+1}
- ▶ $\text{gr}(f) = \{ (f(x), x) : x \in \text{dom}(f) \}$ (graph)
- ▶ $\text{epi}(f) = \{ (v, x) : x \in \text{dom}(f) \wedge v \geq f(x) \}$
(epigraph, we are minimizing)

- ▶ Looking at f in \mathbb{R}^n requires projection:
 - ▶ $L(f, v) = \{ x \in \text{dom}(f) : f(x) = v \}$ (level set)

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- ▶ Looking at f in \mathbb{R}^n requires **projection**:
 - ▶ $L(f, v) = \{ x \in \text{dom}(f) : f(x) = v \}$ (level set)
 - ▶ $S(f, v) = \{ x \in \text{dom}(f) : f(x) \leq v \}$ (sublevel set, we are minimizing)
- ▶ When maximizing, $f(x) = -\infty$ for $x \notin D$, superlevel set and ipograph

- ▶ The other problem: f “jumps wildly”

$$5. \min\{f(x) : x \in [0, 1]\} \text{ with } f(x) = \begin{cases} x & \text{if } x > 0 \\ 1 & \text{if } x = 0 \end{cases}$$

values “near” x do not reliably “predict” what happens there

- ▶ $f : \mathbb{R}^n \rightarrow \mathbb{R}$ continuous at x :

$$\bullet \{x_i\} \rightarrow x \implies \{f(x_i)\} \rightarrow f(x)$$

$$\bullet \forall \varepsilon > 0 \exists \delta > 0 \text{ s.t. } |f(y) - f(x)| < \varepsilon \quad \forall y \in \mathcal{B}(x, \delta)$$

continuous on $S \equiv \forall x \in S$, just “continuous” $\equiv S = \mathbb{R}^n$

- ▶ Intermediate value theorem: $f : \mathbb{R} \rightarrow \mathbb{R}$ continuous on $[a, b]$, $\forall v$ s.t.

$$\min\{f(a), f(b)\} \leq v \leq \max\{f(a), f(b)\} \exists c \in [a, b] \text{ s.t. } f(c) = v$$

- ▶ Continuity easily preserved: f, g continuous at $x \implies$

$$\bullet f + g, f \cdot g \text{ continuous at } x$$

$$\bullet \max\{f, g\}, \min\{f, g\} \text{ continuous at } x$$

$$\bullet f \circ g \equiv f(g(\cdot)) \text{ continuous at } x$$

- ▶ Yet, plenty of non-continuous functions ($\text{sign}(x)$, $1/(x-1)$, ...)

- ▶ Weierstrass extreme value theorem (in our parlance):

$X \subseteq \mathbb{R}^n$ compact and f continuous on $X \implies$

(P) has an optimal solution

- ▶ Works for both min and max

- ▶ In other words:

$X \subseteq \mathbb{R}^n$ compact and f continuous on $X \implies$

all accumulation points of any minimizing sequence are optima
and there is at least one

- ▶ Thus, “ X compact and f continuous (on X)” natural assumptions
- ▶ “ f continuous” basically necessary (recall 5.)
- ▶ But non-bounded X also common, and $f_* = -\infty$ happens

- ▶ f Lipschitz continuous (L.c.) on S if $\exists L > 0$ such that

$$|f(x) - f(y)| \leq L \|x - y\| \quad \forall x, y \in S$$

globally L.c.: $S = \mathbb{R}^n$, locally L.c. at x : $\exists \varepsilon > 0$ s.t. $S \supseteq \mathcal{B}(x, \varepsilon)$

- ▶ Note: L depends on S (locally L.c. $\not\Rightarrow$ globally L.c.)
- ▶ Lipschitz continuity $\equiv f$ cannot change too fast
strong relationships with derivatives (see next)
- ▶ Much stronger property: Lipschitz continuity \implies continuity

Exercise: Prove it

Exercise: Exhibit simple functions that are continuous but not globally L.c.

Exercise: Exhibit a continuous functions that is not L.c. on a compact set

- ▶ Weaker condition: f is lower[upper] semi-continuous (l.[u.]s.c.) at x if

$$\{x_i\} \rightarrow x \implies f(x) \leq \liminf_{i \rightarrow \infty} f(x_i) \quad [f(x) \geq \limsup \dots]$$

- ▶ Also written $\liminf_{y \rightarrow x} f(y) \geq f(x)$, $\limsup_{y \rightarrow x} f(y) \leq f(x)$
- ▶ Can jump down [up] wildly, but can never jump up [down]
- ▶ Particularly useful example: indicator function of $S \subset \mathbb{R}^n$

$$I_S(x) = 0 \text{ if } x \in S, \quad I_S(x) = +\infty \text{ if } x \notin S$$
 (think $S = \text{dom}(f)$) clearly not continuous, but l.s.c.
- ▶ f continuous at $x \iff f$ is both l.s.c. and u.s.c. at x
- ▶ Any l.s.c. f attains minimum (but not maximum) on any compact set X
- ▶ X compact and f l.s.c. \implies all accumulation points of any minimizing sequence are optimal solutions, and there is at least one
- ▶ As a great man said: “(convex) optimization is a one-sided world”

Outline

Motivation

Sets and sequences

Vector spaces and topology

Functions

Derivatives, Gradients and Hessians

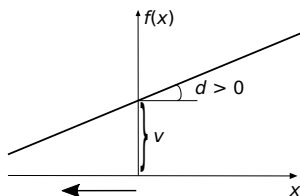
A walkthrough on simple functions

Wrap up & References

- ▶ (the vector) “Space (\mathbb{R}^n) is big. Really big. You just won't believe how vastly, hugely, mind-bogglingly big it is.”

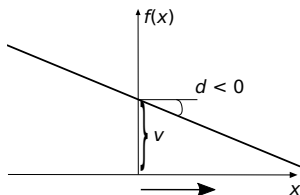
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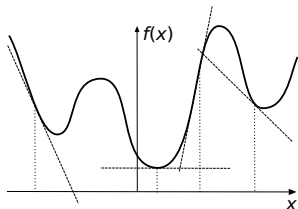
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always left if $d > 0$,

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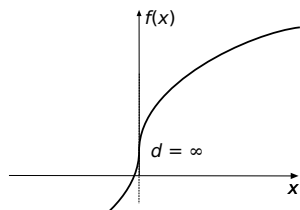
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- ▶ $f(x) := dx + v : \mathbb{R} \rightarrow \mathbb{R}$ (linear) is easy: always left if $d > 0$, right if $d < 0$
- ▶ Obvious idea: use the linear function that best locally approximates f
- ▶ Trusty old derivative:
$$d = f'(x) = \lim_{t \rightarrow 0} [f(x + t) - f(x)] / t$$

- ▶ Easy closed-forms for most reasonable functions

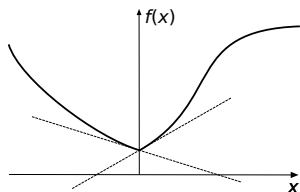
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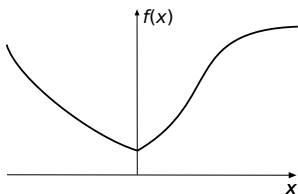
- ▶ Easy closed-forms for most reasonable functions
- ▶ Provided the limit is finite

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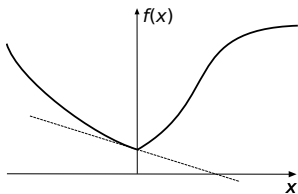


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- ▶ Trusty old derivative:
$$d = f'(x) = \lim_{t \rightarrow 0} [f(x + t) - f(x)] / t$$

- ▶ Easy closed-forms for most reasonable functions
- ▶ Provided the limit is finite ... and it exists at all
- ▶ f differentiable on S if $f'(x)$ exists finite $\forall x \in S$

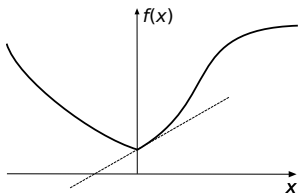


► Left and right derivatives:



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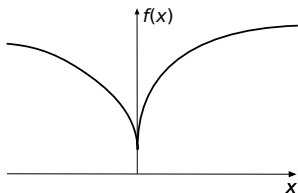
$$f'_-(x) = \lim_{t \rightarrow 0^-} [f(x+t) - f(x)] / t$$



► Left and right derivatives:

$$f'_-(x) = \lim_{t \rightarrow 0_-} [f(x+t) - f(x)] / t$$

$$f'_+(x) = \lim_{t \rightarrow 0_+} [f(x+t) - f(x)] / t$$

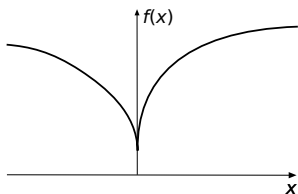


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- ▶ Can be as different as $-\infty$ and $+\infty$



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$$f'_+(x) = \lim_{t \rightarrow 0^+} [f(x+t) - f(x)] / t$$

► Can be as different as $-\infty$ and $+\infty$

► f is differentiable at $x \in \text{int dom}(f) \iff f'_-(x) = f'_+(x)$ (\iff they \exists)

► f differentiable at $x \implies f$ continuous at x

Exercise: Prove it

► f continuously differentiable: f' is also continuous

► Nondifferentiable functions happen (e.g., $|x|$, \sqrt{x})

- $f : \mathbb{R}^n \rightarrow \mathbb{R}$, partial derivative of f w.r.t. x_i at $x \in \mathbb{R}^n$:

$$\frac{\partial f}{\partial x_i}(x) = \lim_{t \rightarrow 0} \frac{f(x_1, \dots, x_{i-1}, x_i + t, x_{i+1}, \dots, x_n) - f(x)}{t}$$

just $f'(x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_n)$ treating x_j for $j \neq i$ as constants

- Gradient = vector of all partial derivatives

$$\nabla f(x) := \left[\frac{\partial f}{\partial x_1}(x), \dots, \frac{\partial f}{\partial x_n}(x) \right]$$

- Directional derivative at x along direction $d \in \mathbb{R}^n$:

$$\frac{\partial f}{\partial d}(x) := \lim_{t \rightarrow 0} \frac{f(x + td) - f(x)}{t}$$

- Of course, $\frac{\partial f}{\partial x_i} = \frac{\partial f}{\partial d}$ with $d = u_i$

- One-sided directional derivative: $\lim_{t \rightarrow 0+} \dots$ (generalizes f'_+ and f'_-)

- f differentiable at x if \exists linear function $\phi(h) = \langle c, h \rangle + f(x)$ s.t.

$$\lim_{\|h\| \rightarrow 0} \frac{|f(x+h) - \phi(h)|}{\|h\|} = 0$$

- ϕ “first order approximation” of f at x
- The error in the approximation vanishes faster than linearly
- f differentiable at $x \implies c = \nabla f(x) \equiv \phi(h) = \langle \nabla f(x), h \rangle + f(x) \implies$ first-order model of f at x : $L_x(y) = \nabla f(x)(y - x) + f(x)$
- Hence, f differentiable $\implies \frac{\partial f}{\partial x_i}(x)$ exists $\forall i$
- The converse is not true
- More in general, f differentiable at $x \implies \exists \frac{\partial f}{\partial d}(x) \forall d \in \mathbb{R}^n$, and

$$\frac{\partial f}{\partial d}(x) = \langle \nabla f(x), d \rangle$$

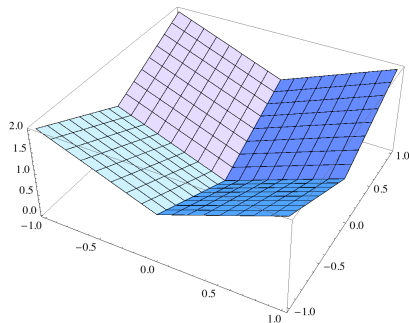
Exercise: prove $-\nabla f(x)$ is the steepest descent direction at $x \equiv$ direction with most negative directional derivative

- ▶ $f : \mathbb{R}^n \rightarrow \mathbb{R}$ differentiable at $x \implies f$ locally Lipschitz continuous at x ;
hence, f differentiable $\implies f$ continuous (but \Leftarrow not true)

Exercise: Prove f differentiable $\implies f$ continuous

- ▶ $\exists \delta > 0$ s.t. $\forall i \frac{\partial f}{\partial x_i}(y)$ continuous $\forall y \in \mathcal{B}(x, \delta) \implies f$ differentiable at x
- ▶ The converse is not true ($\exists f$ differentiable with discontinuous $\frac{\partial f}{\partial x_i}$, weird)
- ▶ The good class for optimization: $C^1 := \nabla f(x)$ continuous everywhere
- ▶ $f \in C^1 \implies f$ differentiable everywhere $\implies f$ continuous everywhere
- ▶ Yet, nondifferentiable functions happen

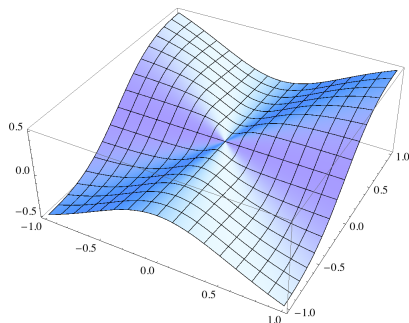
- ▶ $f(x_1, x_2) = \|[x_1, x_2]\|_1 = |x_1| + |x_2|$
- ▶ f continuous everywhere (why?)
- ▶ f non differentiable in $[0, 0]$



Exercise: prove it (hint: compute 4 easy directional derivatives, prove they cannot ever have the form $\langle v, d \rangle$ for any v)

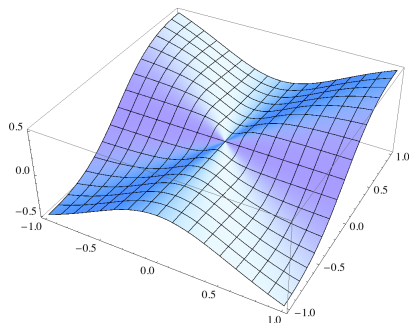
Exercise: where else f is non differentiable? Prove it is not

- ▶ $f(x_1, x_2) = \frac{x_1^2 x_2}{x_1^2 + x_2^2}$
- ▶ Assume $f(0, 0) = 0$ since $\lim_{\alpha \rightarrow 0} f(\alpha d_1, \alpha d_2) = 0$
- ▶ $\exists \frac{\partial f}{\partial d} \quad \forall d \in \mathbb{R}^n \setminus \{[0, 0]\}$
- ▶ f non differentiable in $[0, 0]$



Exercise: prove all this (hint: compute $\lim_{t \rightarrow 0} f(td_1, td_2)/t$, prove it cannot ever have the form $\langle v, d \rangle$ for any v)

- ▶ $f(x_1, x_2) = \frac{x_1^2 x_2}{x_1^2 + x_2^2}$
- ▶ Assume $f(0, 0) = 0$ since $\lim_{\alpha \rightarrow 0} f(\alpha d_1, \alpha d_2) = 0$
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- ▶ f non differentiable in $[0, 0]$



Exercise: prove all this (hint: compute $\lim_{t \rightarrow 0} f(td_1, td_2)/t$, prove it cannot ever have the form $\langle v, d \rangle$ for any v)

Exercise: alternatively, compute ∇f and prove it is not continuous in $[0, 0]$ (hint: look at picture of $\frac{\partial f}{\partial x_2}$ for directions where the limit is \neq)

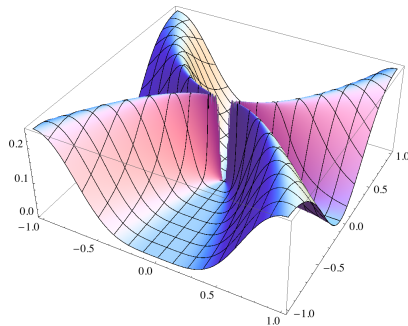
► $f(x_1, x_2) = \left(\frac{x_1^2 x_2}{x_1^4 + x_2^2} \right)^2$ (again, $f(0, 0) = 0$)

► f not continuous \implies
not differentiable at $[0, 0]$

► Yet $\frac{\partial f}{\partial d}(0, 0) = 0 \quad \forall d \in \mathbb{R}^n$

► Directional derivatives
 \exists and are all equal,
yet ∇f does not

► Trick: f does nasty things on curved lines, not straight ones

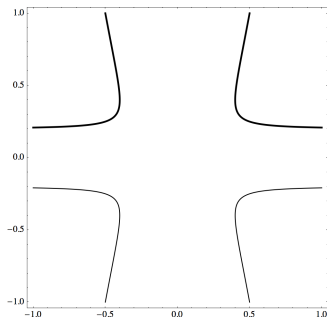


Exercise: prove $\frac{\partial f}{\partial d}(0, 0) = 0$

Exercise: prove f not continuous at $[0, 0]$ (check $\lim_{k \rightarrow \infty} f(1/k, 1/k^2)$)

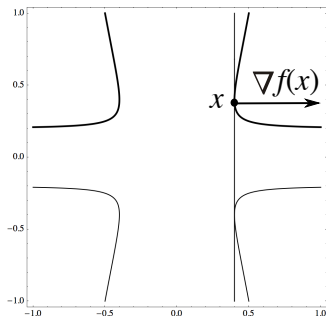
► In \mathbb{R}^n , $S(L_x, f(x))$ is a **line** passing by x and $\nabla f(x) \perp S(L_x, f(x))$

$$f(x_1, x_2) = \frac{x_1^2 x_2}{x_1^2 + x_2^2} \quad , \quad \nabla f(x) = \left[\frac{2x_1 x_2^3}{(x_1^2 + x_2^2)^2}, \frac{x_1^2 (x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2} \right] \quad (\text{cf. Ex. 2})$$



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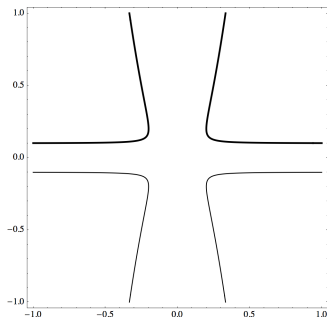


- f differentiable at $x \implies$

$$S(L_x, f(x)) \perp S(f, f(x)) \perp \nabla f(x)$$

- In \mathbb{R}^n , $S(L_x, f(x))$ is a **line** passing by x and $\nabla f(x) \perp S(L_x, f(x))$

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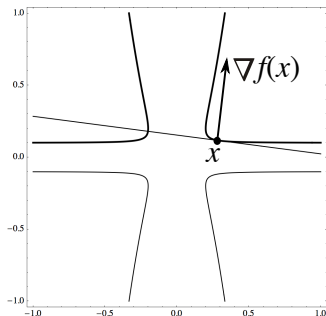


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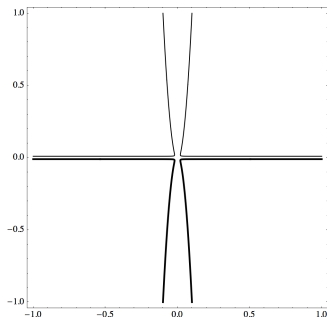
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- f differentiable at $x \implies$
 $S(L_x, f(x)) \perp S(f, f(x)) \perp \nabla f(x)$
- f differentiable at $x \implies$
 $S(f, f(x))$ “smooth”

- In \mathbb{R}^n , $S(L_x, f(x))$ is a **line** passing by x and $\nabla f(x) \perp S(L_x, f(x))$

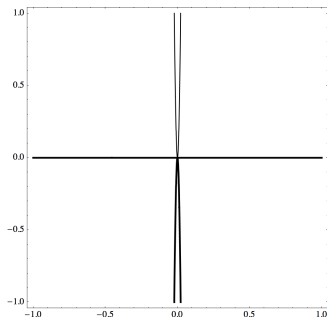
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- f differentiable at $x \implies$
 $S(f, f(x))$ “smooth”
- As $x \rightarrow \bar{x}$ where f **non** differentiable,
 $S(f, f(x))$ “**less and less smooth**”

- In \mathbb{R}^n , $S(L_x, f(x))$ is a **line** passing by x and $\nabla f(x) \perp S(L_x, f(x))$

$$f(x_1, x_2) = \frac{x_1^2 x_2}{x_1^2 + x_2^2} \quad , \quad \nabla f(x) = \left[\frac{2x_1 x_2^3}{(x_1^2 + x_2^2)^2}, \frac{x_1^2(x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2} \right] \quad (\text{cf. Ex. 2})$$



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 $S(L_x, f(x)) \perp S(f, f(x)) \perp \nabla f(x)$
- f differentiable at $x \implies$
 $S(f, f(x))$ “smooth”
- As $x \rightarrow \bar{x}$ where f **non** differentiable,
 $S(f, f(x))$ “**less and less smooth**”
- f **non** differentiable at $x \implies$
 $S(f, f(x))$ has “**kinks**”

- f differentiable \implies all relevant objects in \mathbb{R}^{n+1} and \mathbb{R}^n are smooth
- f non differentiable \implies kinks appear and things break

- ▶ Vector-valued function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$, $f(x) = [f_1(x), f_2(x), \dots, f_m(x)]$
- ▶ Partial derivative: usual stuff, except with **extra index**

$$\frac{\partial f_j}{\partial x_i}(x) = \lim_{t \rightarrow 0} \frac{f_j(x_1, \dots, x_{i-1}, x_i + t, x_{i+1}, \dots, x_n) - f_j(x)}{t}$$

- ▶ **Jacobian** := matrix of all partial derivatives $\in \mathbb{R}^{m,n}$

$$Jf(x) := \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x) & \frac{\partial f_1}{\partial x_2}(x) & \dots & \frac{\partial f_1}{\partial x_n}(x) \\ \frac{\partial f_2}{\partial x_1}(x) & \frac{\partial f_2}{\partial x_2}(x) & \dots & \frac{\partial f_2}{\partial x_n}(x) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(x) & \frac{\partial f_m}{\partial x_2}(x) & \dots & \frac{\partial f_m}{\partial x_n}(x) \end{bmatrix} = \begin{bmatrix} \nabla f_1(x) \\ \nabla f_2(x) \\ \vdots \\ \nabla f_m(x) \end{bmatrix}$$

- ▶ Jacobian = matrix with gradients as rows
- ▶ As usual, much better if **continuous** \equiv **every f_j differentiable**
- ▶ A special case of vector-valued function is particularly important

- ▶ $\frac{\partial f}{\partial x_i} : \mathbb{R}^n \rightarrow \mathbb{R}$, hence has partial derivatives

- ▶ Second order partial derivative
(just do it **twice**)

$$\frac{\partial^2 f}{\partial x_j \partial x_i} = \frac{\partial^2 f}{\partial x_i \partial x_j}$$

- ▶ $\nabla f(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n$, hence has a Jacobian: **Hessian** of f

$$\nabla^2 f(x) := J\nabla f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_1}(x) & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_1}(x) \\ \frac{\partial^2 f}{\partial x_1 \partial x_2}(x) & \frac{\partial^2 f}{\partial x_2^2}(x) & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_2}(x) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_n}(x) & \cdots & \frac{\partial^2 f}{\partial x_n^2}(x) \end{bmatrix}$$

- ▶ $\nabla^2 f$ is f'' : much more complex object, but some things generalise nicely
- ▶ Very important concept: **second-order model** =
first-order model plus **second-order term** (\equiv **better**)

$$Q_x(y) = L_x(y) + \frac{1}{2}(y - x)^T \nabla^2 f(x)(y - x)$$

- ▶ $\exists \delta > 0$ s.t. $\forall y \in \mathcal{B}(x, \delta)$

$\frac{\partial^2 f}{\partial x_j \partial x_i}(y)$ and $\frac{\partial^2 f}{\partial x_i \partial x_j}(y)$ exist and are continuous at x

$$\implies \frac{\partial^2 f}{\partial x_j \partial x_i}(x) = \frac{\partial^2 f}{\partial x_i \partial x_j}(x) \equiv \nabla^2 f \text{ symmetric}$$

- ▶ Symmetry is important: all eigenvalues of $\nabla^2 f$ are real, useful geometric characterization, special cases (all $\geq 0 / \leq 0, \dots$)
- ▶ The very good class: $C^2 := \nabla^2 f(x)$ continuous \implies
 - ▶ $\nabla^2 f(x)$ symmetric
 - ▶ $\nabla f(x)$ continuous (why?)
- ▶ C^2 (strictly speaking C^3) is the best class ever for optimization
- ▶ Second-order information very useful, we will see why

Exercise: $f(x_1, x_2) = x_2^3 / (x_1^2 + x_2^2)$ is non differentiable in $[0, 0]$; check that $\nabla^2 f$ is not symmetric there

Outline

Motivation

Sets and sequences

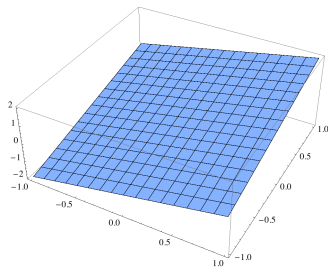
Vector spaces and topology

Functions

Derivatives, Gradients and Hessians

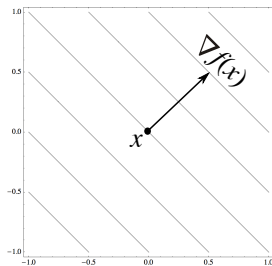
A walkthrough on simple functions

Wrap up & References

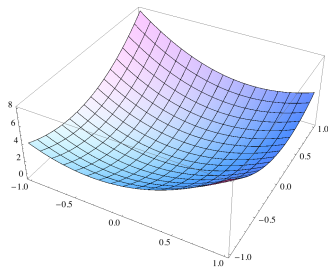


► Linear function: $f(x) = cx$, fixed $c \in \mathbb{R}^n$

► $\nabla f(x) = c$, $\nabla^2 f(x) = 0$



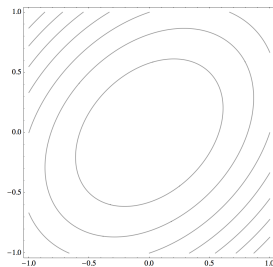
- ▶ Linear function: $f(x) = cx$, fixed $c \in \mathbb{R}^n$
- ▶ $\nabla f(x) = c$, $\nabla^2 f(x) = 0$
- ▶ Level sets are parallel hyperplanes orthogonal to c ($= [1, 1]$ here)



- Quadratic function: $f(x) = \frac{1}{2}x^T Qx + qx$
fixed $Q \in \mathbb{R}^{n \times n}$, $q \in \mathbb{R}^n$; here

$$Q = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix}, \quad q = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

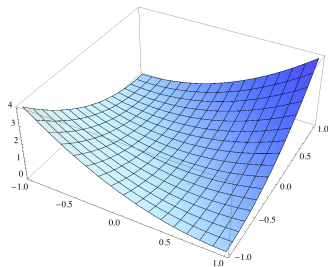
- $\nabla f(x) = Qx + q$, $\nabla^2 f(x) = Q$



- ▶ Quadratic function: $f(x) = \frac{1}{2}x^T Qx + qx$
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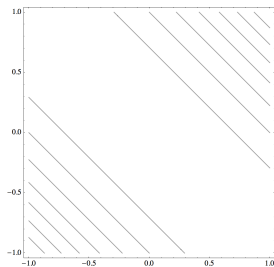
- ▶ $\nabla f(x) = Qx + q$, $\nabla^2 f(x) = Q$
- ▶ Level sets are ellipsoids



- Quadratic function: $f(x) = \frac{1}{2}x^T Qx + qx$
fixed $Q \in \mathbb{R}^{n \times n}$, $q \in \mathbb{R}^n$; here

$$Q = \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}, \quad q = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

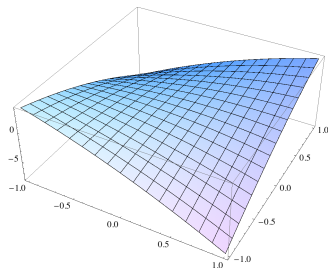
- $\nabla f(x) = Qx + q$, $\nabla^2 f(x) = Q$



- ▶ Quadratic function: $f(x) = \frac{1}{2}x^T Qx + qx$
fixed $Q \in \mathbb{R}^{n \times n}$, $q \in \mathbb{R}^n$; here

$$Q = \begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}, \quad q = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

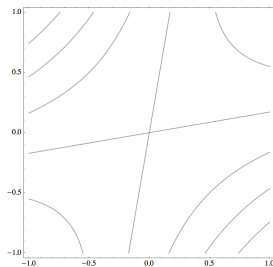
- ▶ $\nabla f(x) = Qx + q$, $\nabla^2 f(x) = Q$
- ▶ Level sets are degenerate ellipsoids



- Quadratic function: $f(x) = \frac{1}{2}x^T Qx + qx$
fixed $Q \in \mathbb{R}^{n \times n}$, $q \in \mathbb{R}^n$; here

$$Q = \begin{bmatrix} -2 & 6 \\ 6 & -2 \end{bmatrix}, \quad q = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

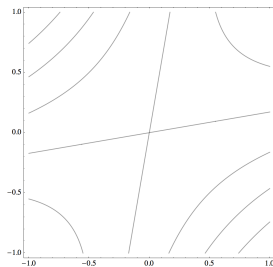
- $\nabla f(x) = Qx + q$, $\nabla^2 f(x) = Q$



- Quadratic function: $f(x) = \frac{1}{2}x^T Qx + qx$
fixed $Q \in \mathbb{R}^{n \times n}$, $q \in \mathbb{R}^n$; here

$$Q = \begin{bmatrix} -2 & 6 \\ 6 & -2 \end{bmatrix}, \quad q = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

- $\nabla f(x) = Qx + q$, $\nabla^2 f(x) = Q$
► Level sets are **hyperboloids**



- Quadratic function: $f(x) = \frac{1}{2}x^T Qx + qx$
 fixed $Q \in \mathbb{R}^{n \times n}$, $q \in \mathbb{R}^n$; here

$$Q = \begin{bmatrix} -2 & 6 \\ 6 & -2 \end{bmatrix}, \quad q = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

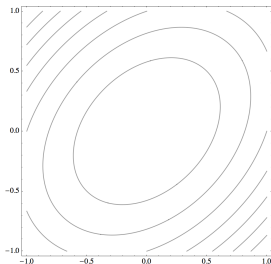
- $\nabla f(x) = Qx + q$, $\nabla^2 f(x) = Q$
 ► Level sets are **hyperboloids**

- Several different cases, let's try to work them out
 ► Can always assume **Q symmetric** \implies has spectral decomposition

$$x^T Qx = [(x^T Qx) + (x^T Qx)^T] / 2 = x^T [(Q + Q^T) / 2]x = \mathbf{H} \mathbf{\Lambda} \mathbf{H}^T$$

- H^i **eigenvectors, orthonormal** ($H_i \perp H_j$, $\|H_i\| = 1$)
 ► $\mathbf{\Lambda}$ **diagonal**, λ_i corresponding **real eigenvalues**
 ► **Sign of eigenvalues** (positive/negative definiteness) \rightarrow shape of level sets

- ▶ Easy case: Q nonsingular $\equiv \lambda_i \neq 0 \forall i$ (regardless of the sign)
- ▶ Then $f(x) = \frac{1}{2}(x - \bar{x})^T Q(x - \bar{x})$ [+ constant] for $\bar{x} = -Q^{-1}q$ (check)
- ▶ \bar{x} center of the ellipsoid, $y = x - \bar{x}$, $f_{\bar{x}}(y) = y^T Q y$ [+ constant]

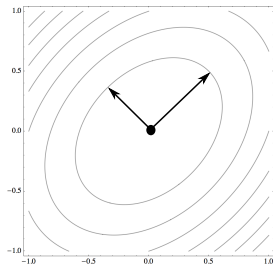


- ▶ Along H_i : $f_i(\alpha) = f_{\bar{x}}(\alpha H_i) = \alpha^2 \lambda_i$ (check)

- ▶ $S(f_{\bar{x}}, 1) \equiv f_i(\alpha) = 1 \equiv \alpha = \sqrt{1/\lambda_i} \implies$

$$Q = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 4 \end{bmatrix}$$

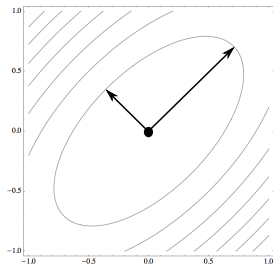
- ▶ Easy case: Q nonsingular $\equiv \lambda_i \neq 0 \forall i$ (regardless of the sign)
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- ▶ Along H_i : $f_i(\alpha) = f_{\bar{x}}(\alpha H_i) = \alpha^2 \lambda_i$ (check)
- ▶ $S(f_{\bar{x}}, 1) \equiv f_i(\alpha) = 1 \equiv \alpha = \sqrt{1/\lambda_i} \implies$
 $H_i \perp$ axes of $S(f_{\bar{x}}, 1)$, length $\sqrt{1/\lambda_i}$

$$Q = \begin{bmatrix} 6 & -2 \\ -2 & 6 \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 4 \end{bmatrix}$$

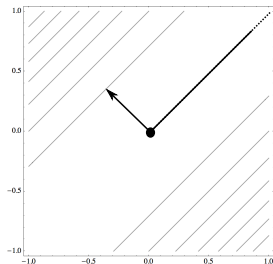
- ▶ Easy case: Q nonsingular $\equiv \lambda_i \neq 0 \forall i$ (regardless of the sign)
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 $H_i \perp$ axes of $S(f_{\bar{x}}, 1)$, length $\sqrt{1/\lambda_i}$
- ▶ The smaller λ_i , the longer the axis

$$Q = \begin{bmatrix} 5 & -3 \\ -3 & 5 \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 2 \end{bmatrix}$$

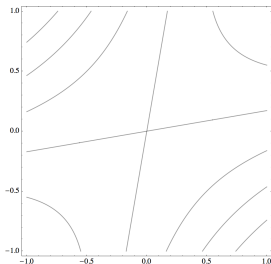
- ▶ Easy case: Q nonsingular $\equiv \lambda_i \neq 0 \forall i$ (regardless of the sign)
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- ▶ \bar{x} center of the ellipsoid, $y = x - \bar{x}$, $f_{\bar{x}}(y) = y^T Q y$ [+ constant]



- ▶ Along H_i : $f_i(\alpha) = f_{\bar{x}}(\alpha H_i) = \alpha^2 \lambda_i$ (check)
- ▶ $S(f_{\bar{x}}, 1) \equiv f_i(\alpha) = 1 \equiv \alpha = \sqrt{1/\lambda_i} \implies$
 $H_i \perp$ axes of $S(f_{\bar{x}}, 1)$, length $\sqrt{1/\lambda_i}$
- ▶ The smaller λ_i , the longer the axis
- ▶ With $\lambda_i = 0$, “axis $\rightarrow \infty$ ” (but Q singular)

$$Q = \begin{bmatrix} 4 & -4 \\ -4 & 4 \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 0 \end{bmatrix}$$

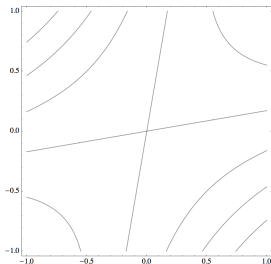
- ▶ Easy case: Q nonsingular $\equiv \lambda_i \neq 0 \forall i$ (regardless of the sign)
- ▶ Then $f(x) = \frac{1}{2}(x - \bar{x})^T Q (x - \bar{x})$ [+ constant] for $\bar{x} = -Q^{-1}q$ (check)
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- ▶ The smaller λ_i , the longer the axis
- ▶ With $\lambda_i = 0$, “axis $\rightarrow \infty$ ” (but Q singular)
- ▶ With $\lambda_i < 0$ sign reverses, no longer “axes”

$$Q = \begin{bmatrix} 3 & -5 \\ -5 & 3 \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ -2 \end{bmatrix}$$

- ▶ Easy case: Q nonsingular $\equiv \lambda_i \neq 0 \forall i$ (regardless of the sign)
- ▶ Then $f(x) = \frac{1}{2}(x - \bar{x})^T Q (x - \bar{x})$ [+ constant] for $\bar{x} = -Q^{-1}q$ (check)
- ▶ \bar{x} center of the ellipsoid, $y = x - \bar{x}$, $f_{\bar{x}}(y) = y^T Q y$ [+ constant]



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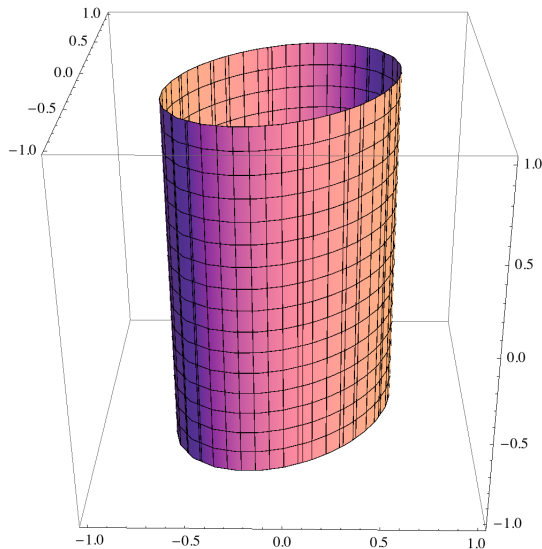
- ▶ The smaller λ_i , the longer the axis
- ▶ With $\lambda_i = 0$, “axis $\rightarrow \infty$ ” (but Q singular)
- ▶ With $\lambda_i < 0$ sign reverses, no longer “axes”

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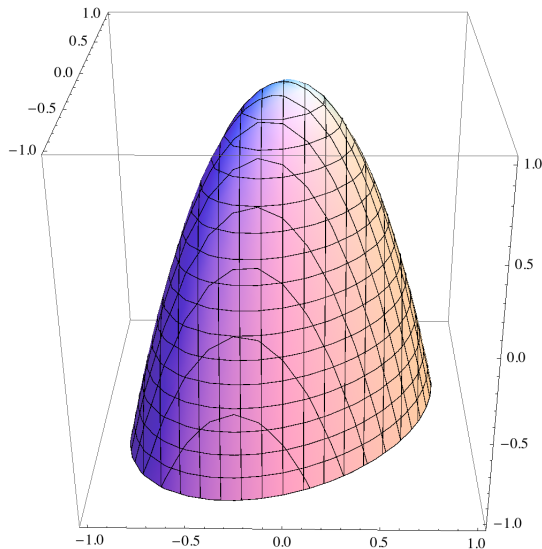
- ▶ $\forall i \lambda_i > 0 \equiv Q \succ 0 \implies \bar{x}$ minimum of f (why?)
- ▶ $\exists i \lambda_i < 0 \equiv Q \not\succ 0 \implies f$ unbounded below (why?)

- ▶ Q singular $\equiv \exists \lambda_i = 0 \equiv \ker(Q) \neq \{0\}$
- ▶ $\mathbb{R}^n = \text{row}(Q) + \ker(Q)$, $\text{row}(Q) \perp \ker(Q)$
 $\text{row}(Q) \equiv$ subspace spanned by rows
 $\ker(Q) \equiv$ subspace spanned by H_i with $\lambda_i = 0$
- ▶ $q = q_+ + q_0$, $q_+ \perp q_0$, where
 $q_+ \in \text{row}(Q) = \text{row}(-Q) \equiv \bar{x}^T(-Q) = q_+^T$ and $q_0 \in \ker(Q) \equiv Qq_0 = 0$
- ▶ Then $f(x) = \frac{1}{2}(x - \bar{x})^T Q(x - \bar{x}) + q_0^T x$ [+ constant] (**check**)
- ▶ f is “truly quadratic” on $\text{row}(Q)$ and linear on $\ker(Q)$
- ▶ Assume $Q \succeq 0$: f has minimum $\iff q_0 = 0 \equiv$
 $\bar{x}^T(-Q) = q_+^T \equiv Q\bar{x} + q = 0 \equiv \nabla f(\bar{x}) = 0$ has solution
- ▶ First example of first-order (global) optimality condition, more to come
- ▶ Linear algebra is crucial for optimization

$$Q = \begin{bmatrix} 6 & -2 & 0 \\ -2 & 6 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad q = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 4 \\ 0 \end{bmatrix}$$

 $S(f, 1)$ 

$$Q = \begin{bmatrix} 6 & -2 & 0 \\ -2 & 6 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad q = \begin{bmatrix} 0 \\ 0 \\ \color{red}{1} \end{bmatrix}, \quad H = \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \lambda = \begin{bmatrix} 8 \\ 4 \\ 0 \end{bmatrix}$$

 $S(f, 1)$ 

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Wrap up & References

- ▶ Optimization **difficult/impossible** in general
- ▶ Need **conditions to make it possible**:
 - ▶ X **closed**, otherwise x_* may be on the unreachable boundary
 - ▶ possibly X **compact** \implies every sequence has accumulation point (but **not always possible**, $f_* = -\infty$ happens)
 - ▶ f (lower semi-) **continuous**, otherwise can “jump away” on would-be x_*
 - ▶ **some sort of derivative information** to tell the way to x_*
- ▶ The more derivatives you have, the better
- ▶ Derivatives \implies first- and second-order **model**
- ▶ f **“complicated”**, model **looks like** f (**close to** x) and **simple**
- ▶ Fundamental concept we will use all the time

- ▶ Boyd, Vandenberghe “Convex optimization” Appendix A
- ▶ Bazaraa, Sherali, Shetty “Nonlinear programming” Appendix A1, A3, A4
- ▶ Nocedal, Wright “Numerical Optimization” Appendix A2
- ▶ Google + Wikipedia; e.g.
https://mathinsight.org/differentiability_multivariable_theorem