

Unconstrained Multivariate Optimality and Convexity

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Outline

Unconstrained multivariate optimization

Gradients, Jacobians, and Hessians

Optimality conditions

A Quick Look to Convex Functions

Wrap up & References

Solutions

- ▶ Back to $f : \mathbb{R}^n \rightarrow \mathbb{R}$, i.e., $f(x_1, x_2, \dots, x_n) = f(x)$
- ▶ Of course need f L-c (exact definition later)
- ▶ **Very bad news**: no algorithm can work in less than $\Omega((LD/\varepsilon)^n)$ [3, p. 413]
- ▶ **Curse of dimensionality**: not really doable unless $n = 3/5/10$ tops
- ▶ Can make it in $O((LD/\varepsilon)^n)$, multidimensional grid with small enough step: the standard approach to hyperparameter optimization (but D, L unknown)
- ▶ If f **analytic**, clever (spatial) B&B can give global optimum
- ▶ If f **black-box** (typically \implies **no derivatives**), many effective heuristics can give good (not provably optimal) solutions [8]
- ▶ In both cases, complexity grows “fast” in practice as n grows
- ▶ **Finding good global solutions hard** in practice, **proving optimality even worse**

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- ▶ In both cases, complexity grows “fast” in practice as n grows
- ▶ **Finding good global solutions hard** in practice, **proving optimality even worse** unless f **convex** \implies **global** \equiv **local**

- ▶ Local optimization much better
- ▶ Results in general surprisingly analogous to (multivariate) quadratic case: most (but not all) convergence results are dimension-independent \equiv complexity does not explicitly depends on n (if it does, not exponentially)
- ▶ Not completely surprising: linear / quadratic models a staple
- ▶ Does not mean all local algorithms are fast:
 - ▶ convergence speed may be rather low (“badly linear” or worse)
 - ▶ cost of f / derivatives computation necessarily increases with n : for large $n \approx 10^9$, even $O(n^2)$ is too much (will see)
 - ▶ some dependency on n may be hidden in $O(\cdot)$ constants
- ▶ Yet, large-scale local optimization is doable if you have derivatives
- ▶ Except, derivatives in \mathbb{R}^n are significantly more complex

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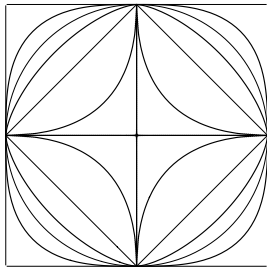
Solutions

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

- ▶ Euclidean norm just one member of a large family:

$$\|x\|_p := \left(\sum_{i=1}^n |x_i|^p \right)^{1/p} \quad p\text{-norm, } p > 0$$

- ▶ Euclidean $\equiv \|x\|_2$, $\|x\|_1 := \sum_{i=1}^n |x_i|$ (Lasso)
- ▶ $\lim_{p \rightarrow \infty} \equiv \|x\|_\infty := \max\{|x_i| : i = 1, \dots, n\}$
- ▶ $\lim_{p \rightarrow 0} \equiv \|x\|_0 := \#\{i : |x_i| > 0\}$ (not norm)



- ▶ Other norms \exists besides p -norm (matrix norms ...)

- ▶ Pictured $S(\|\cdot\|_p, 1) \equiv \mathcal{B}_p(0, 1)$, $p = 0, 1/2, 1, 3/2, 2, 3, \infty$ (grow with p)

- ▶ The norm defines the topology of \mathbb{R}^n , but doesn't really matter:

all is “ \exists ball”, “ \forall small ball”, and all norms are equivalent [9]

$$\forall \|\cdot\|, \|\cdot\|' \exists 0 < \alpha < \beta \text{ s.t. } \alpha\|x\| \leq \|z\|' \leq \beta\|x\| \quad \forall x, z \in \mathbb{R}^n$$

- ▶ **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
- ▶ Note that \mathbb{R}^n “exponentially larger” than $\mathbb{R} \implies$ there are **many more ways** for $\{x_i\} \rightarrow x$ in \mathbb{R}^n than in \mathbb{R}
- ▶ This may lead to more tricky situations / concepts

▶ Same definitions:

▶ f **continuous at x** : $\{x_i\} \rightarrow x \implies \{f(x_i)\} \rightarrow f(x)$

▶ $f \in C^0$: continuous $\forall x \in \mathbb{R}^n$

▶ There are “many” different $\{x_i\} \rightarrow x$, the limit must be = for **all**

▶ **Not** sufficient to only consider “simple” sequences

▶ $f(x_1, x_2) = \left[\frac{x_1^2 x_2}{x_1^4 + x_2^2} \right]^2$ $f(0, 0) = ??$

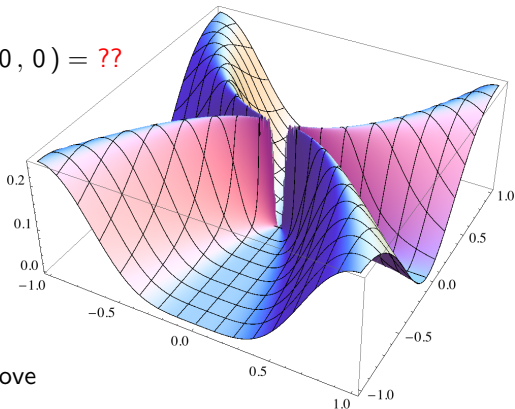
▶ Limit = “on straight lines”

$$\forall [d_1, d_2] \in \mathbb{R}^2$$

$$\lim_{k \rightarrow \infty} f(d_1/k, d_2/k) = 0$$

▶ Limit \neq on “curved” line

$$\lim_{k \rightarrow \infty} f(1/k, 1/k^2) = 1/4$$



Exercise: Prove the two limits above

- ▶ $f : \mathbb{R}^n \rightarrow \mathbb{R}$, directional derivative at $x \in \mathbb{R}^n$ along direction $d \in \mathbb{R}^n$:

$$\frac{\partial f}{\partial d}(x) := \lim_{t \rightarrow 0} \frac{f(x+td) - f(x)}{t} = \varphi'_{x,d}(0)$$

- ▶ Scales linearly with $\|d\|$: $\frac{\partial f}{\partial \beta d}(x) = \beta \frac{\partial f}{\partial d}(x)$ (sounds familiar?) (check)
- ▶ One-sided directional derivative: $\lim_{t \rightarrow 0_{\pm}} \dots = [\varphi_{x,d}]'_{\pm}(0)$
- ▶ The derivative of the (x, d) -tomography (in 0): how can it be computed?
- ▶ Special case: partial derivative of f w.r.t. x_i at $x \in \mathbb{R}^n$

$$\frac{\partial f}{\partial x_i}(x) := \lim_{t \rightarrow 0} \frac{f(x_1, \dots, x_{i-1}, x_i+t, x_{i+1}, \dots, x_n) - f(x)}{t} = [f'_x]^i(x) = \frac{\partial f}{\partial u^i}(x)$$

- ▶ The derivative of the restriction of f to x_i is easy to compute: just

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

- ▶ Gradient = (column) vector of all partial derivatives, “easy to compute” [6]

$$\nabla f(x) := \left[\frac{\partial f}{\partial x_1}(x), \dots, \frac{\partial f}{\partial x_n}(x) \right]^T \in \mathbb{R}^n$$

- ▶ $f(x) = \langle b, x \rangle \implies \nabla f(x) = b$

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- ▶ $f(x) = \frac{1}{2}x^T Qx + qx \implies \nabla f(x) = Qx + q$

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

$$\lim_{\|h\| \rightarrow 0} \frac{|f(x+h) - \phi(h)|}{\|h\|} = 0 \quad [\implies \phi(0) = f(x) \implies c = f(x)]$$

$\varphi \equiv$ “first order model” of f at x , the error “vanishes faster than linearly”

- ▶ f differentiable at $x \implies b = \nabla f(x)$ [5, Th. 5.3.6]

$$\implies \frac{\partial f}{\partial x_i}(x) \text{ exists } \forall i \quad (\text{but } \longleftarrow \text{ not true})$$

$$\implies \text{first-order model of } f \text{ at } x: L_x(z) = \langle \nabla f(x), z - x \rangle + f(x)$$

- ▶ f differentiable at $x \implies \nabla f(x)$ gives all $\frac{\partial f}{\partial d}$ [5, Ex 5.3.19]:

$$\forall d \in \mathbb{R}^n \quad \frac{\partial f}{\partial d}(x) = \langle \nabla f(x), d \rangle \quad (\longleftarrow \exists)$$

- ▶ [5, Th. 5.3.10, Th. 5.3.7] $\exists \delta > 0$ s.t. $\forall i \frac{\partial f}{\partial x_i}(z)$ continuous $\forall z \in \mathcal{B}(x, \delta)$

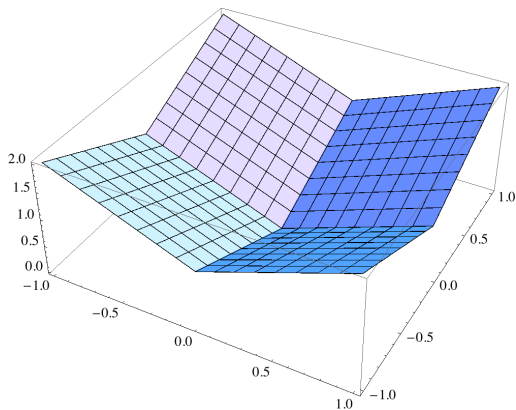
$$\implies f \text{ differentiable at } x \implies f \text{ continuous at } x$$

- ▶ $\frac{\partial f}{\partial x_i} \in C^0 \implies f$ differentiable everywhere $\equiv f \in C^1$

(but $\not\leftarrow$, \exists weird f differentiable with discontinuous $\frac{\partial f}{\partial x_i}$ [5, Ex. 5.3.9])

- ▶ (non)differentiability in \mathbb{R}^n is much weirder than in \mathbb{R}

- ▶ $f(x_1, x_2) = \|[x_1, x_2]\|_1 = |x_1| + |x_2|$
- ▶ f continuous everywhere (why?)
- ▶ $\exists d \in \mathbb{R}^n$ s.t. $\nexists \frac{\partial f}{\partial d}(0, 0)$
- ▶ f non differentiable in $[0, 0]$



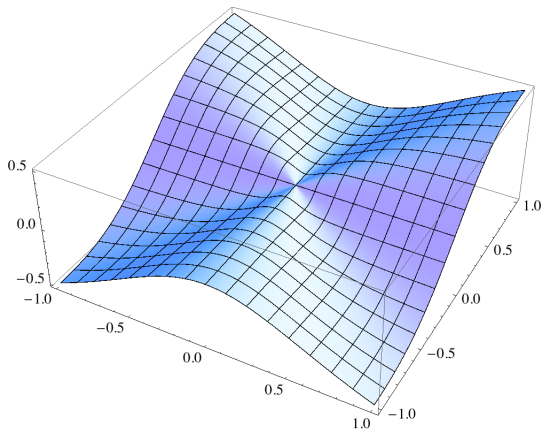
Exercise: where else f is non differentiable? Prove it is not

Non-differentiability II

▶ $f(x_1, x_2) = \frac{x_1^2 x_2}{x_1^2 + x_2^2}$

▶ Can take $f(0, 0) = 0$ as
$$\lim_{[x_1, x_2] \rightarrow [0, 0]} f(x_1, x_2) = 0$$

▶ $\exists \frac{\partial f}{\partial d} \forall d \in \mathbb{R}^n$, but
 f non differentiable in $[0, 0]$

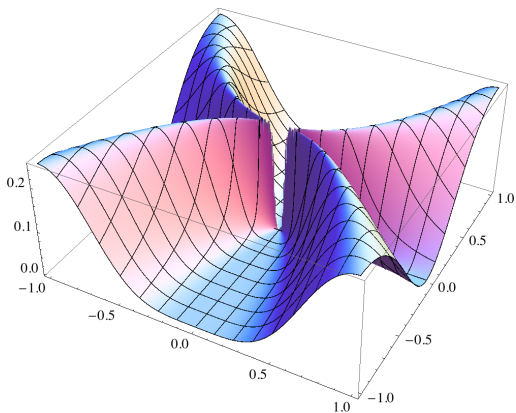


Exercise: prove $\lim_{x \rightarrow 0} f(x) = 0$, first “along lines” then in general

Exercise: prove all this (hint: compute $[\partial f / \partial d](0, 0)$ for generic $d = [d_1, d_2]$, prove it cannot 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 $\partial f / \partial x_2$ for directions where the limit is \neq)

- ▶ $f(x_1, x_2) = \left[\frac{x_1^2 x_2}{x_1^4 + x_2^2} \right]^2$
- ▶ f not continuous \implies
not differentiable at $[0, 0]$
- ▶ $\frac{\partial f}{\partial d}(0, 0) = 0 \quad \forall d \in \mathbb{R}^n$
- ▶ $\nexists \nabla f$, but $\exists v (= 0)$ s.t.
 $\frac{\partial f}{\partial d} = \langle v, d \rangle \quad \forall d \in \mathbb{R}^n$
- ▶ f does nasty things on **curved lines**, not **straight ones**

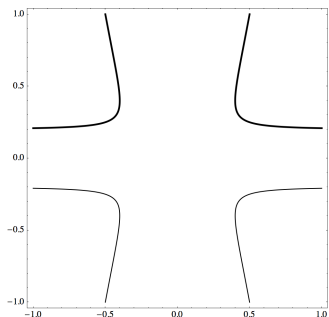


Exercise: prove $\frac{\partial f}{\partial d}(0, 0) = 0$

- ▶ In \mathbb{R}^2 , $L(L_x, f(x))$ is a **line** passing by x and $\nabla f(x) \perp L(L_x, f(x))$

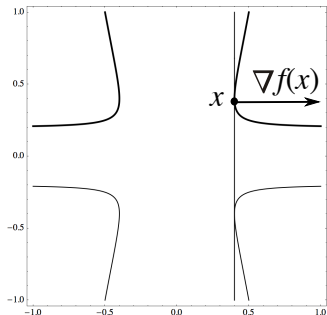
► In \mathbb{R}^n , $L(L_x, f(x))$ is a **surface** passing by x and $\nabla f(x) \perp L(L_x, f(x))$

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



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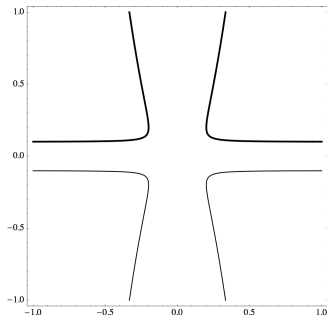


► f differentiable at $x \implies$

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

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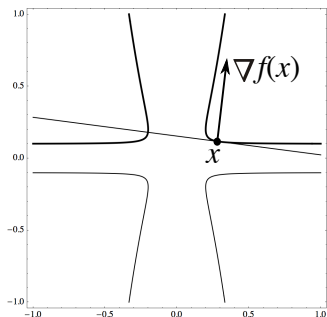


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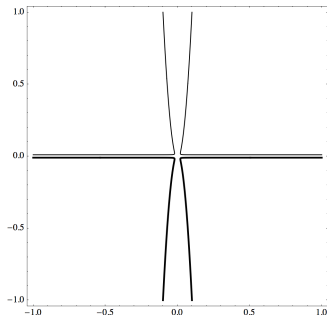
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 $L(L_x, f(x)) \perp L(f, f(x)) \perp \nabla f(x)$
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 $L(f, f(x))$ “smooth”

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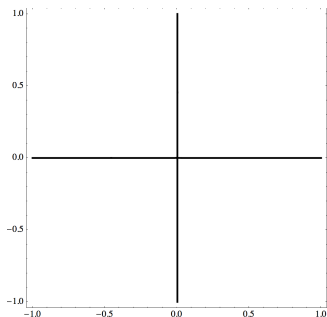
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- ▶ As $x \rightarrow \bar{x}$ where f non differentiable,
 $L(f, f(x))$ “less and less smooth”
- ▶ f non differentiable at $x \implies$
 $L(f, f(x))$ has “kinks”
- ▶ f differentiable \implies all relevant objects in \mathbb{R}^{n+1} and \mathbb{R}^n 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 $m \cdot n$ partial derivatives

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

= $m \times n$ matrix with **gradients as rows**

- ▶ Will come in handy later on for constrained optimization
- ▶ A special vector-valued function is particularly important already

▶ $\frac{\partial f}{\partial x_i} : \mathbb{R}^n \rightarrow \mathbb{R} \implies$ has partial derivatives itself

▶ Second order partial derivative
(just do it twice) $\frac{\partial^2 f}{\partial x_j \partial x_i} = \frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_i^2} = [f''_x]^j$

▶ $\nabla f(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n \implies$ has a Jacobian: Hessian (matrix) of f at x

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

$O(n^2)$ to store and (at least) compute (unless sparse), bad when n large

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

$O(n^2)$ to store and (at least) compute (unless sparse), bad when n large

▶ $f(x) = \frac{1}{2}x^T Qx + qx \implies \nabla^2 f(x) = Q$

▶ $\frac{\partial f}{\partial x_i} : \mathbb{R}^n \rightarrow \mathbb{R} \implies$ has partial derivatives itself

▶ Second order partial derivative
(just do it twice) $\frac{\partial^2 f}{\partial x_j \partial x_i} = \frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_i^2} = [f''_x]^j$

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▶ $f(x) = \frac{1}{2}x^T Qx + qx \implies \nabla^2 f(x) = Q$

▶ Second-order model = first-order model + second-order term (= better)

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

a (non-homogeneous) quadratic function \implies simple

- ▶ [5, Th. 5.3.3] $\exists \delta > 0$ s.t. $\forall z \in \mathcal{B}(x, \delta)$

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

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

\implies all eigenvalues of $\nabla^2 f(x)$ real

- ▶ Yet, extremely difficult to construct examples of **not** symmetric $\nabla^2 f$

- ▶ $f \in C^2 := \nabla^2 f(x)$ continuous everywhere $\equiv \partial^2 f / \partial x_j \partial x_i \in C^0 \forall i, j$

$\implies \nabla^2 f(x)$ symmetric everywhere and

$$\nabla f(x) \in C^1 \implies \nabla f(x) \in C^0 \implies f(x) \in C^0$$

- ▶ C^2 (strictly speaking C^3) is the best class ever for optimization, but it is sometimes necessary to make do with (much) less than that

Outline

Unconstrained multivariate optimization

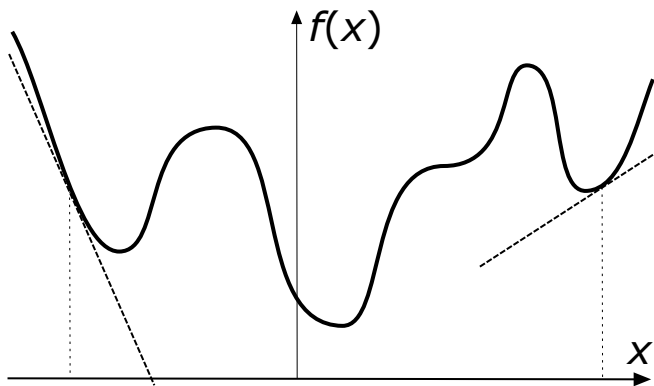
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Optimality conditions

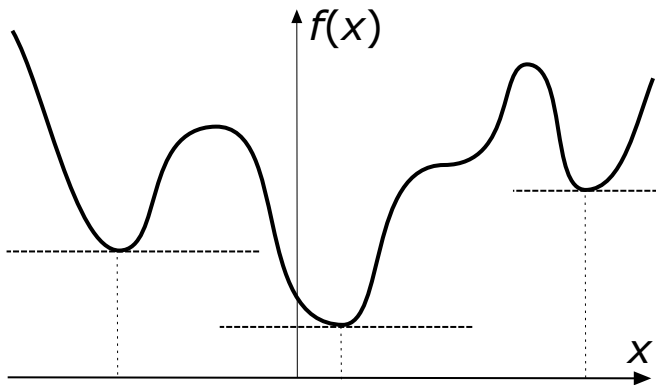
A Quick Look to Convex Functions

Wrap up & References

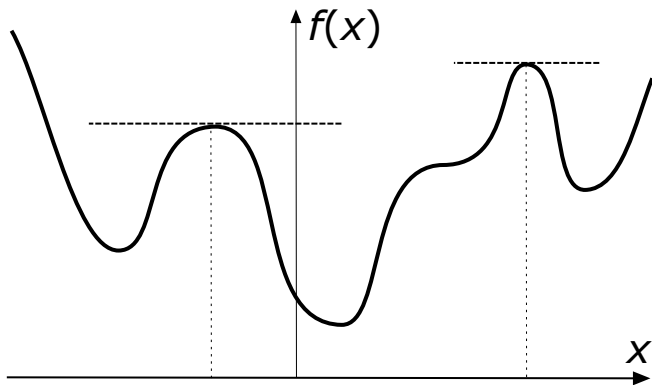
Solutions



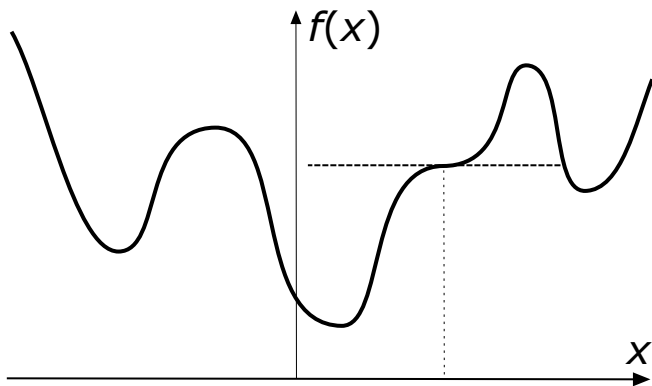
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- ▶ However, $f'(x) = 0$ also in local (hence global) maxima
... as well as in saddle points

- ▶ f differentiable at x and x local minimum $\implies \nabla f(x) = 0$
 \equiv stationary point (\nleftarrow , previous pictures for $n = 1$)
- ▶ The proof, because theorems' proofs breed algorithms
- ▶ By contradiction: x local minimum but $\nabla f(x) \neq 0$
- ▶ Prove x not local minimum not straightforward ($\nexists \equiv \forall /$):
 $\forall \varepsilon > 0$ "small enough" $\exists z \in \mathcal{B}(x, \varepsilon)$ s.t. $f(z) < f(x)$
 \equiv have to construct ∞ -ly many z better than x arbitrarily close to it
- ▶ Luckily all the z can be taken along a single $d \in \mathbb{R}^n$: $z = x + \alpha d$, $\alpha > 0$
- ▶ Can choose d , use "best" one: steepest descent direction at x
 $\equiv d$ with $\|d\| = 1$ s.t. $\frac{\partial f}{\partial d}(x)$ is most negative
 \equiv the (normalised) anti-gradient $-\nabla f(x) / \|\nabla f(x)\|$

Exercise: prove $-\nabla f(x) / \|\nabla f(x)\|$ is the steepest descent direction at x

Exercise: Why are we insisting that $\|d\| = 1$? Discuss

- ▶ Tomography $\varphi(\alpha) = \varphi_{x, -\nabla f(x)}(\alpha)$ (better **not** normalise d)
- ▶ Want to prove: $\exists \bar{\alpha} > 0$ s.t. $\varphi(\alpha) < f(x) = \varphi(0) \forall \alpha \in [0, \bar{\alpha}]$ (⚡)
- ▶ **Remainder** of first-order model at z : $R(z - x) = f(z) - L_x(z)$
- ▶ Definition of $f \in C^1$: $\lim_{h \rightarrow 0} R(h) / \|h\| = 0 \equiv R(h) \rightarrow 0$ “faster than $h \rightarrow 0$ ”
- ▶ $\varphi(\alpha) = f(x - \alpha \nabla f(x)) = f(x) + \langle -\alpha \nabla f(x), \nabla f(x) \rangle + R(-\alpha \nabla f(x))$
 $= f(x) - \alpha \|\nabla f(x)\|^2 + R(-\alpha \nabla f(x))$
negative term linear in α + (possibly) **positive “more than linear” one**
- ▶ As $\alpha \rightarrow 0$ ($\implies \|h = -\alpha \nabla f(x)\| \rightarrow 0$), it is clear who wins:

$$\lim_{\alpha \rightarrow 0} R(-\alpha \nabla f(x)) / \|\alpha \nabla f(x)\| = \lim_{h \rightarrow 0} R(h) / \|h\| = 0$$

$$\equiv \forall \varepsilon > 0 \exists \bar{\alpha} > 0 \text{ s.t. } R(-\alpha \nabla f(x)) / \|\alpha \nabla f(x)\| \leq \varepsilon \quad \forall \alpha \in [0, \bar{\alpha}]$$
- ▶ **Take $\varepsilon < \|\nabla f(x)\|$** to get $R(-\alpha \nabla f(x)) < \alpha \|\nabla f(x)\|^2 \implies$
 $\varphi(\alpha) = f(x) - \alpha \|\nabla f(x)\|^2 + R(-\alpha \nabla f(x)) < f(x)$
- ▶ Proof shows: **a small enough step along $-\nabla f(x)$ ($\neq 0$) yields a better z**

- ▶ Stationary point $\not\Rightarrow$ local minimum: **how to tell them apart?**
- ▶ **First-order model can't**, it is “flat”: need to look at **curvature** of f
- ▶ If f were **quadratic** I would know: **look at eigenvalues** of $Q = \nabla^2 f(x)$
- ▶ Obvious idea: **approximate f with a quadratic function** =
second-order model = $Q_x(z) = L_x(z) + \frac{1}{2}(z-x)^T \nabla^2 f(x)(z-x)$
- ▶ $\nabla Q_x(x) = \nabla L_x(x) = \nabla f(x) \implies \nabla Q_x(x) = 0$ (**check**)
- ▶ Hence, $\nabla^2 f(x) \succeq 0 \iff x$ (global) minimum of Q_x
- ▶ Can prove it (almost) holds for f , too:

$$f \in C^2: x \text{ local minimum} \implies \nabla^2 f(x) \succeq 0$$

- ▶ Requires **second-order Taylor's theorem** [5, Th. 5.4.9]:

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

with $\lim_{h \rightarrow 0} R(h) / \|h\|^2 = 0 \equiv R(h) \rightarrow 0$ faster than “ $h^2 \rightarrow 0$ ”

\equiv the remainder vanishes “faster than quadratically”

Mathematically speaking: 2nd-order optimality conditions, the proof 19

- ▶ By contradiction: $f \in C^2$, x local minimum but $\nabla^2 f(x) \not\preceq 0 \equiv \exists d$ s.t. $d^T \nabla^2 f(x) d < 0$ (w.l.o.g. $\|d\| = 1$)
- ▶ $d =$ direction of negative curvature, $\varphi(\alpha) = \varphi_{x,d}(\alpha)$
- ▶ Second-order Taylor + $\nabla f(x) = 0 \equiv L_x(z) = f(x) \implies \varphi(\alpha) = f(x) + \frac{1}{2}\alpha^2 d^T \nabla^2 f(x) d + R(\alpha d)$
negative quadratic term in α + (possibly) positive “more than quadratic” one
- ▶ As α ($= \|h = \alpha d\|$ since $\|d\| = 1$) $\rightarrow 0$, it is clear who wins:
 $\lim_{\alpha \rightarrow 0} R(\alpha d) / \alpha^2 = \lim_{h \rightarrow 0} R(h) / \|h\|^2 = 0 \equiv \forall \varepsilon > 0 \exists \bar{\alpha} > 0$ s.t. $R(\alpha d) \leq \varepsilon \alpha^2 \quad \forall \alpha \in [0, \bar{\alpha}]$
- ▶ Take $(0 <) \varepsilon < -\frac{1}{2}d^T \nabla^2 f(x) d$ to get $R(\alpha d) < -\frac{1}{2}\alpha^2 d^T \nabla^2 f(x) d \implies \varphi(\alpha) = f(x) + \frac{1}{2}\alpha^2 d^T \nabla^2 f(x) d + R(\alpha d) < f(x) \quad \forall \alpha \in [0, \bar{\alpha}] \quad \nexists$
- ▶ In a local minimum, there cannot be directions of negative curvature: “when the first derivative is 0, second-order effects prevail”

- ▶ Necessary condition **almost** also sufficient: $f \in C^2$,
 $\nabla f(x) = 0$ and $\nabla^2 f(x) \succ 0 \implies x$ local minimum
- ▶ Avoids “bad case” $d^T \nabla^2 f(x) d = 0 \equiv$ zero-curvature direction
 $\equiv x$ saddle point $\approx f''(x) = 0$: would need even higher-order derivatives
- ▶ Proof: second-order Taylor $f(x+d) = f(x) + \frac{1}{2} d^T \nabla^2 f(x) d + R(d)$ with
 $\lim_{d \rightarrow 0} R(d) / \|d\|^2 = 0 \equiv \forall \varepsilon > 0 \exists \delta > 0$ s.t. $R(d) / \|d\|^2 \geq -\varepsilon$
 $\equiv R(d) \geq -\varepsilon \|d\|^2 \quad \forall d$ s.t. $\|d\| < \delta$
 $\lambda_n > 0$ min eigenvalue of $\nabla^2 f(x) \implies d^T \nabla^2 f(x) d \geq \lambda_n \|d\|^2$
 Take $\varepsilon < \lambda_n / 2$: then, $\forall d$ s.t. $\|d\| < \delta$
 $f(x+d) = f(x) + \frac{1}{2} d^T \nabla^2 f(x) d + R(d) \geq f(x) + \frac{\lambda_n - \varepsilon}{2} \|d\|^2$
- ▶ It **proves more than we asked**: f grows “at least quadratically around x ”
 $\exists \delta > 0$ and $\gamma > 0$ s.t. $f(z) \geq f(x) + \gamma \|z - x\|^2 \quad \forall z \in \mathcal{B}(x, \delta)$
 \equiv strong (local) optimality

Outline

Unconstrained multivariate optimization

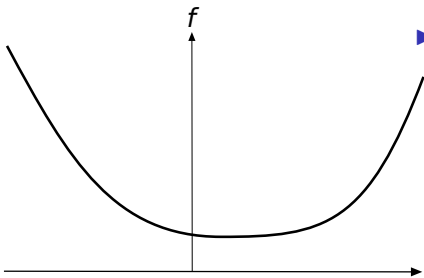
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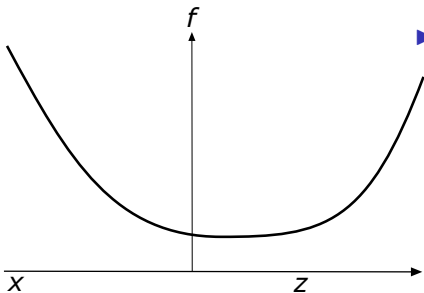
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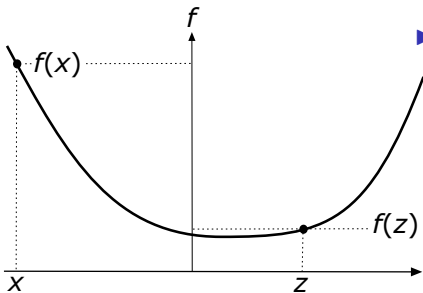
Solutions



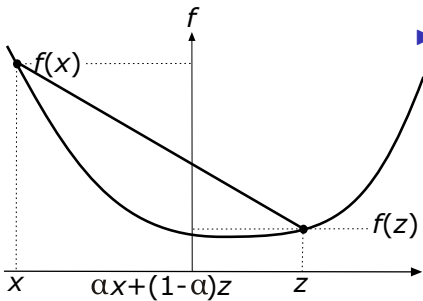
► f convex \equiv



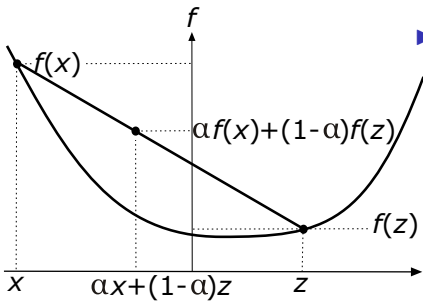
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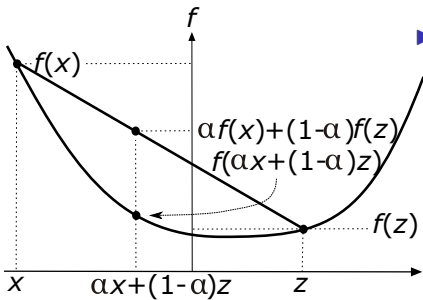


► f convex $\equiv \forall x, z \in \mathbb{R}^n, \alpha \in [0, 1]$

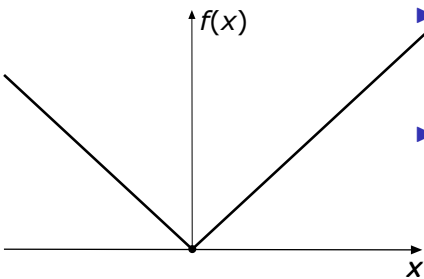


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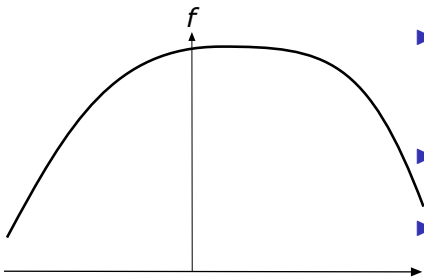
$$\alpha f(x) + (1 - \alpha)f(z)$$



- f convex $\equiv \forall x, z \in \mathbb{R}^n, \alpha \in [0, 1]$
 $\alpha f(x) + (1-\alpha)f(z) \geq f(\alpha x + (1-\alpha)z)$



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- ▶ Convex $\not\Rightarrow C^1$ (ex. $\|\cdot\|_1$)

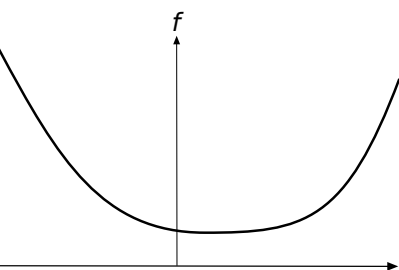


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 $\alpha f(x) + (1 - \alpha)f(z) \geq f(\alpha x + (1 - \alpha)z)$
- ▶ Convex $\not\Rightarrow C^1$ (ex. $\|\cdot\|_1$)
- ▶ f concave $\equiv -f$ convex

- ▶ $\max\{f(x) : x \in \mathbb{R}^n\} = +\infty$ (unless $f(x) = c$); sounds familiar?
- ▶ In fact, f quadratic convex $\equiv Q \succeq 0$
- ▶ Exactly the opposite for f concave ($Q \preceq 0$): as a great man said,
 “(convex) optimization is a one-sided world”
- ▶ Only f both convex and concave: linear
- ▶ How do you tell if a function is convex?

▶ $f \in C^1$ convex $\iff \nabla f$ monotone: $\langle \nabla f(z) - \nabla f(x), z - x \rangle \geq 0 \quad \forall x, z$

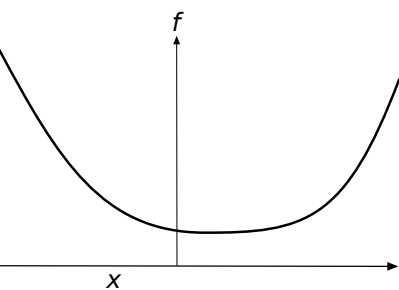
Exercise: Justify why that property is called “monotone”



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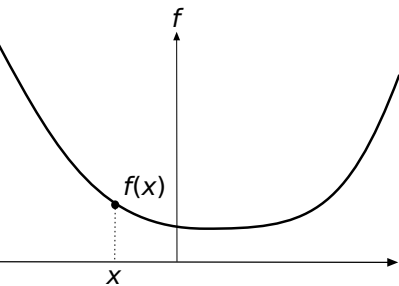
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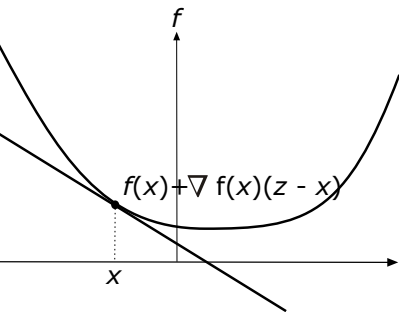
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 $L_x(z) = f(x)$

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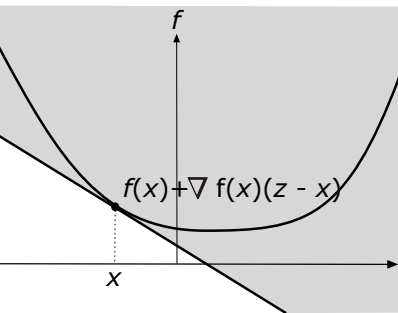
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Exercise: prove \implies “by prime principles”

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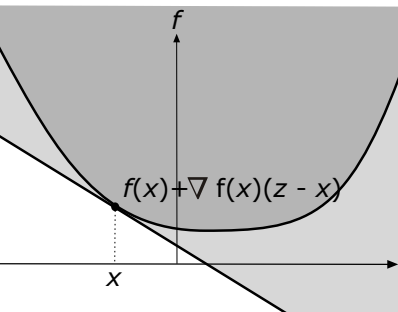
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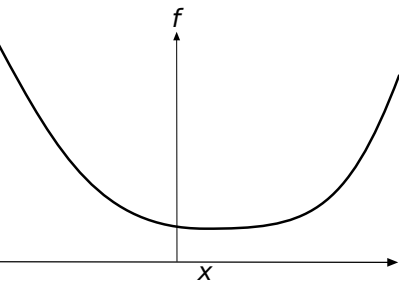
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- Geometrically: the **epigraph** is an half-space that contains that of f ($\text{epi}(L_x) \supseteq \text{epi}(f)$)

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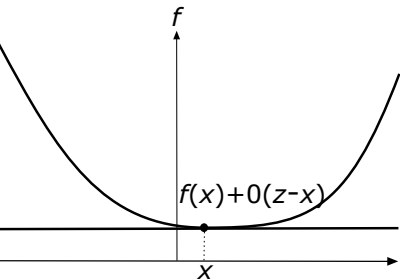
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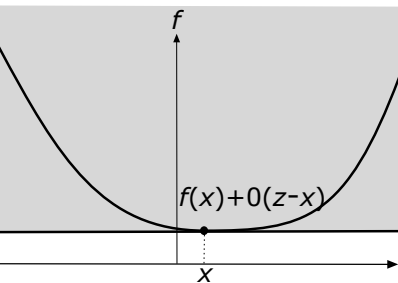
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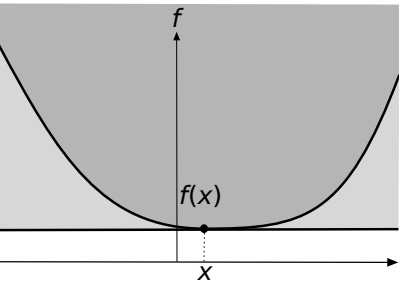
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- ▶ Geometrically: the **epigraph** is an half-space that contains that of f ($\text{epi}(L_x) \supseteq \text{epi}(f)$)

- ▶ $\nabla f(x) = 0 \implies f(z) \geq f(x) \quad \forall z \in \mathbb{R}^n$
- ▶ $f \in C^1$ convex: $\nabla f(x) = 0 \iff x$ **global** minimum
- ▶ $f \in C^2$: f convex $\equiv \nabla^2 f(x) \succeq 0 \quad \forall x \in \mathbb{R}^n$
- ▶ $f \in C^2$ with $\nabla^2 f \succeq \tau I$ with $\tau > 0$ the **best case** for optimization
- ▶ Sometimes the best way to prove f convex, **unless it is by construction**

► Some functions are (more or less obviously) convex:

1. $f(x) = bx + c$ (affine) \iff both convex and concave (check) [nontrivial]
2. $f(x) = \frac{1}{2}x^T Qx + qx$ (quadratic) convex $\iff Q \succeq 0$
3. $f(x) = e^{ax}$ for any $a \in \mathbb{R}$
4. restricted to $x \geq 0$, $f(x) = -\ln(x)$
5. restricted to $x \geq 0$, $f(x) = x^a$ for $a \geq 1$ or $a \leq 0$
6. $f(x) = \|x\|_p$ for $p \geq 1$
7. $f(x) = \max\{x_1, \dots, x_n\}$
8. $Q \in \mathbb{R}^{n \times n}$ symmetric, eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \lambda_n$:
 $f_m(Q) = \sum_{i=1}^m \lambda_i$ (sum of m largest eigenvalues)

Exercise: Prove 3., 4. and 5.; for the latter, which a make x^a convex on all \mathbb{R} ?

Exercise: is $f(x) = \min\{x_1, \dots, x_n\}$ convex?

Mathematically speaking: Convexity-preserving operations [2, § 3.2] 24

1. f, g convex, $\delta, \beta \in \mathbb{R}_+ \implies \delta f + \beta g$ convex (non-negative combination)
2. $\{f_i\}_{i \in I}$ (∞ -ly many) convex functions $\implies f(x) = \sup_{i \in I} \{f_i(x)\}$ convex
3. f convex $\implies f(Ax + b)$ convex (pre-composition with linear mapping)
4. $f : \mathbb{R}^n \rightarrow \mathbb{R}$ convex, $g : \mathbb{R} \rightarrow \mathbb{R}$ convex increasing $\implies g(f(x))$ convex (post-composition with increasing convex function)
5. f_1, f_2 convex $\implies f(x) = \inf\{f_1(x_1) + f_2(x_2) : x_1 + x_2 = x\}$ convex (infimal convolution)
6. g convex $\implies f(x) = \inf\{g(z) : Az = x\}$ convex (value function of convex constrained problem)
7. $g(x, z) : \mathbb{R}^{n+m} \rightarrow \mathbb{R}$ convex $\implies f(x) = \inf\{g(x, z) : z \in \mathbb{R}^m\}$ convex (partial minimization)
8. $f(x)$ convex $\implies p(x, u) = uf(x/u)$ convex on $u > 0$ (perspective or dilation function of f)

Exercise: Prove 1. “from prime principles” (at least 2., 3. analogous)

- ▶ $n = 1$: f unimodal \iff **quasi**convex [1, Ex. 3.57] \equiv
 $\alpha f(x) + (1 - \alpha)f(z) \leq \max\{f(x), f(z)\}$ (??)
- ▶ f **quasi**convex $\iff \forall$ nonempty **sublevel** set $S(f, l) = \{x : f(x) \leq l\}$ is a (possibly, infinite) **interval** (in fact a **convex set**, will see) [1, Th. 3.5.2]

Exercise: Prove: f convex $\implies f$ quasiconvex, \Leftarrow not true

- ▶ Issue: algebra of quasiconvex (**not** convex) functions “weaker”
- ▶ f quasiconvex, $\delta \in \mathbb{R}_+$ $\implies \delta f$ quasiconvex **true**
- ▶ But f, g quasiconvex $\implies f + g$ quasiconvex **false**

Exercise: Prove the two statements above

- ▶ No (or much weaker) Disciplined **Quasi**Convex Programming [7],
 f “naturally” quasiconvex unlikely
- ▶ Does **not** mean impossible, you may be lucky, in fact **NN** often \approx quasiconvex

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Gradients, Jacobians, and Hessians

Optimality conditions

A Quick Look to Convex Functions

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- ▶ Multivariate local optimality “easy” with the right (first-order) information: $f \in C^1$ (but one often has to **make do with less**, will see)
- ▶ **Local optimization** \approx **nonlinear system** $\nabla f(x) = 0$, surely nontrivial
- ▶ “ f simple” (quadratic) \implies “ $\nabla f(x) = 0$ simple” (**linear** system): **quadratic models** are going to be useful
- ▶ However, **stationary points not always local minima** (may be maxima)

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- ▶ Time to move to multivariate **algorithms**

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Solutions

- ▶ For $y = 1/k \rightarrow 0$, $f(d_1y, d_2y) = [d_1^2 d_2 y^3 / ((d_1y)^4 + (d_2y)^2)]^2 \rightarrow 0$ (the degree of the numerator is $>$ of the min degree at the denominator, i.e., the numerator goes to 0 faster than the denominator) however chosen d_1 and d_2 . In the second case $f(y, y^2) = [y^4 / (y^4 + y^4)]^2 = 1/4$ **[back]**
- ▶ $\frac{\partial f}{\partial \beta d}(x) = \lim_{t \rightarrow 0} (f(x + t(\beta d)) - f(x)) / t =$
 $= \lim_{t \rightarrow 0} \beta (f(x + (t\beta)d) - f(x)) / (\beta t)$. $p = \beta t, t \rightarrow 0 \implies p \rightarrow 0$
 $\implies \frac{\partial f}{\partial \beta d}(x) = \lim_{p \rightarrow 0} \beta (f(x + pd) - f(x)) / p = \beta \frac{\partial f}{\partial d}(x)$ **[back]**
- ▶ In all points $[0, x_2]$: for $d = [1, 0]$, $\varphi[0, x_2], d(\alpha) = |\alpha| + |x_2|$ is nondifferentiable in 0, i.e., $\partial f / \partial d \nexists$; analogous for $[x_1, 0]$ **[back]**

- Fix any $[d_1, d_2]$: $\lim_{t \rightarrow 0} f(td_1, td_2) = \lim_{t \rightarrow 0} \frac{t^3 d_1^2 d_2}{t^2(d_1^2 + d_2^2)} = 0$. For the general result we use the definition of limit: for any $\varepsilon > 0$ we find $\delta > 0$ s.t. $\|[x_1, x_2]\| \leq \delta \implies |f(x_1, x_2)| \leq \varepsilon$. $\|[x_1, x_2]\| = \sqrt{x_1^2 + x_2^2} \leq \delta$ implies $|x_2| \leq \delta$. Hence,

$$|f(x_1, x_2) - 0| \leq |x_2| \left(\frac{x_1^2}{x_1^2 + x_2^2} \right) \leq |x_2| \leq \delta$$

whenever $\|[x_1, x_2]\| \leq \delta$; thus, taking $\delta = \varepsilon$ works, proving that the limit is indeed 0 however chosen the converging sequence. **[back]**

- $\frac{\partial f}{\partial [d_1, d_2]}(0, 0) = \lim_{t \rightarrow 0} \frac{f(td_1, td_2) - f(0, 0)}{t} = \lim_{t \rightarrow 0} \frac{t^3 d_1^2 d_2}{t^3(d_1^2 + d_2^2)} = f(d_1, d_2)$, clearly not a linear function **[back]**

- $\nabla f(x_1, x_2) = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2} \right] = \left[\frac{2x_1 x_2^3}{(x_1^2 + x_2^2)^2}, \frac{x_1^2 (x_1^2 - x_2^2)}{(x_1^2 + x_2^2)^2} \right]$; for $g(x_1, x_2) = \partial f / \partial x_2$, it is easy to check that $g(\alpha, 0) = 1$ while $g(0, \alpha) = 0$, i.e., the limit along the directions $[1, 0]$ and $[0, 1]$ is different **[back]**

- ▶ Strictly speaking, defining $\frac{\partial f}{\partial d}(0, 0)$ requires $f(0, 0)$, which is undefined. However, we can take any generic direction $d = [d_1, d_2] \neq 0$ and prove that $\lim_{\alpha \rightarrow 0} f(\alpha d) = d_1^4 d_2^4 \alpha^4 / (d_2^2 + d_1^4 \alpha^2)^2 = 0$ however chosen d . In fact, if either $d_2 = 0$ or $d_1 = 0$ the numerator is always 0 while the denominator is not (they cannot be both 0). If they are both nonzero, the numerator goes to 0 while the denominator goes to $d_2^4 > 0$. Thus, only looking along lines it would be safe to define $f(0, 0) = 0$ by continuity, and therefore to have $\frac{\partial f}{\partial d}(0, 0) = 0$ for all $d \neq 0$, which gives $\frac{\partial f}{\partial d}(0, 0) = \langle [0, 0], d \rangle$ [back]

- ▶ We know that $\frac{\partial f}{\partial d}(x) = \langle \nabla f(x), d \rangle = \|\nabla f(x)\| \|d\| \cos(\theta) = \|\nabla f(x)\| \cos(\theta)$ (as $\|d\| = 1$). Clearly, this number is minimum when $\cos(\theta)$ is, i.e., $\theta = \pi \equiv \cos(\theta) = -1$. This corresponds to d being collinear to $\nabla f(x)$ with opposite direction, i.e., $d = -\nabla f(x) / \|\nabla f(x)\|$ [back]

- ▶ Because $\frac{\partial f}{\partial \beta d} = \beta \frac{\partial f}{\partial d}$, hence $\|d\| \rightarrow \infty \implies \frac{\partial f}{\partial d} \rightarrow -\infty$ (with right d) [back]

- ▶ $Q_x(z) = f(x) + \langle \nabla f(x), z - x \rangle + \frac{1}{2}(z - x)^T \nabla^2 f(x)(z - x) \implies \nabla Q_x(z) = \nabla f(x) + \nabla^2 f(x)(z - x)$, thus evaluated at $z = x$ gives $\nabla f(x)$. The derivation handily reveals that $\nabla Q_x(z)$ is a linear (vector) function of z that coincides with $\nabla f(x)$ at $z = x$, i.e., it is the first-order model of ∇f at x (in fact it uses the “gradient of the gradient”, that is, the Hessian) **[back]**

- ▶ In the univariate case the condition is $(f'(z) - f'(x))(z - x) \geq 0$, i.e., “ $f'(z) - f'(x)$ and $z - x$ have the same sign”. In other words, $z \geq x \implies f'(z) \geq f'(x)$ and $z \leq x \implies f'(z) \leq f'(x)$, i.e., f' is monotone nonincreasing **[back]**

- ▶ $\forall \alpha \in [0, 1] \alpha f(z) + (1 - \alpha)f(x) \geq f(\alpha z + (1 - \alpha)x) \implies \alpha(f(z) - f(x)) + f(x) \geq f(\alpha(z - x) + x) \implies f(z) - f(x) \geq [f(\alpha(z - x) + x) - f(x)]/\alpha$
 send $\alpha \rightarrow 0$ to get $\frac{\partial f}{\partial(z-x)}(x) = \langle \nabla f(x), z - x \rangle$ **[back]**

- This is surprisingly nontrivial. We want to prove: f both concave and convex (BCC) $\iff f(x) = \langle b, x \rangle + c$ for some $b \in \mathbb{R}^n$, $c \in \mathbb{R}$.

$$\text{BCC} \equiv f((1-\alpha)x + \alpha z) \text{ [both } \geq \text{ and } \leq \implies] = (1-\alpha)f(x) + \alpha f(z)$$

$$f(x) = \langle b, x \rangle + c \implies f((1-\alpha)x + \alpha z) = \langle b, (1-\alpha)x + \alpha z \rangle + c =$$

$$(1-\alpha)\langle b, x \rangle + \alpha\langle b, z \rangle + [(1-\alpha)c + \alpha c] =$$

$$(1-\alpha)(\langle b, x \rangle + c) + \alpha(\langle b, z \rangle + c) = (1-\alpha)f(x) + \alpha f(z); \text{ note how this crucially depends on } (1-\alpha) + \alpha = 1, \text{ it would not be true for generic } \gamma x + \delta z$$

For \impliedby , define $g(x) = f(x) - f(0)$ so that $g(0) = 0$. Since f is BCC, then also g is (trivial, or see point 1. in next slide). Hence

$$0 = g(0) = g((1 - (1/2))x + (1/2)(-x)) =$$

$$= (1 - (1/2))g(x) + (1/2)g(-x) \implies g(-x) = -g(x) \text{ (antisymmetric)}$$

We now prove: i. $g(\gamma x) = \gamma g(x)$, ii. $g(x + z) = g(x) + g(z)$

$$\text{For i., } 0 \leq \gamma \leq 1 \implies g(\gamma x) = g(\gamma x + (1-\gamma)0) =$$

$$= \gamma g(x) + (1-\gamma)g(0) = \gamma g(x). \text{ If } \gamma > 1, \text{ then } g(x) = g((1/\gamma)\gamma x) =$$

$$= g((1/\gamma)\gamma x + (1 - 1/\gamma)0) = (1/\gamma)g(\gamma x) + (1 - 1/\gamma)g(0) =$$

$$= (1/\gamma)g(\gamma x); \text{ multiply both sides by } \gamma \text{ to get } \gamma g(x) = g(\gamma x). \text{ Finally, if}$$

$$\gamma < 0 \text{ then } g(\gamma x) = g((- \gamma)(-x)) = (-\gamma)g(-x) \text{ (using the previous}$$

$$\text{results with } -\gamma > 0) = (-\gamma)(-g(x)) \text{ (using } g(-x) = -g(x)) = \gamma g(x)$$

For ii., $g(x+z) = g((1/2)2x + (1/2)2z) = (1/2)g(2x) + (1/2)g(2z) = (1/2)2g(x) + (1/2)2g(z) = g(x) + g(z)$ (using i. with $\gamma = 2$)

i. and ii. are the alternative definition of linear function, hence $\exists b \in \mathbb{R}^n$ s.t. $g(x) = \langle b, x \rangle$; thus, $f(x) = g(x) + f(0)$ is affine with $c = f(0)$, as desired **[back]**

- ▶ $[e^{ax}]'(x) = ae^{ax}$, which is positive increasing if $a > 0$, negative increasing if $a < 0$. $[-\ln(\cdot)]'(x) = -1/x$, which is negative increasing. $[x^a]'(x) = ax^{a-1}$; for $a < 0$ this is negative increasing, for $a \geq 1$ this is positive increasing. Only positive even integer a make x^a convex on all \mathbb{R} , since then ax^{a-1} is positive increasing (as the second derivative, $a(a-1)x^{a-2}$, is always positive). **[back]**
- ▶ No: consider $f(x_1, x_2) = \min\{x_1, x_2\}$ on the line $x_1 + x_2 = 0 \equiv x_2 = -x_1$, i.e., $\min\{x_1, -x_1\} = -|x_1|$ which is concave (and not linear, hence it cannot be convex) **[back]**

- ▶ $\alpha f(x) + (1 - \alpha)f(z) \geq f(\alpha x + (1 - \alpha)z) \implies$
 $\delta[\alpha f(x) + (1 - \alpha)f(z)] \geq \delta f(\alpha x + (1 - \alpha)z).$
 $\alpha g(x) + (1 - \alpha)g(z) \geq g(\alpha x + (1 - \alpha)z) \implies$
 $\beta[\alpha g(x) + (1 - \alpha)g(z)] \geq \beta g(\alpha x + (1 - \alpha)z).$
 Hence, $\delta[\alpha f(x) + (1 - \alpha)f(z)] + \beta[\alpha g(x) + (1 - \alpha)g(z)] =$
 $= \alpha(\delta f(x) + \beta g(x)) + (1 - \alpha)(\delta f(z) + \beta g(z)) \geq$
 $\delta f(\alpha x + (1 - \alpha)z) + \beta g(\alpha x + (1 - \alpha)z) \quad \text{[back]}$
- ▶ Take x s.t. $f(x) \leq l$, z s.t. $f(z) \leq l$, and any $\alpha \in [0, 1]$: then, by convexity
 $f(\alpha x + (1 - \alpha)z) \leq \alpha f(x) + (1 - \alpha)f(z) \leq \alpha l + (1 - \alpha)l = l$, i.e.,
 $\alpha x + (1 - \alpha)z \in S(f, l) \implies S(f, l)$ is a (possibly, infinite) interval (in
 general a convex set)
 On the other hand, consider the “downward spike function centered at c ”, i.e.,
 $s_c(x) = \min\{|x - c|, 1\}$. Clearly, s_c is quasiconvex: in fact, $S(f, l) = \emptyset$ if
 $l < 0$, $S(f, l) = [c - l, c + l]$ if $0 \leq l < 1$, and $S(f, l) = \mathbb{R}$ if $l \geq 1$.
 However, s_0 is not convex: in fact,
 $(1/2)s_0(0) + (1/2)s_0(2) = 1/2 < 1 = s_0((1/2)0 + (1/2)2) = s_0(1) \quad \text{[back]}$

- $S(\delta f, l) = \{x : \delta f(x) \leq l\} = \{x : \delta f(x) \leq l/\delta\} = S(f, l/\delta)$: since the latter is an interval (convex set), the former also is
To prove \nLeftarrow consider $f(x) = s_{-1}(x) + s_1(x)$ (cf. previous exercise). Clearly, $f(-1) = f(1) = 0$ but $f(x) > 0$ for all other values of x , i.e., $S(f, 0) = \{-1, 1\}$ is not an interval **[back]**