ORF522 – Linear and Nonlinear Optimization

15. Subgradient methods

Ed forum

- Convex functions rule: nonincreasing (instead of decreasing) and nondecreasing (instead of increasing)
- Without strong convexity, objective error acts better than variable error. Does this mean that
 generally, we choose objective error in our algorithms for functions without strong convexity
 and objective error for functions with strong convexity? Or can we always look at the objective
 error for different functions?
 (We can look at both. The truth: we look at what's easiest to prove:))
- If we don't have L-smooth and strong convex in the whole domain, but within some subset of the domain, and the initial point is close to the optimal, can we still get linear convergence? It seems to me that as long as the quadratic approximation is relatively accurate, we can achieve similar result.
 - (Yes, local strong convexity. There are also other conditions: regularity condition, Polyak-Lojasiewicz (PL) condition)

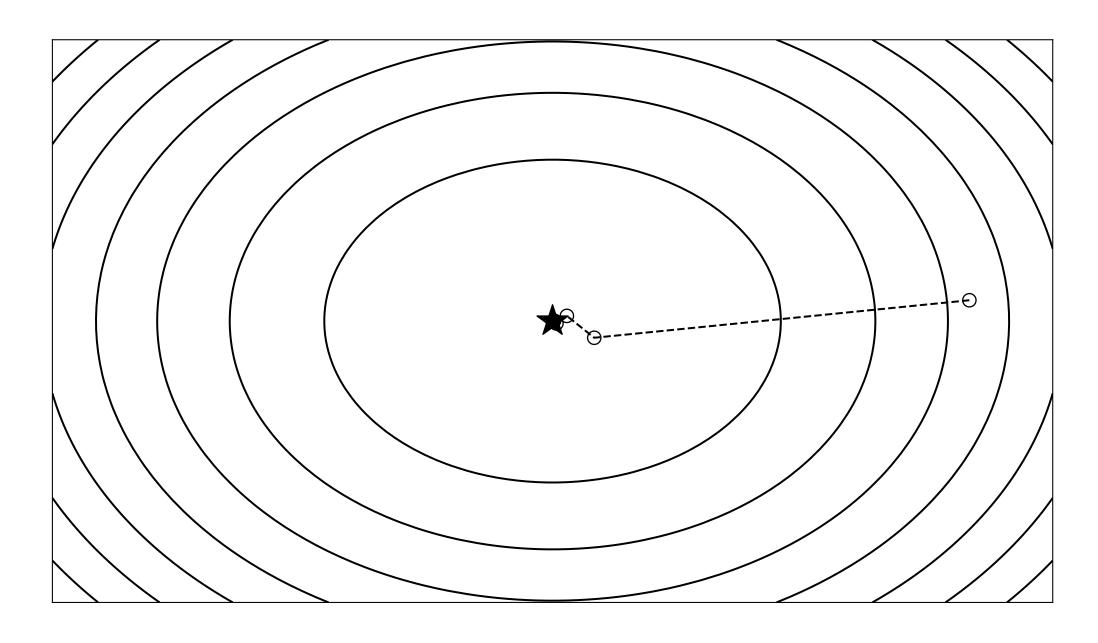
Recap

Slow convergence

Very dependent on scaling

$$f(x) = (x_1^2 + 20x_2^2)/2$$

$$f(x) = (x_1^2 + 2x_2^2)/2$$

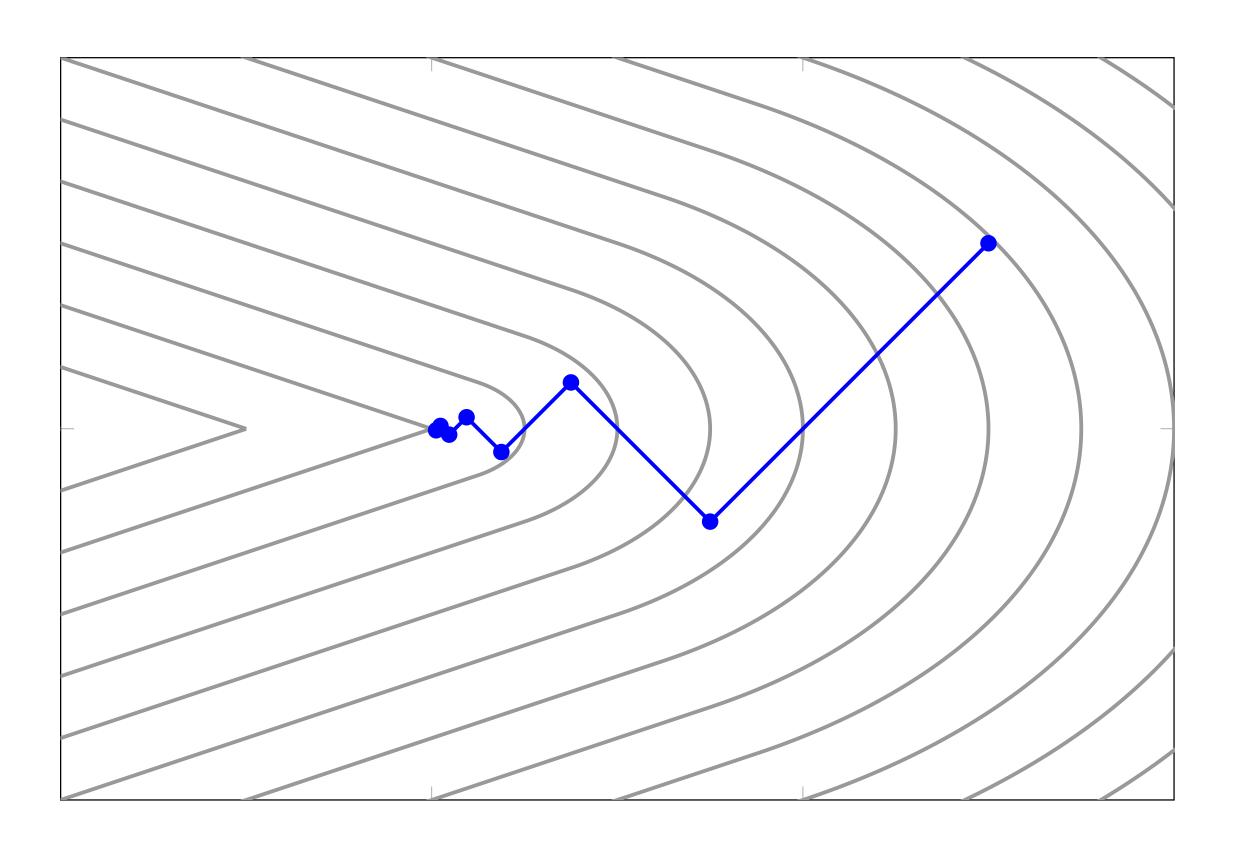


Faster

Non-differentiability

Wolfe's example

$$f(x) = \begin{cases} \sqrt{x_1^2 + \gamma x_2^2} & |x_2| \le x_1 \\ \frac{x_1 + \gamma |x_2|}{\sqrt{1 + \gamma}} & |x_2| > x_1 \end{cases}$$



Gradient descent with exact line search gets stuck at x = (0,0)

In general: gradient descent cannot handle non-differentiable functions and constraints

Today's lecture

[Chapter 3 and 8, First Order Methods in Optimization, Beck] [ee364b Lecture notes, Boyd] [Chapter 3, Lectures on Convex Optimization, Nesterov]

Subgradient methods

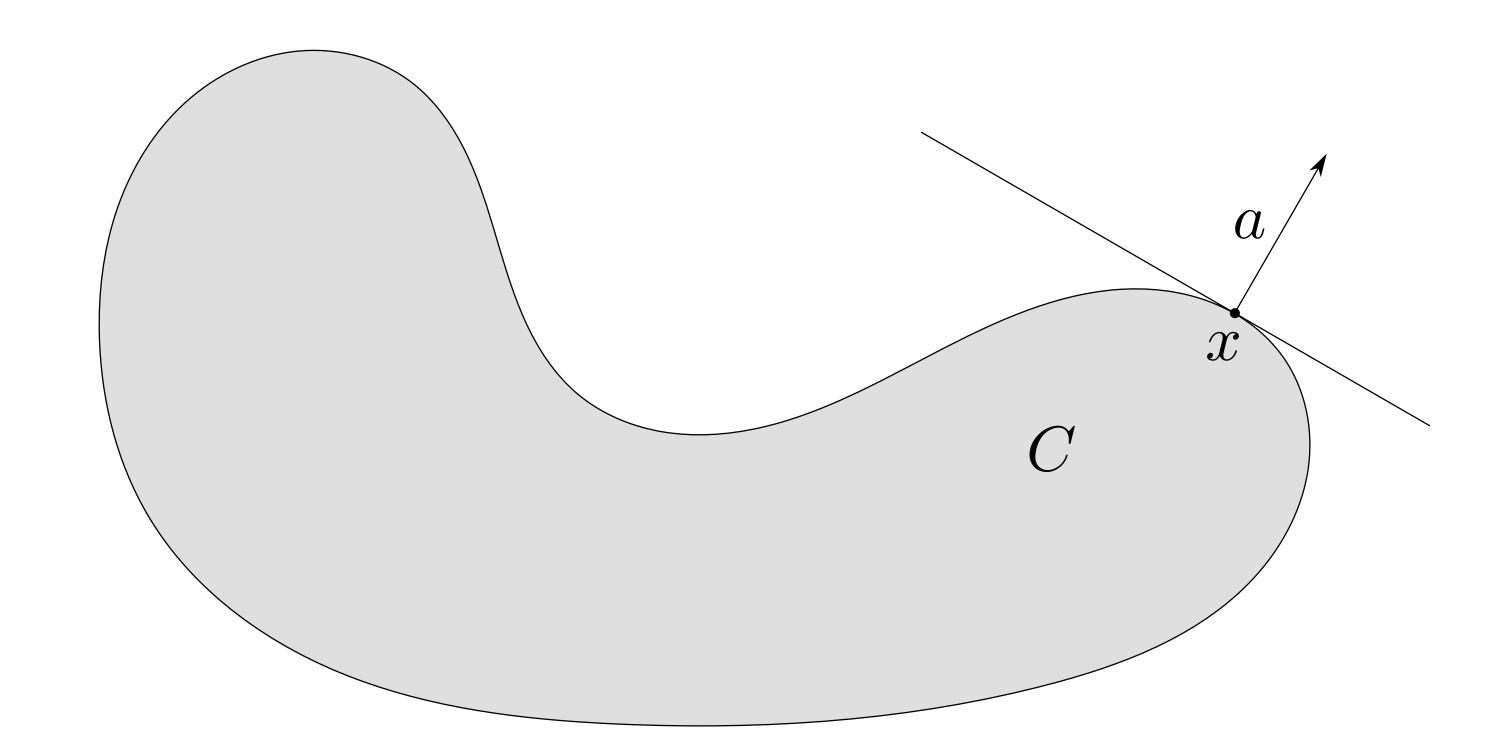
- Geometric definitions
- Subgradients
- Subgradient calculus
- Optimality conditions based on subgradients
- Subgradient methods

Geometric definitions

Supporting hyperplanes

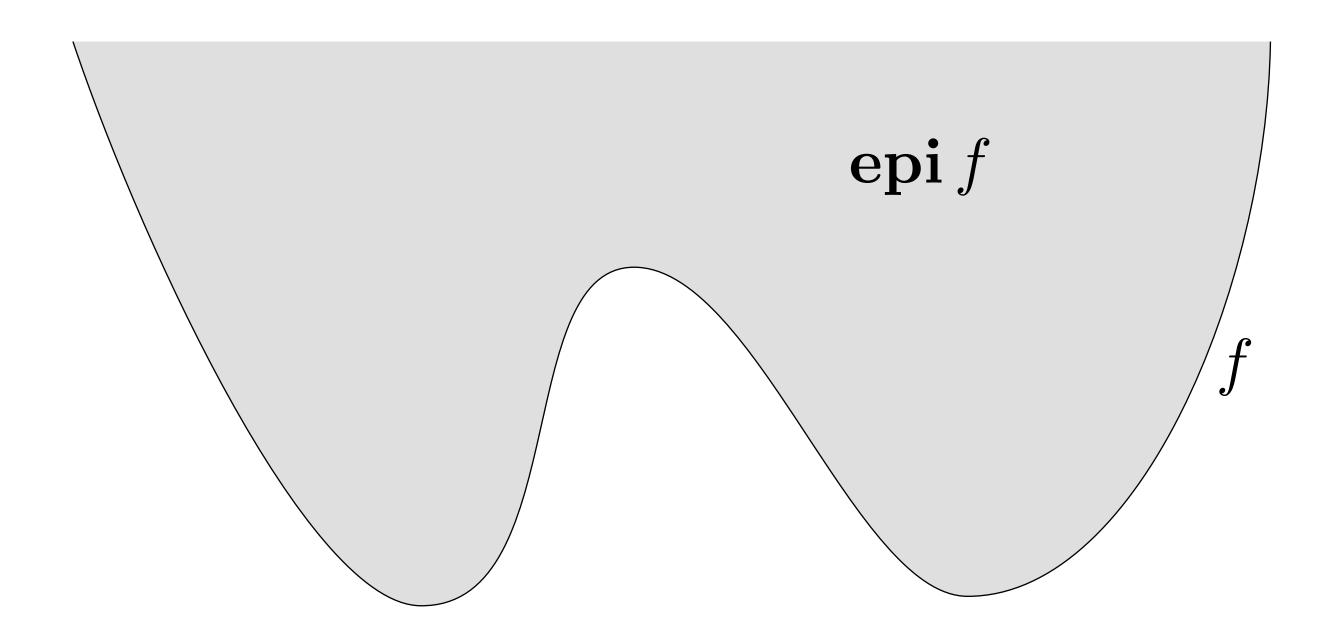
Given a set C point x at the boundary of C a hyperplane $\{z \mid a^Tz = a^Tx\}$ is a supporting hyperplane if

$$a^T(y-x) \le 0, \quad \forall y \in C$$



Function epigraph

$$\mathbf{epi} f = \{(x, t) \mid x \in \mathbf{dom} f, \ f(x) \le t\}$$

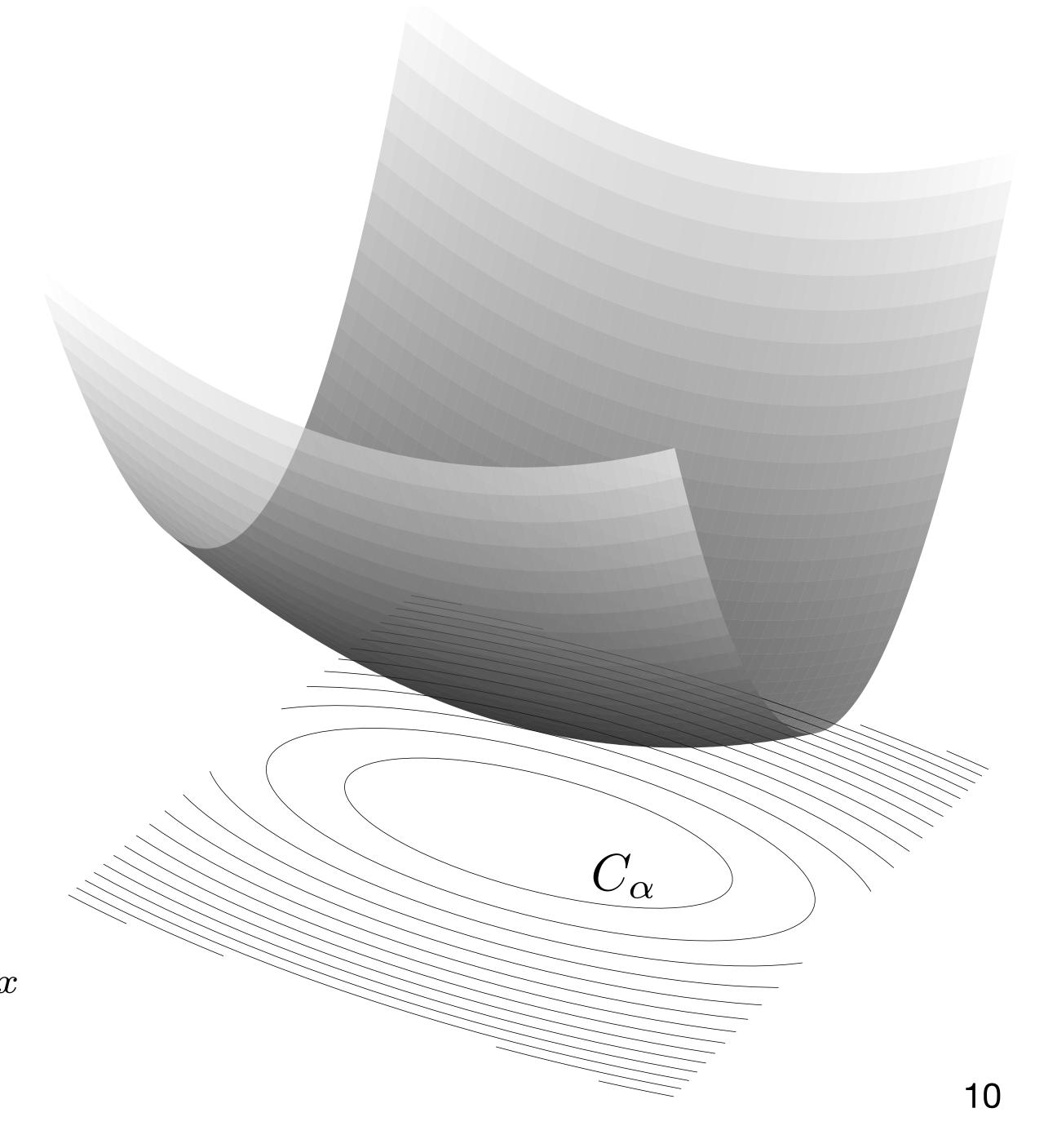


f is convex if and only if epi f is a convex set

Sublevel sets

$$C_{\alpha} = \{ x \in \mathbf{dom} \, f \mid f(x) \le \alpha \}$$

If f is convex, then C_{α} is convex $\forall \alpha$ Note converse not true, e.g., $f(x) = -e^x$



Subgradients

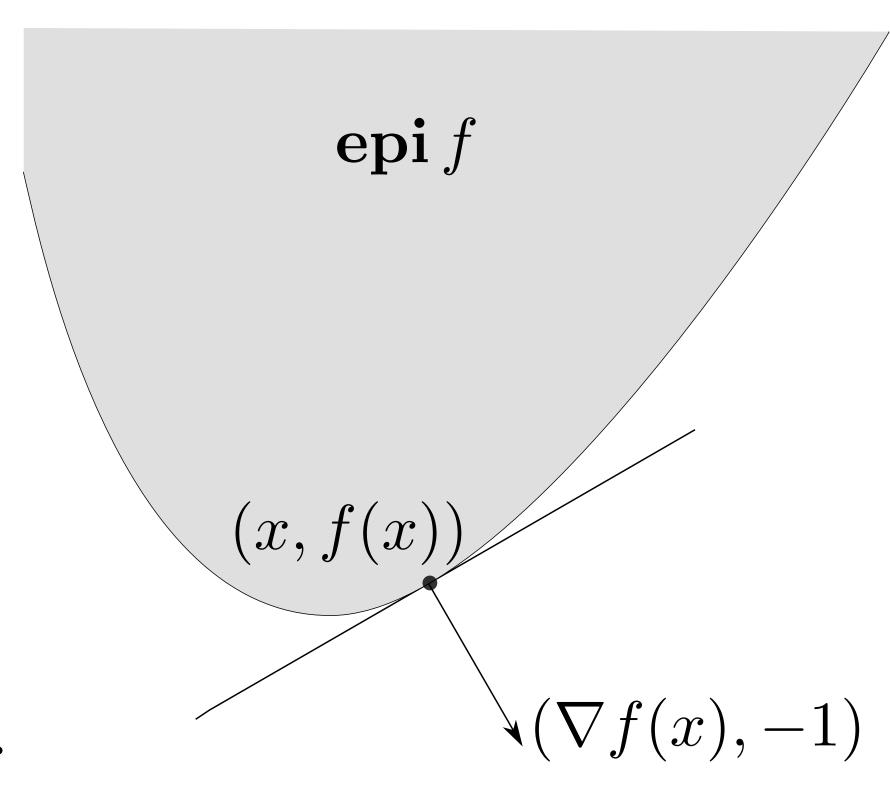
Gradients and epigraphs

For a convex differentiable function f, i.e.

$$f(y) \ge f(x) + \nabla f(x)^T (y - x), \quad \forall y \in \mathbf{dom} f$$

 $(\nabla f(x), -1)$ defines a supporting hyperplane to epigraph of f at (x, f(x))

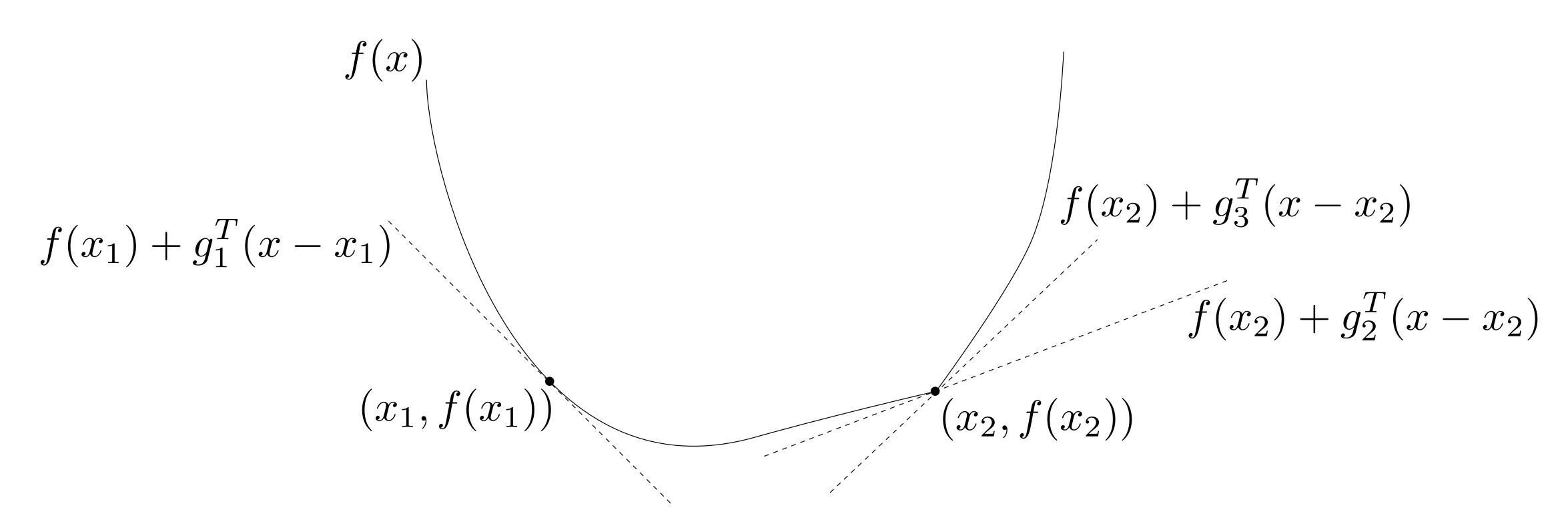
$$\begin{bmatrix} \nabla f(x) \\ -1 \end{bmatrix}^T \left(\begin{bmatrix} y \\ t \end{bmatrix} - \begin{bmatrix} x \\ f(x) \end{bmatrix} \right) \le 0, \quad \forall (y, t) \in \mathbf{epi} f$$



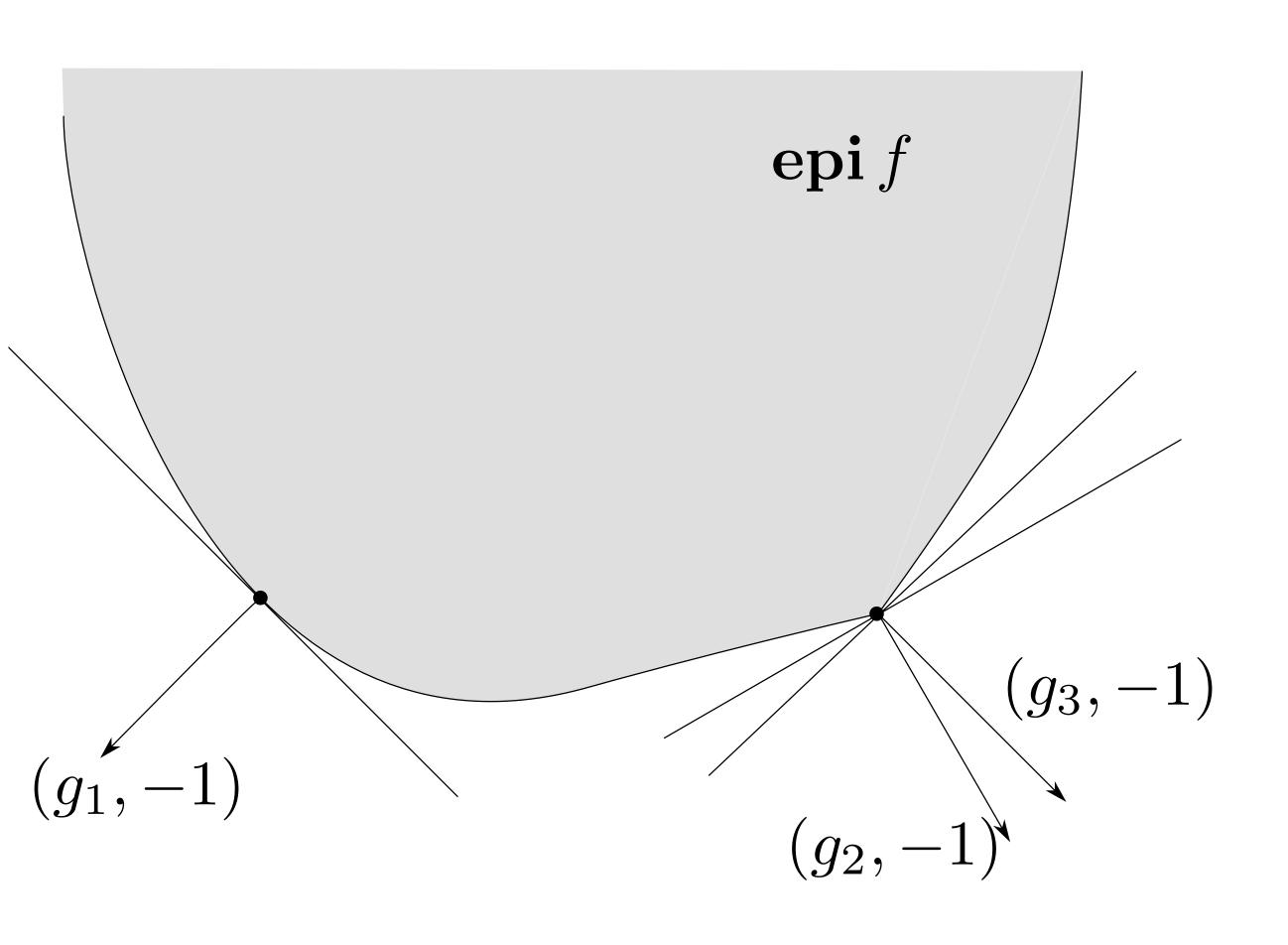
Subgradient

We say that g is a **subgradient** of function f at point x if

$$f(y) \ge f(x) + g^T(y - x), \quad \forall y$$



Subgradient properties



g is a subgradient of f at x iff (g, -1) supports $\operatorname{epi} f$ at (x, f(x))

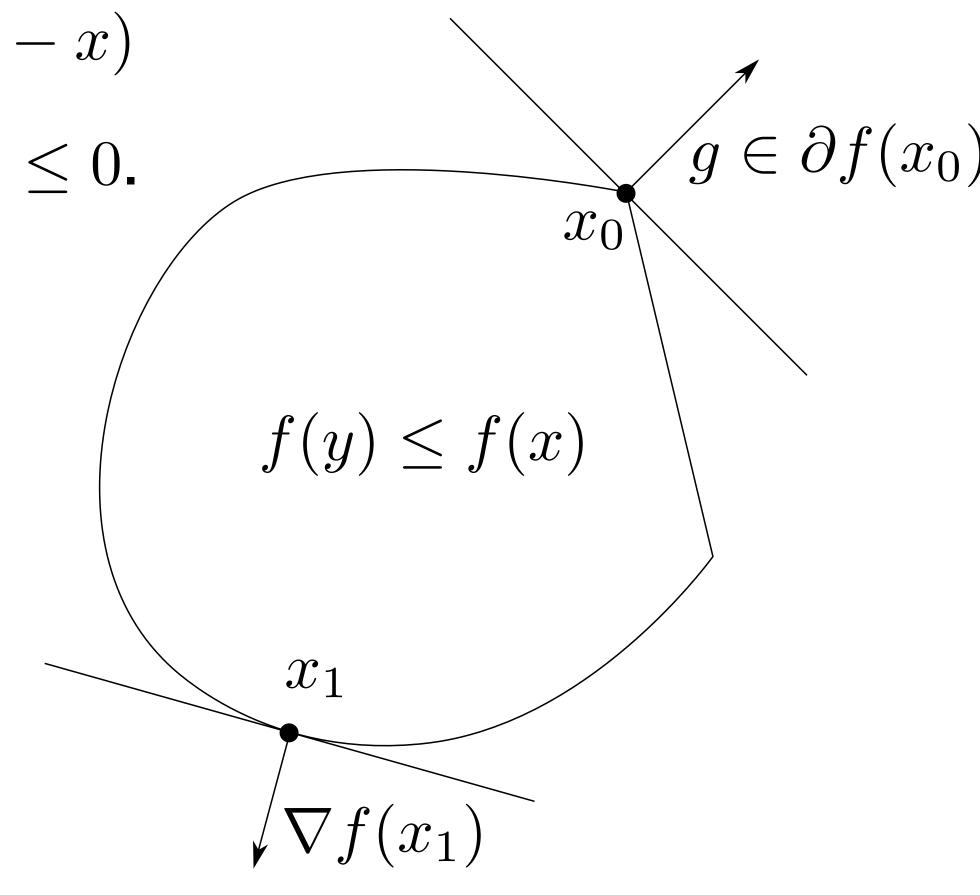
g is a subgradient of f iff $f(x) + g^T(y - x)$ is a global underestimator of f

If f is convex and differentiable, $\nabla f(x)$ is a subgradient of f at x

(Sub)gradients and sublevel sets

g being a subgradient of f means $f(y) \geq f(x) + g^T(y-x)$

Therefore, if $f(y) \le f(x)$ (sublevel set), then $g^T(y-x) \le 0$.



f differentiable at x

 $\nabla f(x)$ is normal to the sublevel set $\{y \mid f(y) \leq f(x)\}$

f nondifferentiable at x subgradients define supporting hyperplane to sublevel set through x

Subdifferential

The subdifferential $\partial f(x)$ of f at x is the set of all subgradients

$$\partial f(x) = \{ g \mid g^T(y - x) \le f(y) - f(x), \quad \forall y \in \mathbf{dom} \, f \}$$

Properties

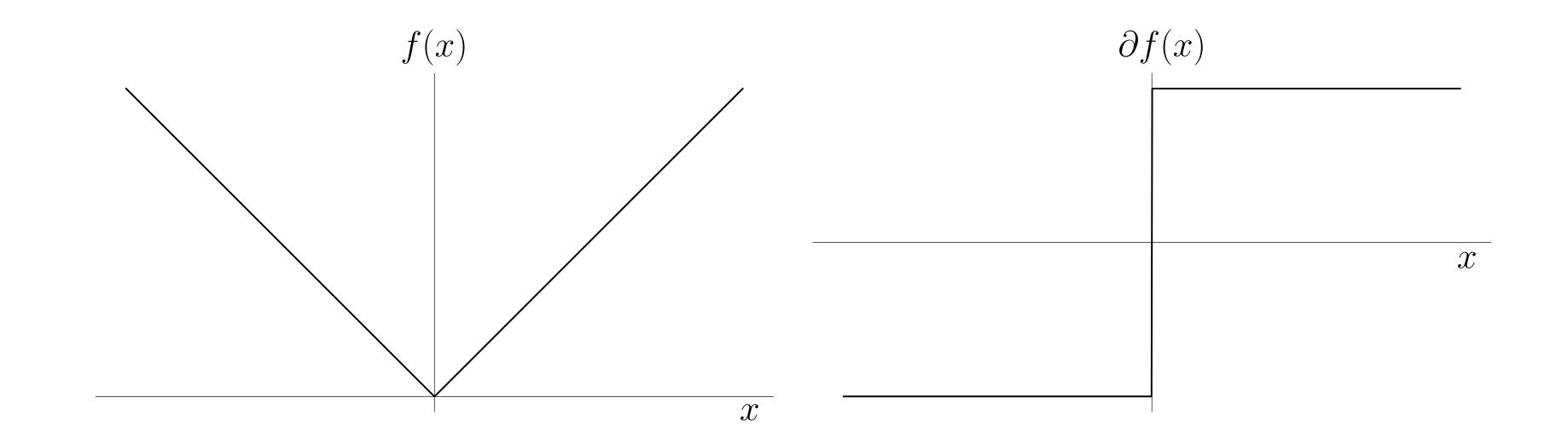
- $\partial f(x)$ is always closed and convex, also for nonconvex f. (intersection of halfspaces)
- If $\partial f(x) \neq \emptyset$, $\forall x$ then f is convex (converse not true)
- If f is convex and differentiable at x, then $\partial f(x) = {\nabla f(x)}$
- If f is convex and $\partial f(x) = \{g\}$, then f is differentiable at x and $g = \nabla f(x)$

Example

Absolute value

$$f(x) = |x|$$

$$\partial f(x) = \begin{cases} \{-1\} & x < 0 \\ [-1,1] & x = 0 \\ \{1\} & x > 0 \end{cases} = \begin{cases} \mathbf{sign}(x) & x \neq 0 \\ [-1,1] & x = 0 \end{cases}$$



Subgradient calculus

Subgradient calculus

Strong subgradient calculus

Formulas for finding the whole subdifferential $\partial f(x)$ ———— Hard

Weak subgradient calculus

Formulas for finding *one* subgradient $g \in \partial f(x)$ ———— Easy

In practice, most algorithms require only one subgradient g at point x

Basic rules

Nonnegative scaling: $\partial(\alpha f) = \alpha \partial f$ with $\alpha > 0$

Addition: $\partial (f_1 + f_2) = \partial f_1 + \partial f_2$

Affine transformation: f(x) = h(Ax + b), then

$$\partial f(x) = A^T \partial h(Ax + b)$$

Basic rules

Pointwise maxima

Finite pointwise maximum $f(x) = \max_{i=1,...,m} f_i(x)$, then

$$\partial f(x) = \mathbf{conv}\left(\bigcup\{\partial f_i(x) \mid f_i(x) = f(x)\}\right)$$
 (convex hull of active functions)

General pointwise maximum $f(x) = \max_{s \in S} f_s(x)$, then

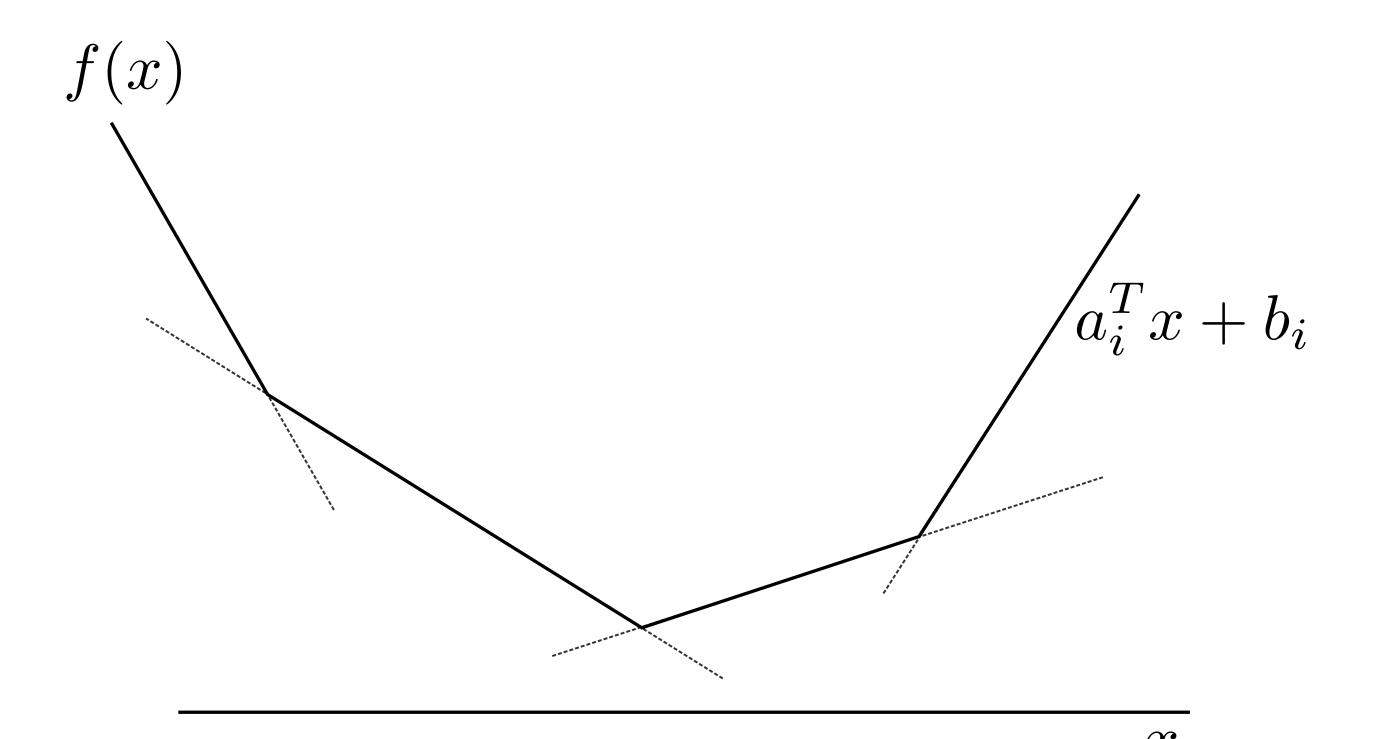
$$\partial f(x) = \mathbf{cl}\left(\mathbf{conv}\left(\bigcup\{\partial f_s(x)\mid f_s(x)=f(x)\}\right)\right)$$
 (closure of the hull)

Note: Equality requires some regularity assumptions (otherwise \supseteq) (e.g. S compact and f_s is continuous in s)

Example

Piecewise linear function

$$f(x) = \max_{i=1,...,m} (a_i^T x + b_i)$$



Subdifferential is a polyhedron

$$\partial f(x) = \mathbf{conv}\{a_i \mid i \in I(x)\}$$

$$I(x) = \{i \mid a_i^T x + b_i = f(x)\}$$

Example

Norms

Given $f = ||x||_p$ we can express it as

$$||x||_p = \max_{\|z\|_q \le 1} z^T x,$$

where q such that 1/p + 1/q = 1 defines the dual norm. Therefore,

$$\partial f(x) = \underset{\|z\|_q \le 1}{\operatorname{argmax}} z^T x$$

Example:
$$f(x) = ||x||_1 = \max_{\|s\|_{\infty} \le 1} s^T x$$

$$\partial f(x) = J_1 \times \dots \times J_n$$
 where $J_i = \begin{cases} \{-1\} & x < 0 \\ [-1,1] & x = 0 \\ \{1\} & x > 0 \end{cases}$

Weak result alternative

$$\mathbf{sign}(x) \in \partial f(x)$$

Basic rules

Composition

$$f(x) = h(f_1(x), \dots, f_k(x)), \quad h \text{ convex nondecreasing, } f_i \text{ convex}$$

$$g = q_1 g_1 + \dots + q_k g_k \in \partial f(x)$$

where
$$q \in \partial h(f_1(x), \dots, f_k(x))$$
 and $g_i \in \partial f_i(x)$

Proof

$$f(y) = h(f_1(y), \dots, f_k(y))$$

$$\geq h(f_1(x) + g_1^T(y - x), \dots, f_k(x) + g_k^T(y - x))$$

$$\geq h(f_1(x), \dots, f_k(x)) + q^T(g_1^T(y - x), \dots, g_k^T(y - x))$$

$$= f(x) + g^T(y - x)$$

Optimality conditions

Fermat's optimality condition

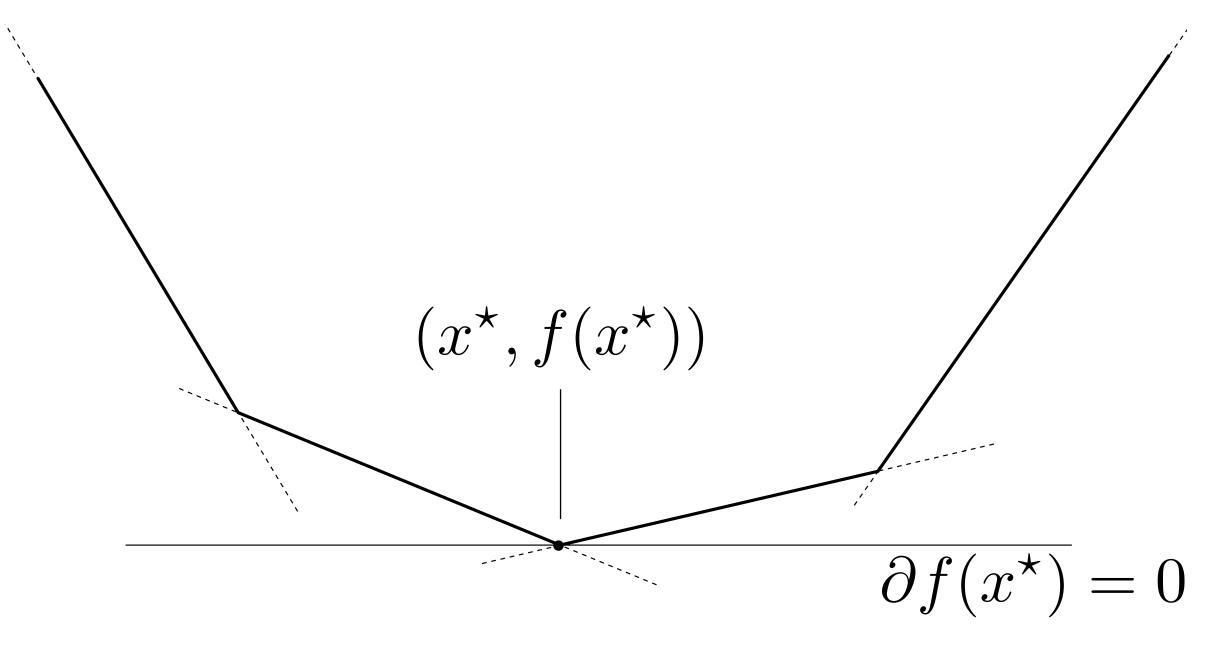
For any (not necessarily convex) function f where $\partial f(x^*) \neq \emptyset$, x^* is a local minimizer if and only if

$$0 \in \partial f(x^*)$$

Proof

A subgradient g = 0 means that, for all y

$$f(y) \ge f(x^*) + 0^T (y - x^*) = f(x^*)$$



Note differentiable case with $\partial f(x) = \{\nabla f(x)\}$

Example: piecewise linear function

Optimality condition

$$f(x) = \max_{i=1,...,m} (a_i^T x + b_i)$$
 $0 \in \partial f(x) = \mathbf{conv}\{a_i \mid a_i^T x + b_i = f(x)\}$

In other words, x^* is optimal if and only if $\exists \lambda$ such that

$$\lambda \geq 0, \quad \mathbf{1}^T \lambda = 1, \quad \sum_{i=1}^m \lambda_i a_i = 0$$
 where $\lambda_i = 0$ if $a_i^T x^\star + b_i < f(x^\star)$

Same KKT optimality conditions as the primal-dual problems

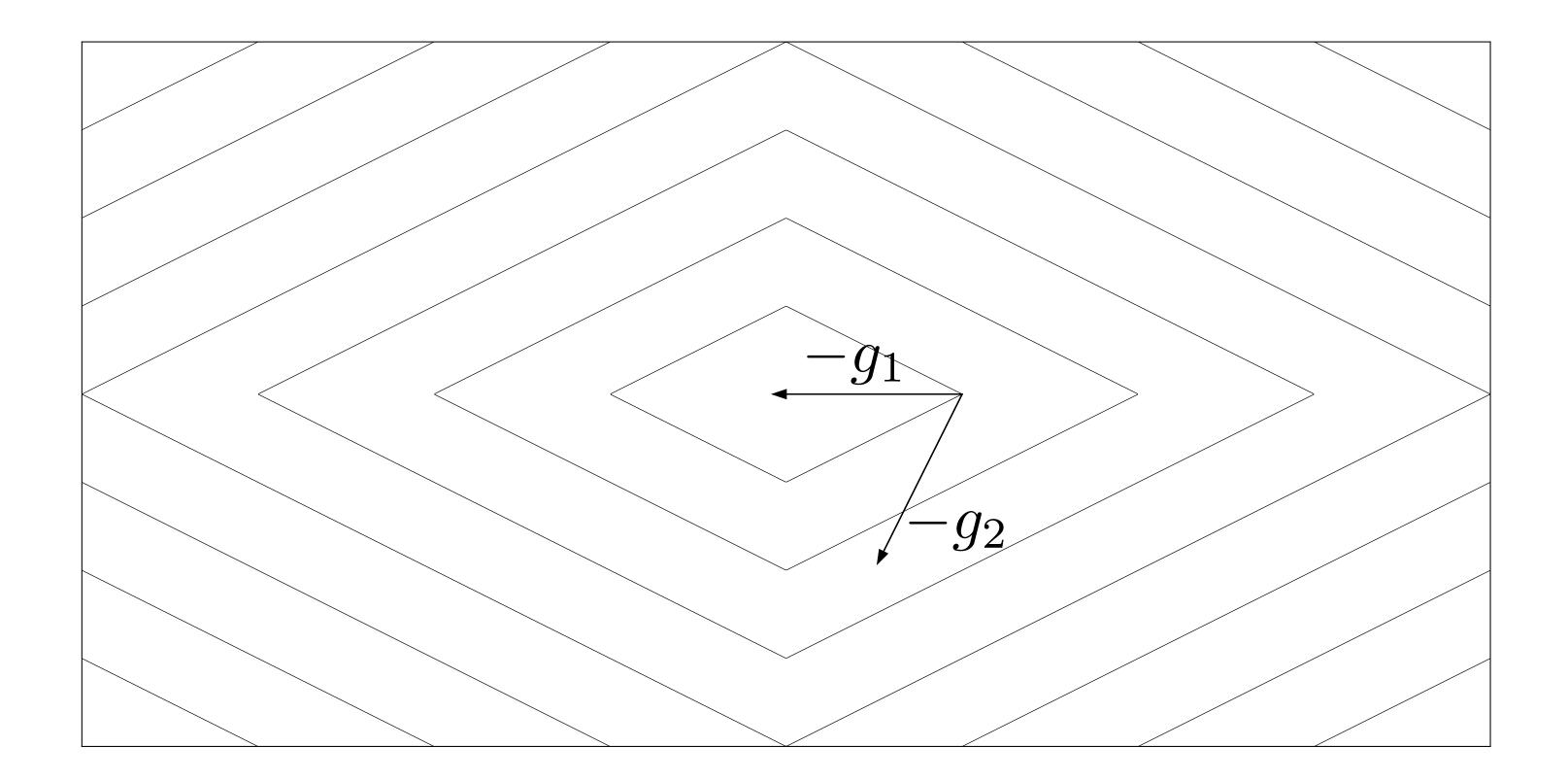
minimize
$$t$$
 subject to $Ax + b \le t\mathbf{1}$

maximize
$$b^T\lambda$$
 subject to $A^T\lambda=0$
$$\lambda \geq 0, \quad \mathbf{1}^T\lambda=1$$

Subgradient method

Negative subgradients are not necessarily descent directions

$$f(x) = |x_1| + 2|x_2|$$



$$x = (1, 0)$$

$$g_1=(1,0)\in\partial f(x)$$
 and $-g_1$ is a descent direction

$$g_2=(1,2)\in\partial f(x)$$
 and $-g_2$ is not a descent direction

Subgradient method

Convex optimization problem

minimize f(x) (optimal cost f^*)

Iterations

$$x^{k+1} = x^k - t_k g^k, \qquad g^k \in \partial f(x^k)$$

 g^k is any subgradient of f at x^k

Not a descent method, keep track of the best point

$$f_{\text{best}}^k = \min_{i=1,\dots,k} f(x^i)$$

Step sizes

Line search can lead to suboptimal points

Step sizes *pre-specified*, not adaptively computed (different than gradient descent)

Fixed:
$$t_k = t$$
 for $k = 0, \dots$

$$\sum_{k=0}^{\infty} t_k^2 < \infty, \quad \sum_{k=0}^{\infty} t_k = \infty$$

Square summable but not summable (goes to 0 but not too fast)

e.g.,
$$t_k = O(1/k)$$

Assumptions

- f is convex with $dom f = \mathbf{R}^n$
- $f(x^*) > -\infty$ (finite optimal value)
- f is Lipschitz continuous with constant G > 0, i.e.

$$|f(x) - f(y)| \le G||x - y||_2, \quad \forall x, y$$

which is equivalent to $||g||_2 \leq G$, $\forall g \in \partial f(x), \ \forall x$

Lipschitz continuity equivalence

f is Lipschitz continuous with constant G > 0, i.e.

$$|f(x) - f(y)| \le G||x - y||_2, \quad \forall x, y$$

which is equivalent to $||g||_2 \leq G$, $\forall g \in \partial f(x), \ \forall x$

Proof

If $||g|| \leq G$ for all subgradients, pick $x, g_x \in \partial f(x)$ and $y, g_y \in \partial f(y)$. Then,

$$g_x^T(x - y) \ge f(x) - f(y) \ge g_y^T(x - y)$$

$$\implies G||x - y||_2 \ge f(x) - f(y) \ge -G||x - y||_2$$

If $||g||_2 > G$ for some $g \in \partial f(x)$. Take $y = x + g/||g||_2$ such that $||x - y||_2 = 1$:

$$f(y) \ge f(x) + g^{T}(y - x) = f(x) + ||g||_{2} > f(x) + G$$

Theorem

Given a convex, G-Lipschitz continuous f with finite optimal value, the subgradient method obeys

$$f_{\text{best}}^k - f^* \le \frac{R^2 + G^2 \sum_{i=0}^k t_i^2}{2 \sum_{i=0}^k t_i}$$

where $||x^0 - x^*||_2 \le R$

Proof

Key quantity: euclidean distance to optimal set (not function value)

$$||x^{k+1} - x^*||_2^2 = ||x^k - t_k g^k - x^*||_2^2$$

$$= ||x^k - x^*||_2^2 - 2t_k (g^k)^T (x^k - x^*) + t_k^2 ||g^k||_2^2$$

$$\leq ||x^k - x^*||_2^2 - 2t_k (f(x^k) - f^*) + t_k^2 ||g^k||_2^2$$

using
$$f^* = f(x^*) \ge f(x^k) + (g^k)^T (x^* - x^k)$$

Proof (continued)

Apply inequality recursively, obtaining

$$||x^{k+1} - x^*||_2^2 \le ||x^0 - x^*||_2^2 - 2\sum_{i=0}^k t_i (f(x^i) - f^*) + \sum_{i=0}^k t_i^2 ||g^i||_2^2$$

$$\le R^2 - 2\sum_{i=0}^k t_i (f(x^i) - f^*) + G^2 \sum_{i=0}^k t_i^2$$

Using $||x^{k+1} - x^*||_2^2 \ge 0$ we get

$$2\sum_{i=0}^{k} t_i (f(x^i) - f^*) \le R^2 + G^2 \sum_{i=0}^{k} t_i^2$$

Proof (continued)

$$2\sum_{i=0}^{k} t_i (f(x^i) - f^*) \le R^2 + G^2 \sum_{i=0}^{k} t_i^2$$

Combine it with

$$\sum_{i=0}^{k} t_i (f(x^i) - f(x^*)) \ge \left(\sum_{i=0}^{k} t_i\right) \min_{i=0,\dots,k} (f(x^i) - f^*) = \left(\sum_{i=0}^{k} t_i\right) (f_{\text{best}}^k - f^*)$$

to get

$$f_{\text{best}}^k - f^* \le \frac{R^2 + G^2 \sum_{i=0}^k t_i^2}{2 \sum_{i=0}^k t_i}$$

Implications for step size rules

$$f_{\text{best}}^k - f^* \le \frac{R^2 + G^2 \sum_{i=0}^k t_i^2}{2 \sum_{i=0}^k t_i}$$

Fixed:

$$t_k = t$$
 for $k = 0, \dots$

$$f_{\text{best}}^k - f^* \le \frac{R^2 + G^2(k+1)t^2}{2(k+1)t}$$

May be suboptimal

$$\lim_{k \to \infty} f_{\text{best}}^k \le f^* + \frac{G^2 t}{2}$$

Diminishing:
$$\sum_{k=0}^{\infty} t_k^2 < \infty, \quad \sum_{k=0}^{\infty} t_k = \infty$$

e.g.,
$$t_k = \tau/(k+1)$$
 or $t_k = \tau/\sqrt{k+1}$

Optimal

$$\lim_{k \to \infty} f_{\text{best}}^k = f^*$$

Optimal step size and convergence rate

For a tolerance $\epsilon > 0$, let's find the optimal t_k for a fixed k:

$$\frac{R^2 + G^2 \sum_{i=0}^{k} t_i^2}{2 \sum_{i=0}^{k} t_i} \le \epsilon$$

Convex and symmetric in (t_0, \ldots, t_k) Hence, minimum when $t_i = t$

$$\frac{R^2 + G^2(k+1)t^2}{2(k+1)t}$$

Optimal choice
$$t = \frac{R}{G\sqrt{k+1}}$$

Convergence rate

$$f_{\text{best}}^k - f^* \le \frac{RG}{\sqrt{k+1}}$$

Iterations required

$$k = O(1/\epsilon^2)$$

(gradient descent $k = O(1/\epsilon)$)

Stopping criterion

Terminating when

$$\frac{R^2 + G^2 \sum_{i=0}^{k} t_i^2}{2 \sum_{i=0}^{k} t_i} \le \epsilon$$

is really, really slow.

Bad news

There is not really a good stopping criterion for the subgradient method

Optimal step size when f^* is known

Polyak step size

$$t_k = \frac{f(x^k) - f^*}{\|g^k\|_2^2}$$

Motivation: minimize righthand side of

$$||x^{k+1} - x^*||_2^2 \le ||x^k - x^*||_2^2 - 2t_k(f(x^k) - f^*) + t_k^2||g^k||_2^2$$

Obtaining
$$(f(x^k) - f^*)^2 \le (\|x^{k+1} - x^*\|_2^2 - \|x^k - x^*\|_2^2) G^2$$

Applying recursively,
$$f_{\mathrm{best}}^k - f^\star \leq \frac{GR}{\sqrt{k+1}}$$

Iterations required

$$k = O(1/\epsilon^2)$$

still not great

Example: 1-norm minimization

minimize $f(x) = ||Ax - b||_1$ $g = A^T \operatorname{sign}(Ax - b) \in \partial f(x)$ Diminishing step size Fixed step size t = 0.0010 $0.01/\sqrt{k+1}$ = 0.0005 10^{0} $0.001/\sqrt{k+1}$ t = 0.00010.01/(k+1) $\underset{\leftarrow}{\star} 10^{-1}$ t = 0.0001 10^{-1} Polyak 10^{-4} 10^{-4} 10^{-5} 1000 3000 2000 3000 4000 5000 6000 2000 4000 6000 5000

Efficient packages to automatically compute (sub)gradients: *Python:* JAX, PyTorch *Julia:* Zygote.jl, ForwardDiff.jl, ReverseDiff.jl

Summary subgradient method

- Simple
- Handles general nondifferentiable convex functions
- Very slow convergence $O(1/\epsilon^2)$
- No good stopping criterion

Can we do better?

Can we incorporate constraints?

Subgradient methods

Today, we learned to:

- Define subgradients
- Apply subgradient calculus
- Derive optimality conditions from subgradients
- Define subgradient method and analyze its convergence

Next lecture

Proximal algorithms