ORF522 – Linear and Nonlinear Optimization

15. Subgradient methods

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Ed Forum

- Can similar convergence results be made for stochastic gradient descent?
- In backtracking line search, do we choose and fix α and β for each iteration, and if so, what is the interpretation/significance of the value chosen?
- For the first-order characterization (Lipschitz continuous gradient) for L-smoothness of convex functions, how should I show that it is necessary and sufficient (if a convex function is L-smooth, then it has Lipschitz continuous gradient?

Recap

Equivalent L-smoothness conditions

A convex function f is L-smooth if the following equivalent conditions hold

- $\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2, \quad \forall x, y$
- $f(y) \leq f(x) + \nabla f(x)^T (y - x) + \frac{L}{2}\|y - x\|^2, \quad \forall x, y$
- $\nabla^2 f(x) \preceq LI, \quad \forall x$

Detailed proofs: Theorem 5.8 and 5.12 FMO book

Backtracking line search

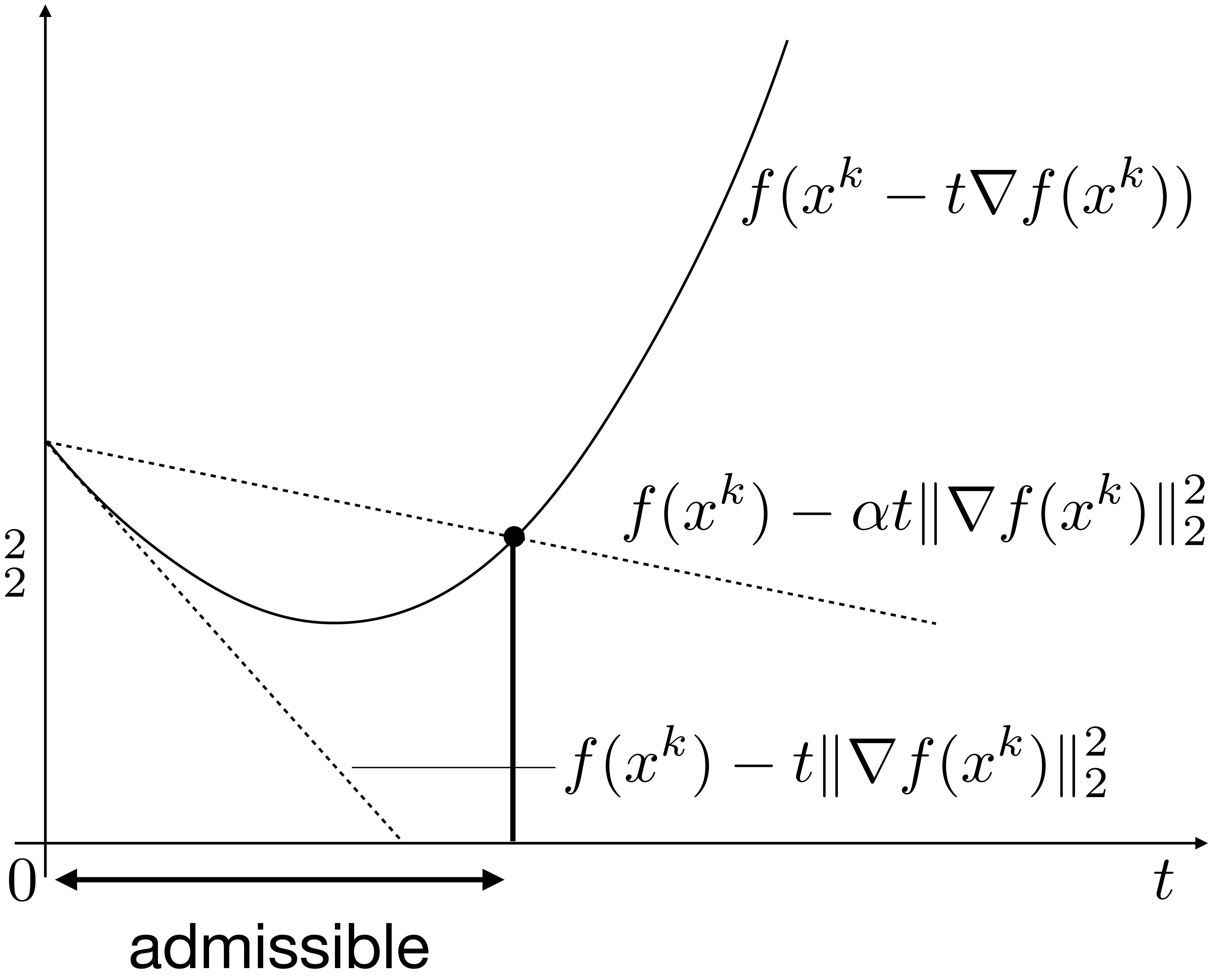
Iterations

initialization

$$t = 1, \quad 0 < \alpha \leq 1/2, \quad 0 < \beta < 1$$

while $f(x^k - t\nabla f(x^k)) > f(x^k) - \alpha t \|\nabla f(x^k)\|_2^2$

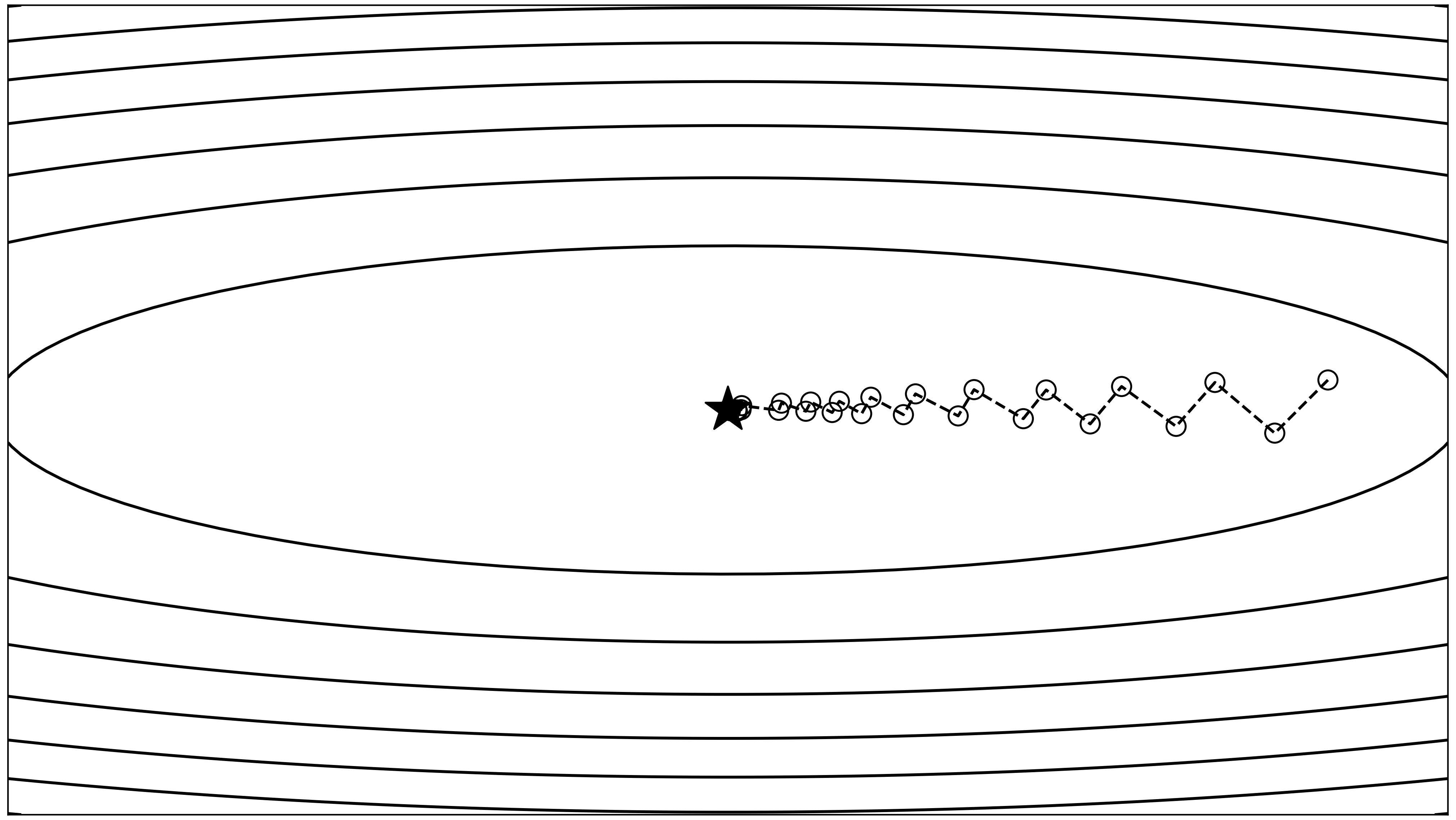
$\quad t \leftarrow \beta t$



Slow convergence

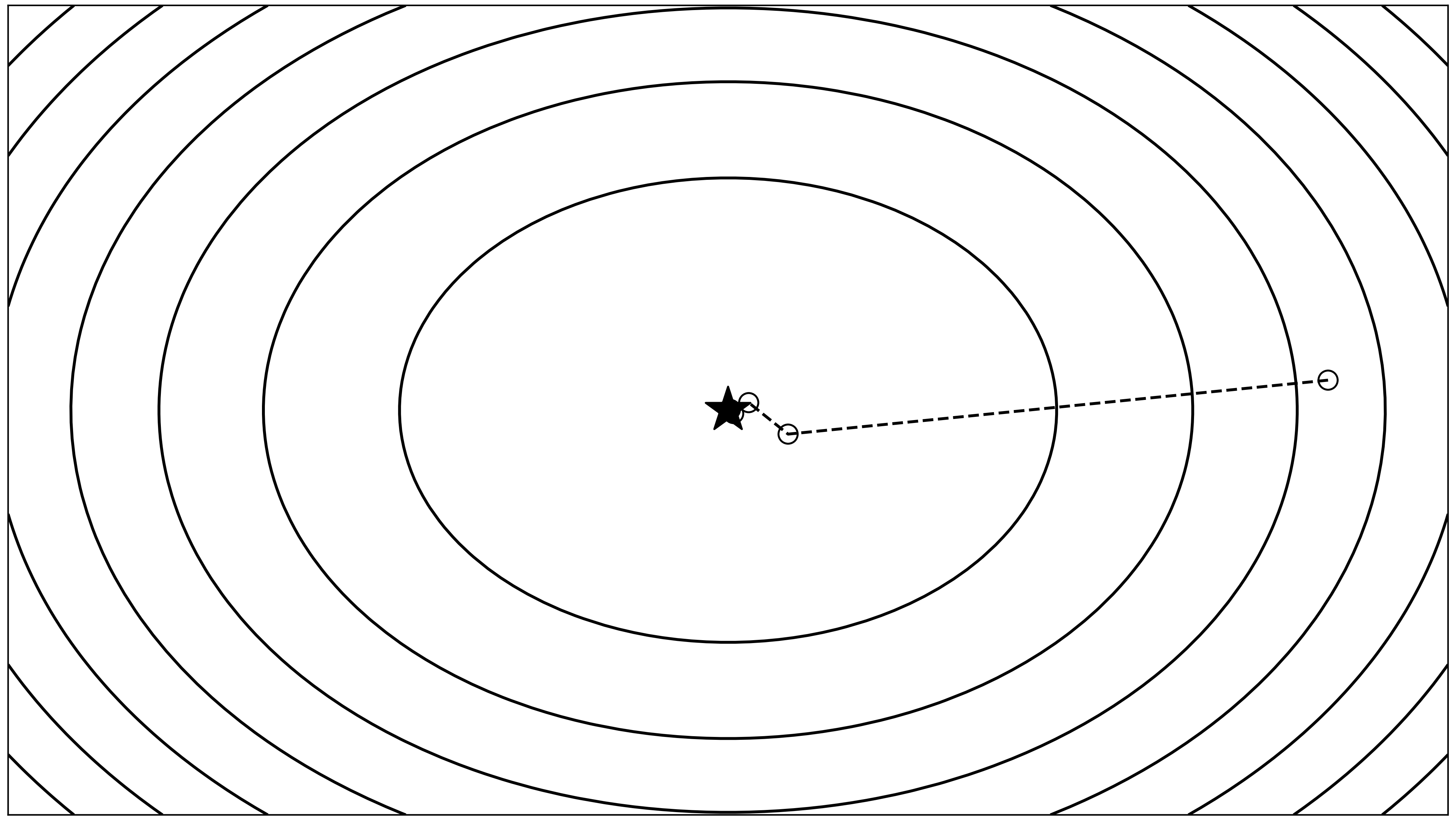
Very dependent on scaling

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



Slow convergence

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

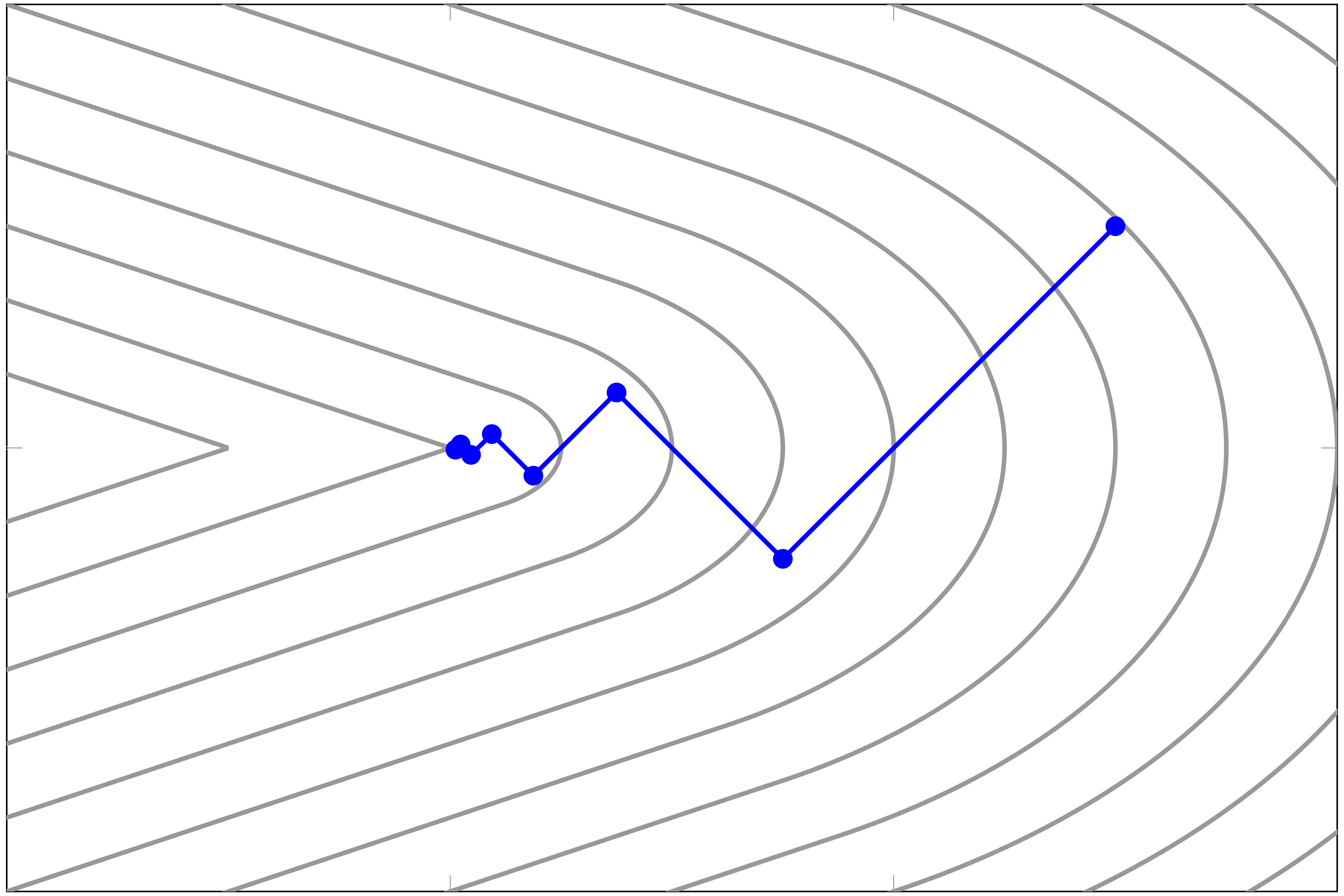


Faster

Non-differentiability

Wolfe's example

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



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, FMO][ee364b][Chapter 3, ILCO]

Subgradient methods

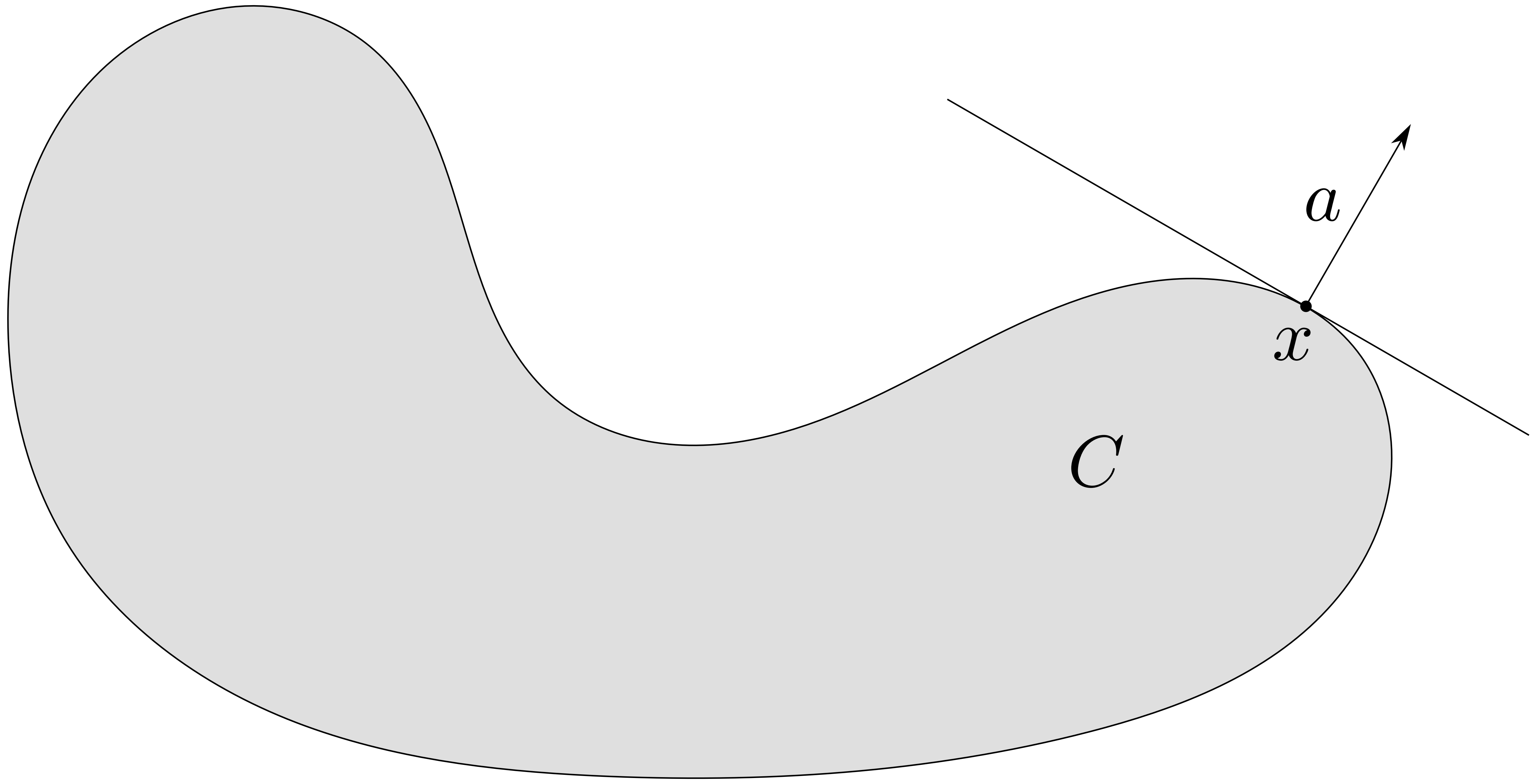
- Geometric definitions
- Subgradients
- Subgradient calculus
- Optimality conditions based on subgradients
- Subgradient methods

Geometric definitions

Supporting hyperplanes

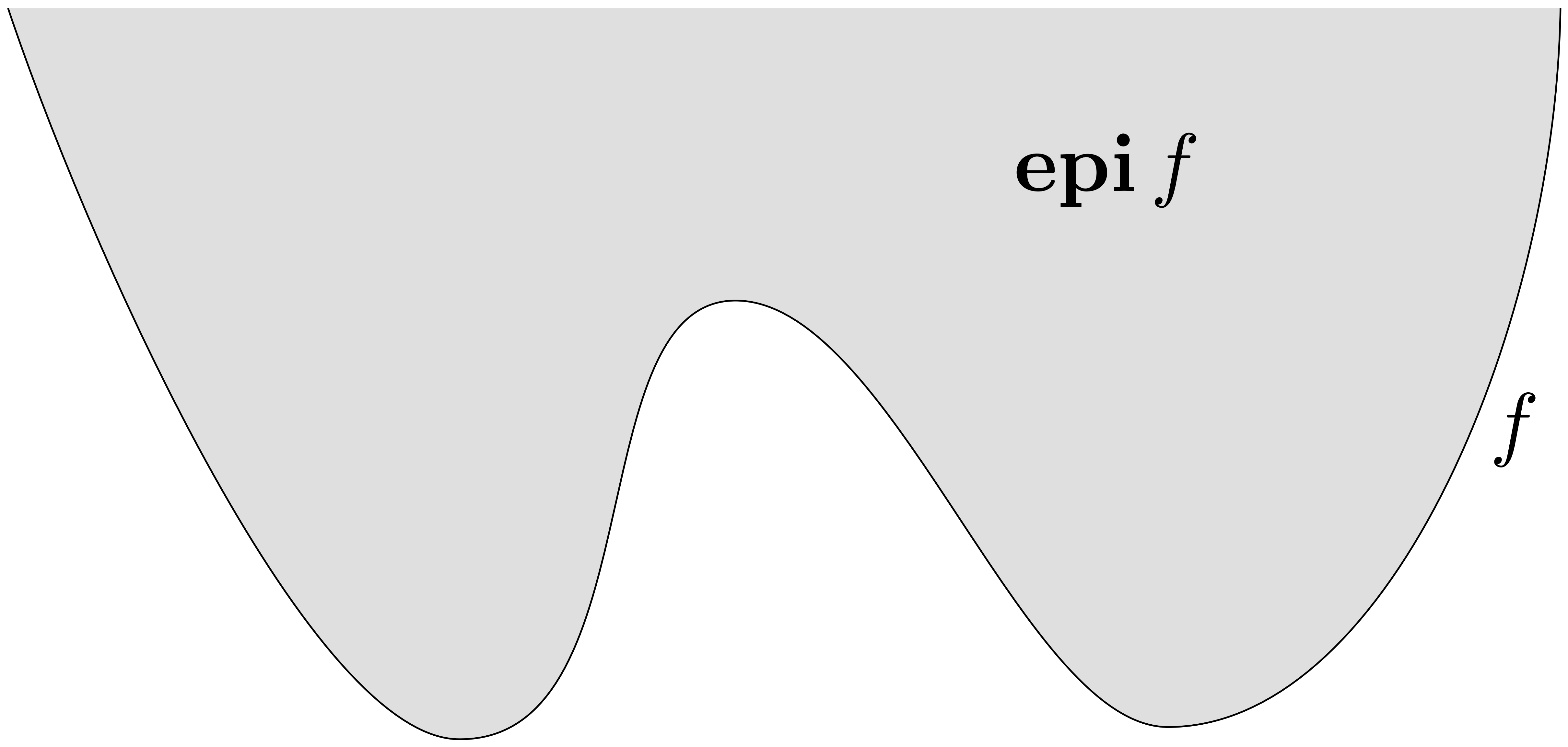
Given a set C point x at the boundary of C
a hyperplane $\{z \mid a^T z = a^T x\}$ is a **supporting hyperplane** if

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



Function epigraph

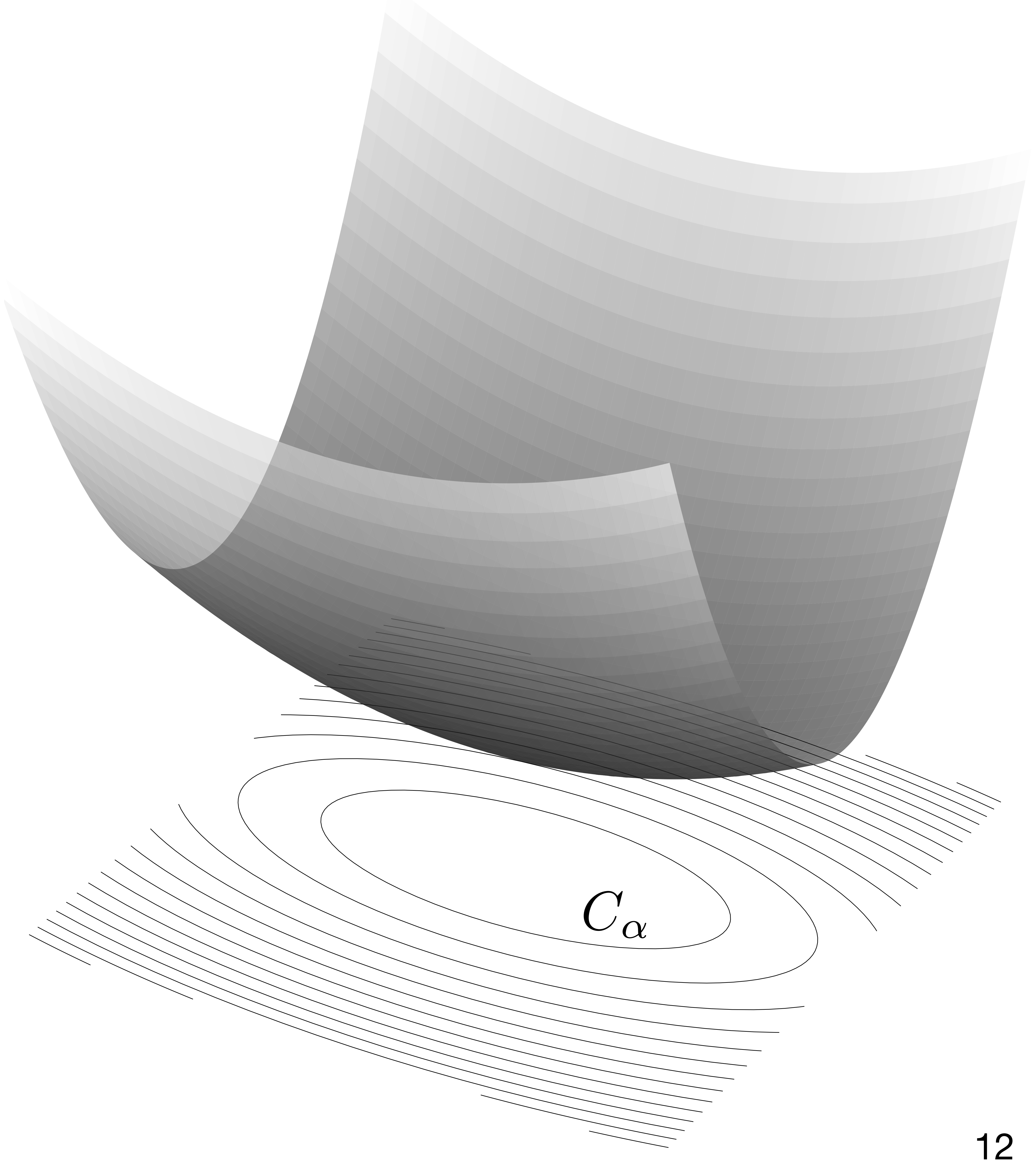
$$\mathbf{epi}\, f = \{(x,t) \mid x \in \mathbf{dom}\, f,\ f(x) \le t\}$$



f is convex if and only if $\mathbf{epi}\, f$ is a convex set

Sublevel sets

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



If f is convex, then C_α is convex $\forall \alpha$

Note converse not true, e.g., $f(x) = -e^x$

Subgradients

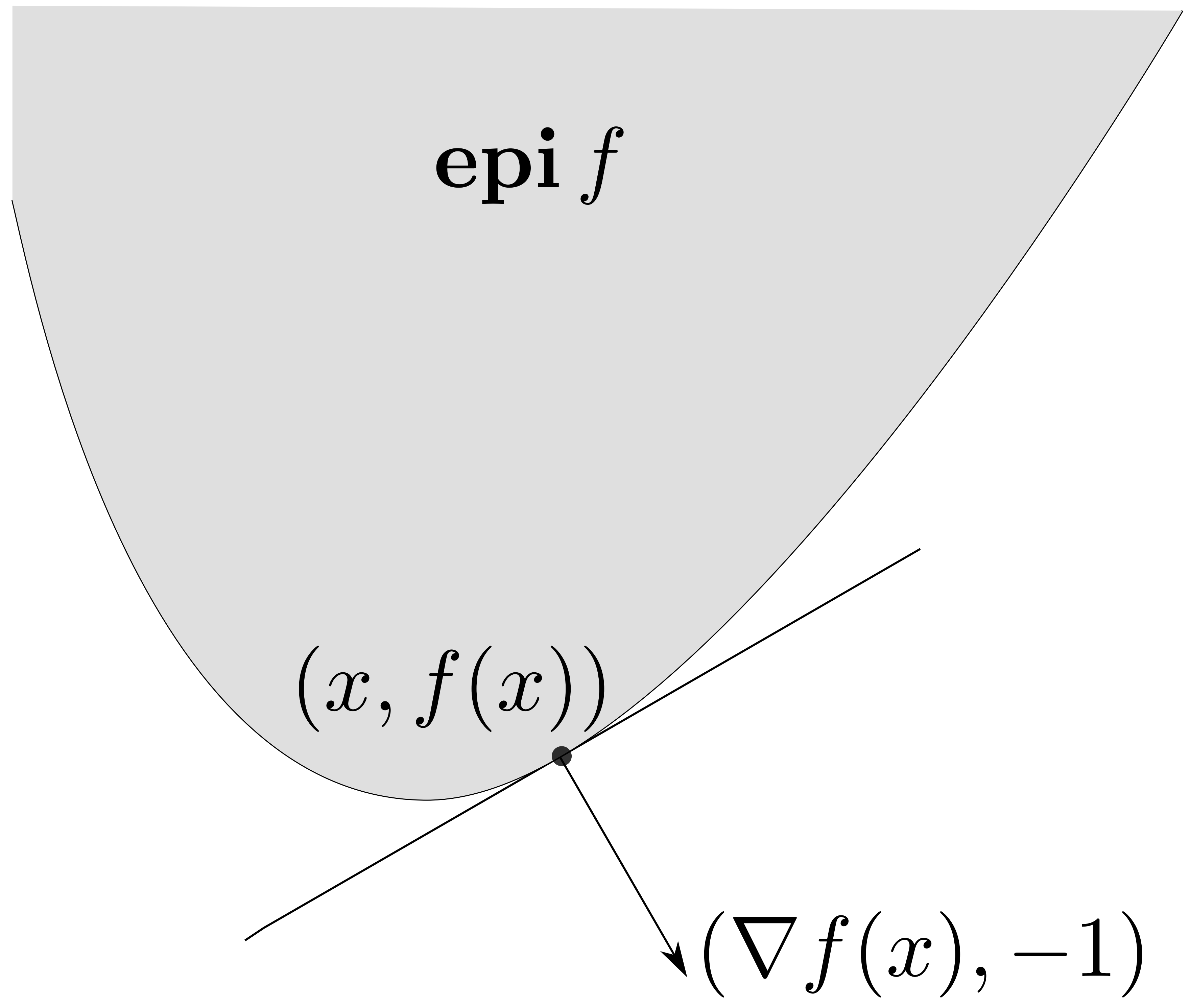
Gradients and epigraphs

For a convex differentiable function f, i.e.

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

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

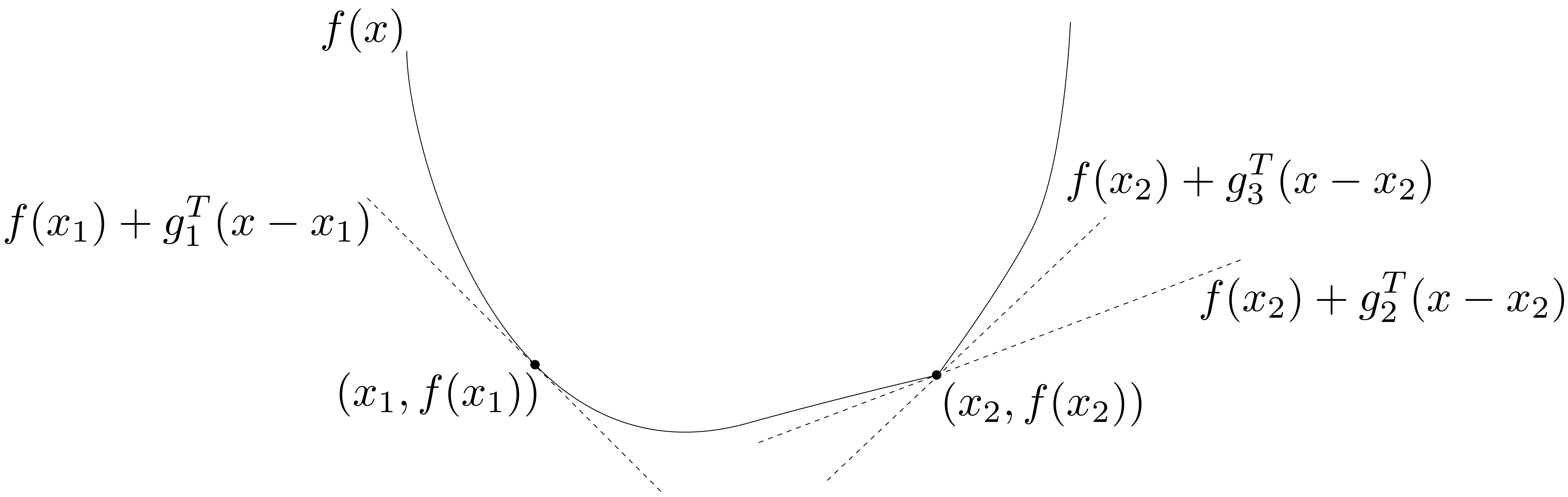
$$\begin{bmatrix} \nabla f(x) \\ -1 \end{bmatrix}^T \left(\begin{bmatrix} y \\ t \end{bmatrix} - \begin{bmatrix} x \\ f(x) \end{bmatrix} \right) \leq 0, \quad \forall (y, t) \in \mathbf{epi}\, f$$



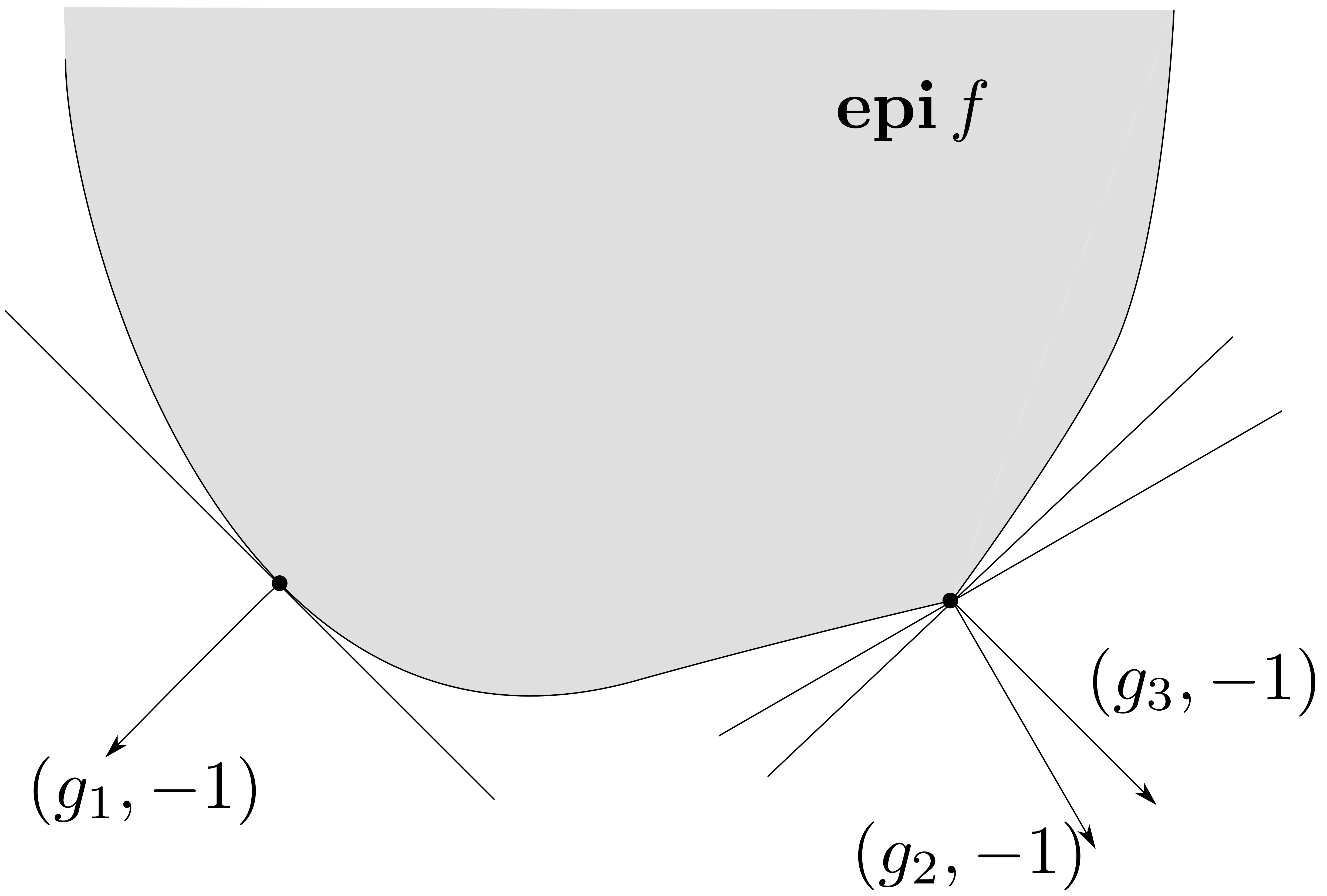
Subgradient

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

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



Subgradient properties



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

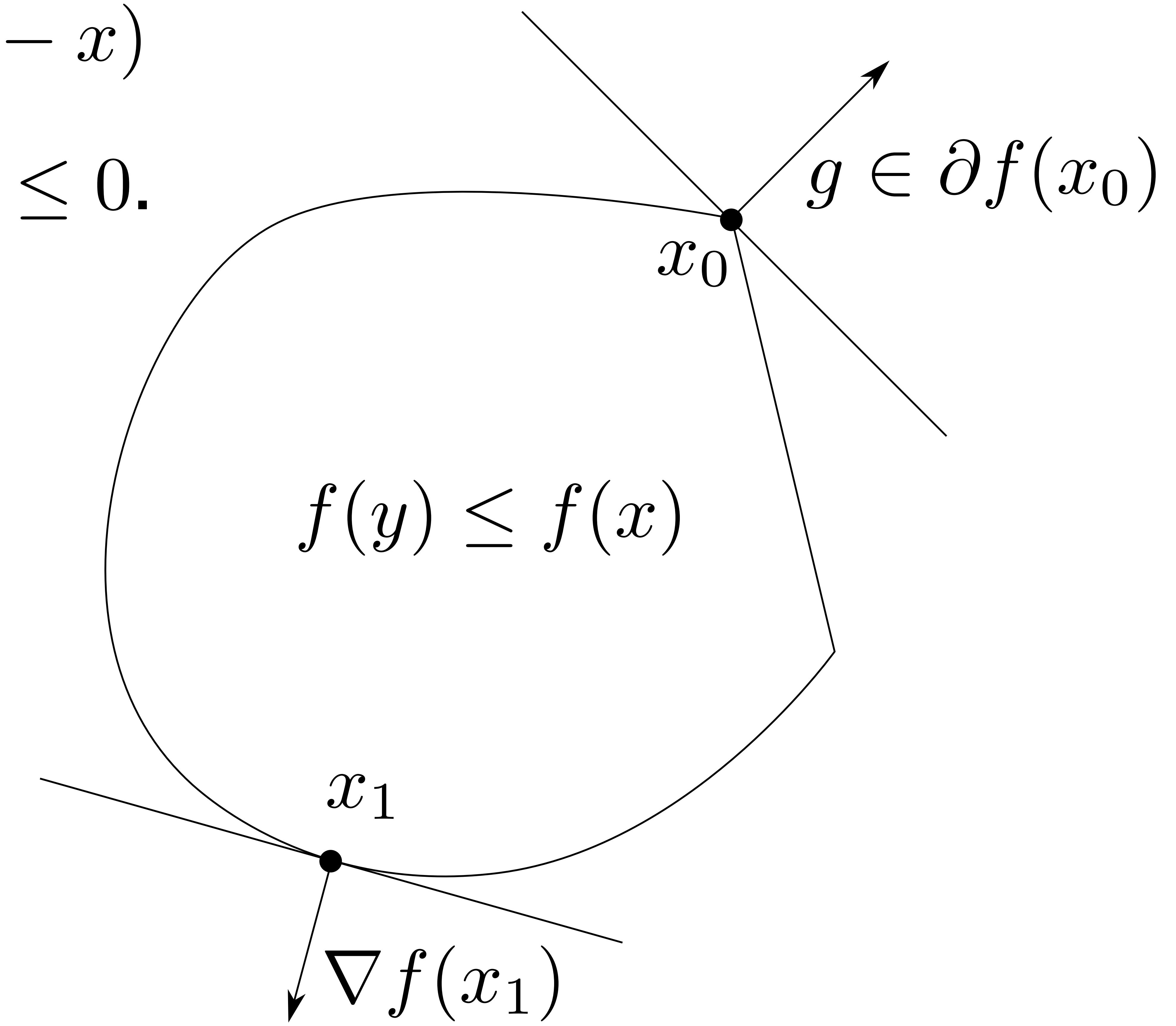
g is a subgradient of f iff $f(x) + g^T(y - x)$ is a global underestimator of f

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



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 throgh x

Subdifferential

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

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

Properties

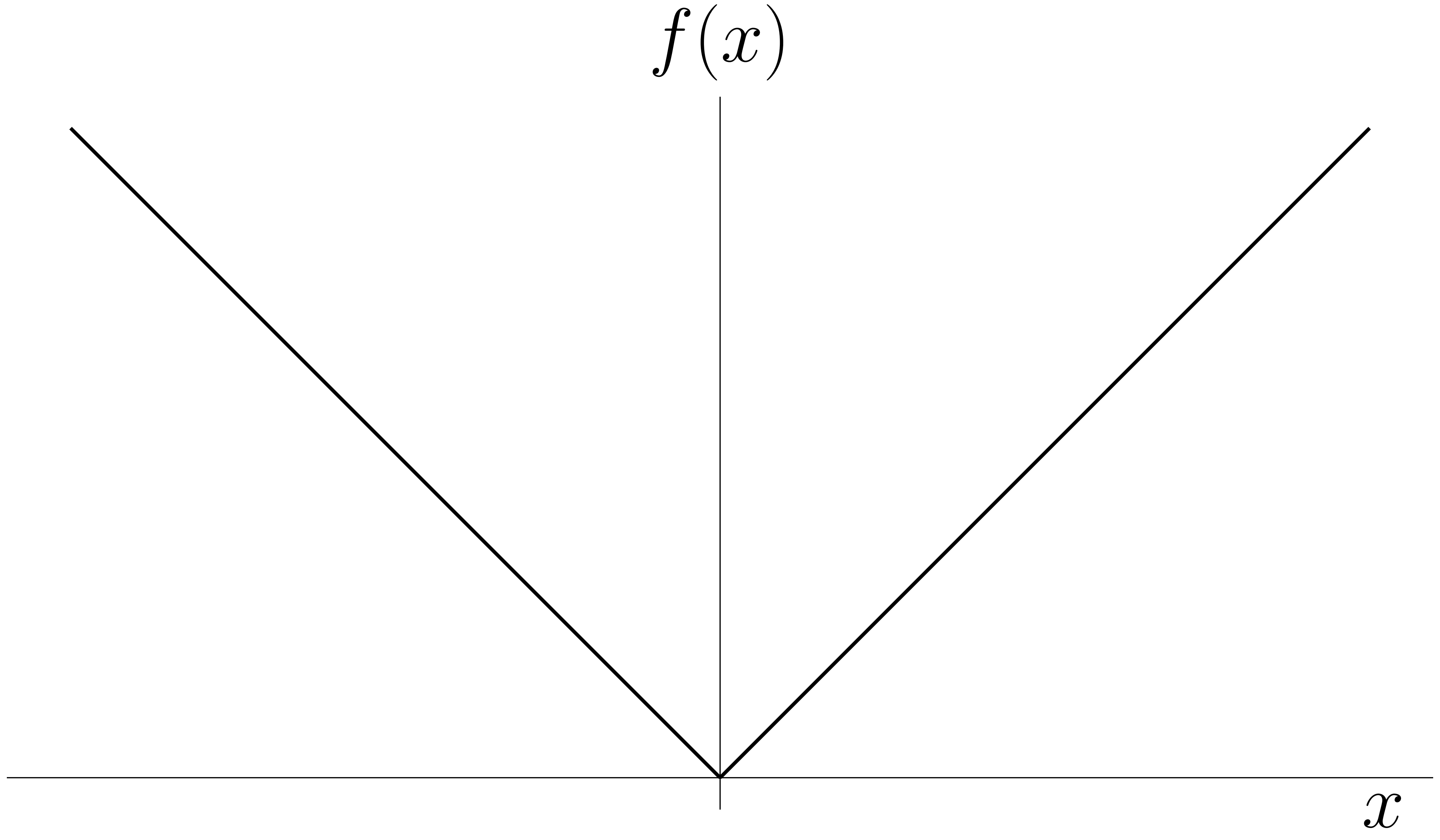
- $\partial f(x)$ is always closed and convex, also for nonconvex f.
  (intersection of halfspaces)
- If $\partial f(x) \neq \emptyset,\ \forall x$ then f is convex (converse not true)
- If f is convex and differentiable at x, then $\partial f(x) = \{\nabla f(x)\}$
- If f is convex and $\partial f(x)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

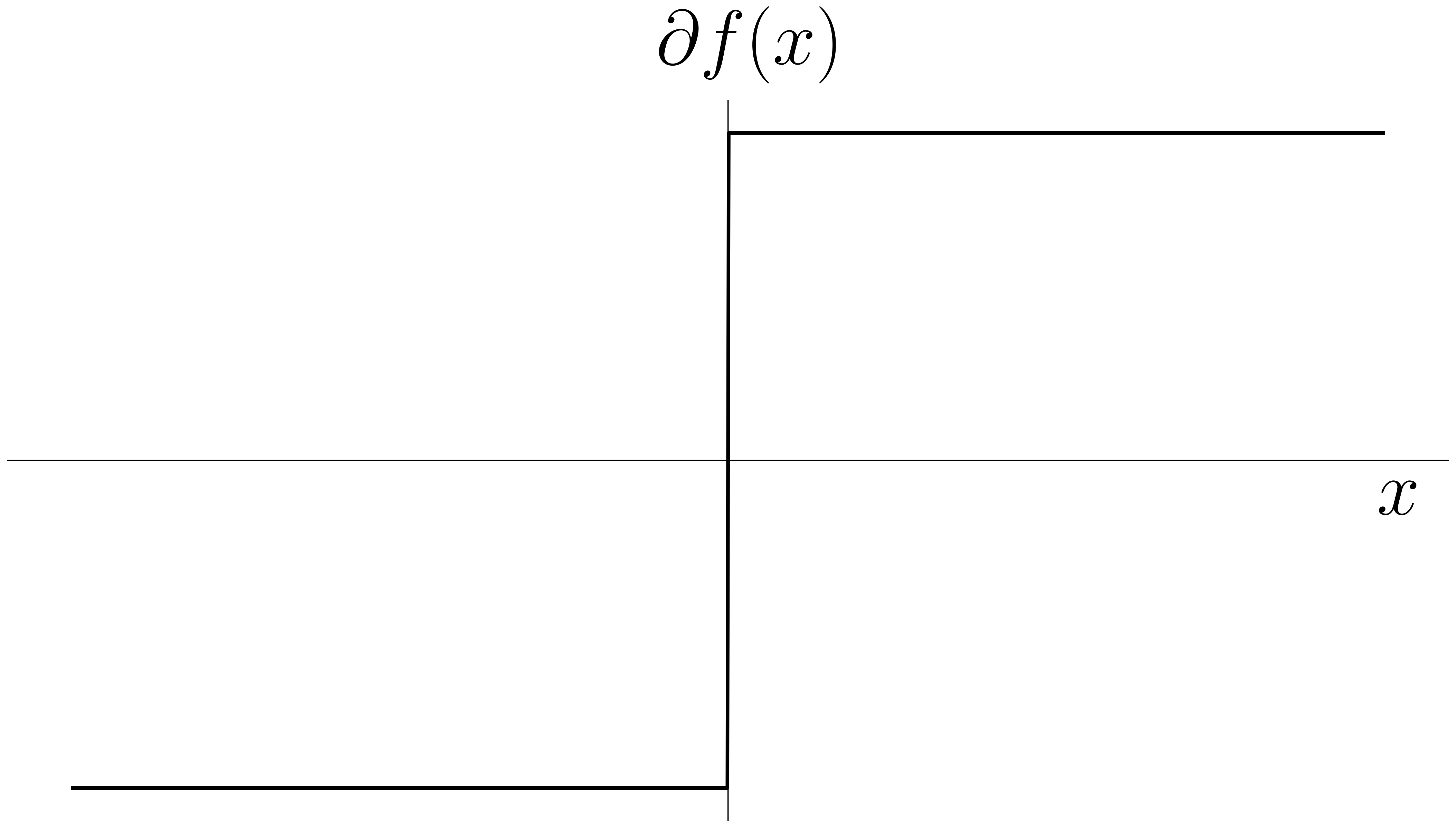
Example

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 $f(x) = \max_{i=1,\dots,m} f_i(x)$, 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 (supremum) $f(x) = \max_{s \in S} f_s(x)$, then

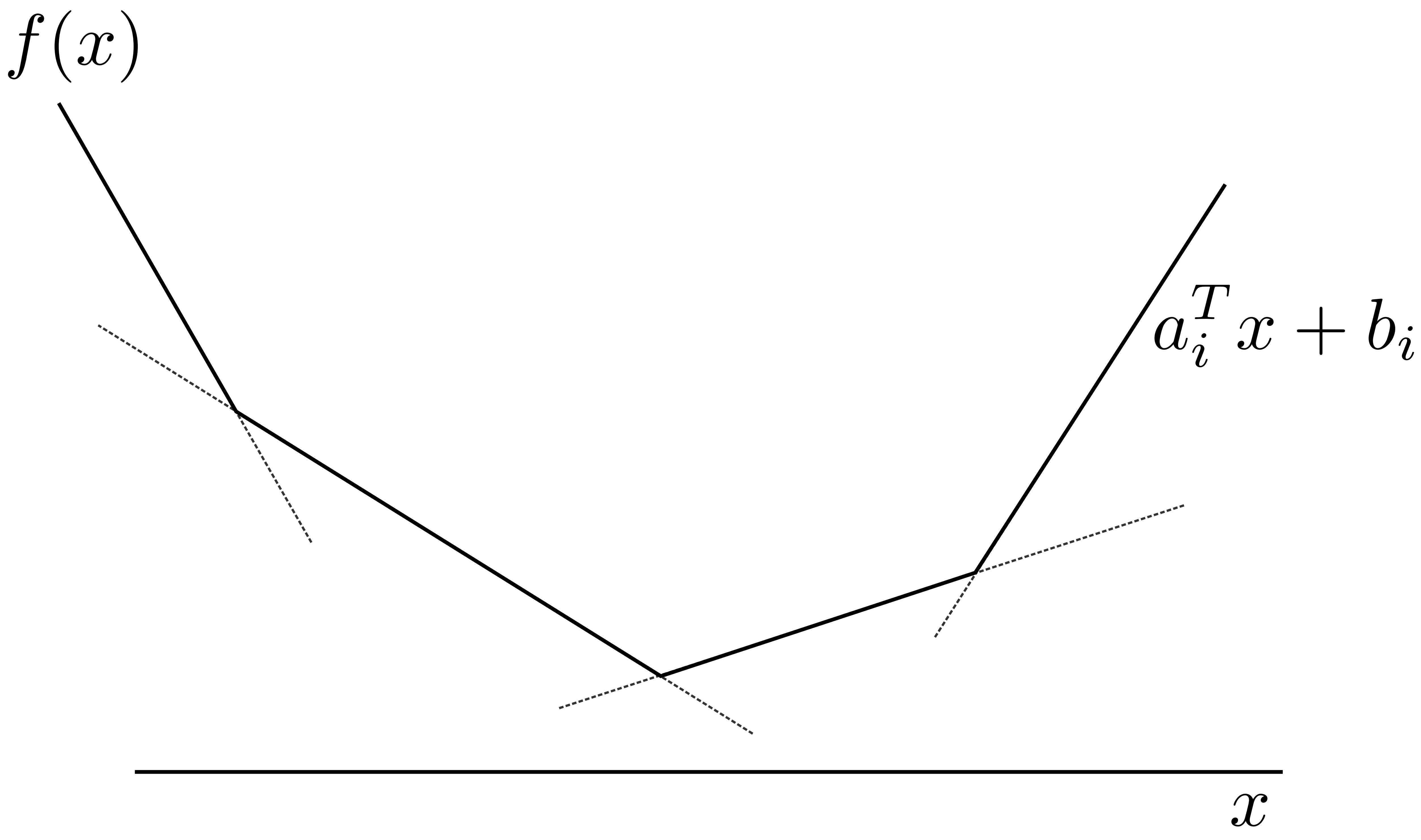
$$\partial f(x) \supseteq \mathbf{conv}\left(\bigcup\{\partial f_s(x) \mid f_s(x) = f(x)\}\right)$$

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

Example

Piecewise linear function

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



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

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

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

$$\partial f(x) = \underset{\|z\|_q \leq 1}{\text{argmax}} \; z^T x$$

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

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

weak result

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

Basic rules

Composition

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

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

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

Proof

$$\begin{aligned}
f(y) &= h(f_1(y), \dots, f_k(y)) \\
&\geq h(f_1(x) + g_1^T(y - x), \dots, f_k(x) + g_k^T(y - x)) \\
&\geq h(f_1(x), \dots, f_k(x)) + q^T(g_1^T(y - x), \dots, g_k^T(y - x)) \\
&= f(x) + g^T(y - x)
\end{aligned}$$

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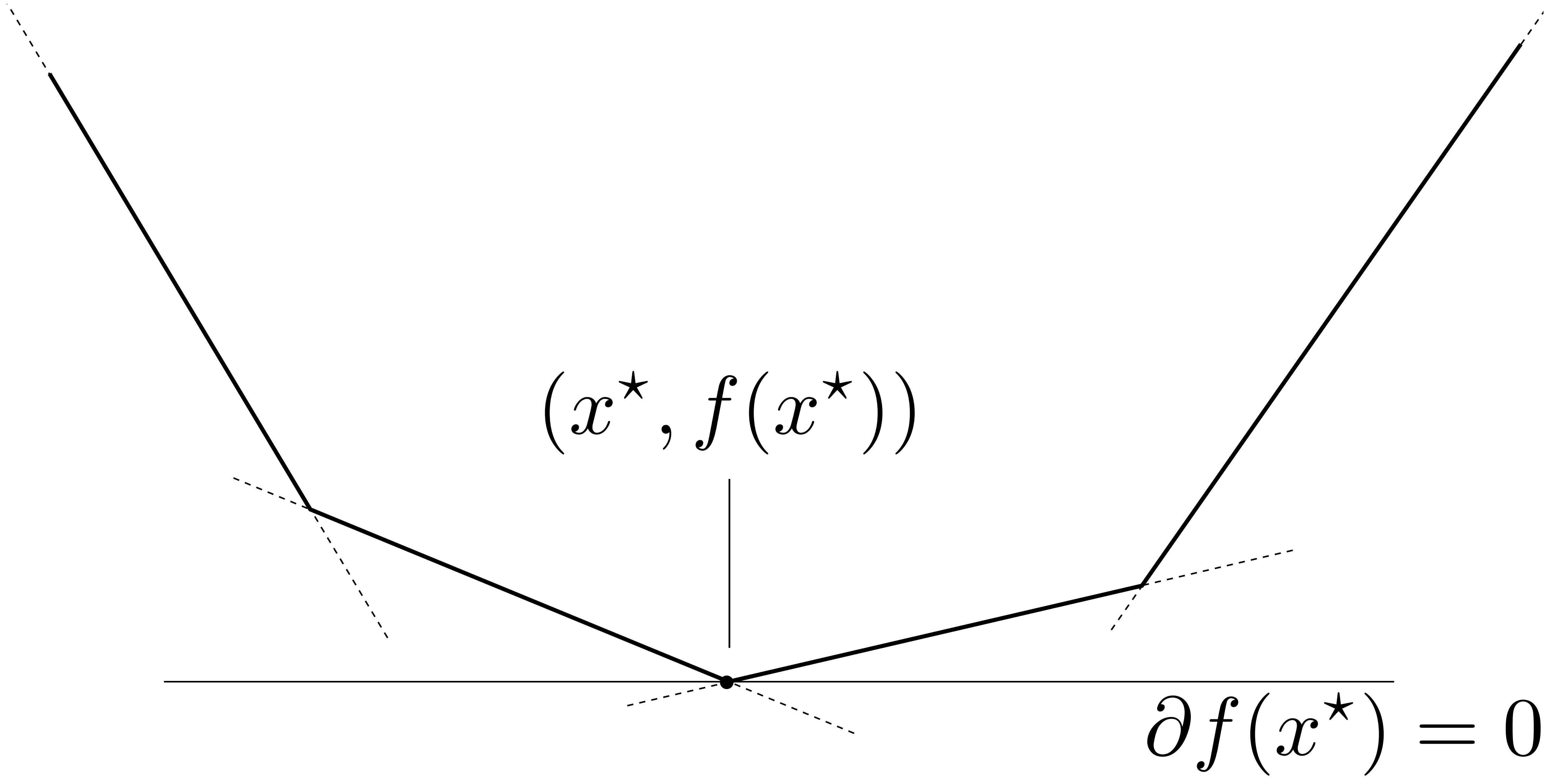
Optimality conditions

Fermat's optimality condition

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

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



Proof

A subgradient $g = 0$ means that, for all y

$$f(y) \geq f(x^\star) + 0^T(y - x^\star) = f(x^\star) \quad \blacksquare$$

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

Example: piecewise linear function

Optimality condition

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

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

$$\lambda \geq 0, \quad \mathbf{1}^T\lambda = 1, \quad \sum_{i=1}^m \lambda_i a_i = 0 \longleftarrow (0 \in \partial f(x))$$

where $\lambda_i = 0$ if $a_i^T x^\star + b_i < f(x^\star)$

Same KKT optimality conditions as the primal-dual problems

$$\begin{array}{ll} \text{minimize} & t \\ \text{subject to} & Ax + b \leq t\mathbf{1} \end{array}$$

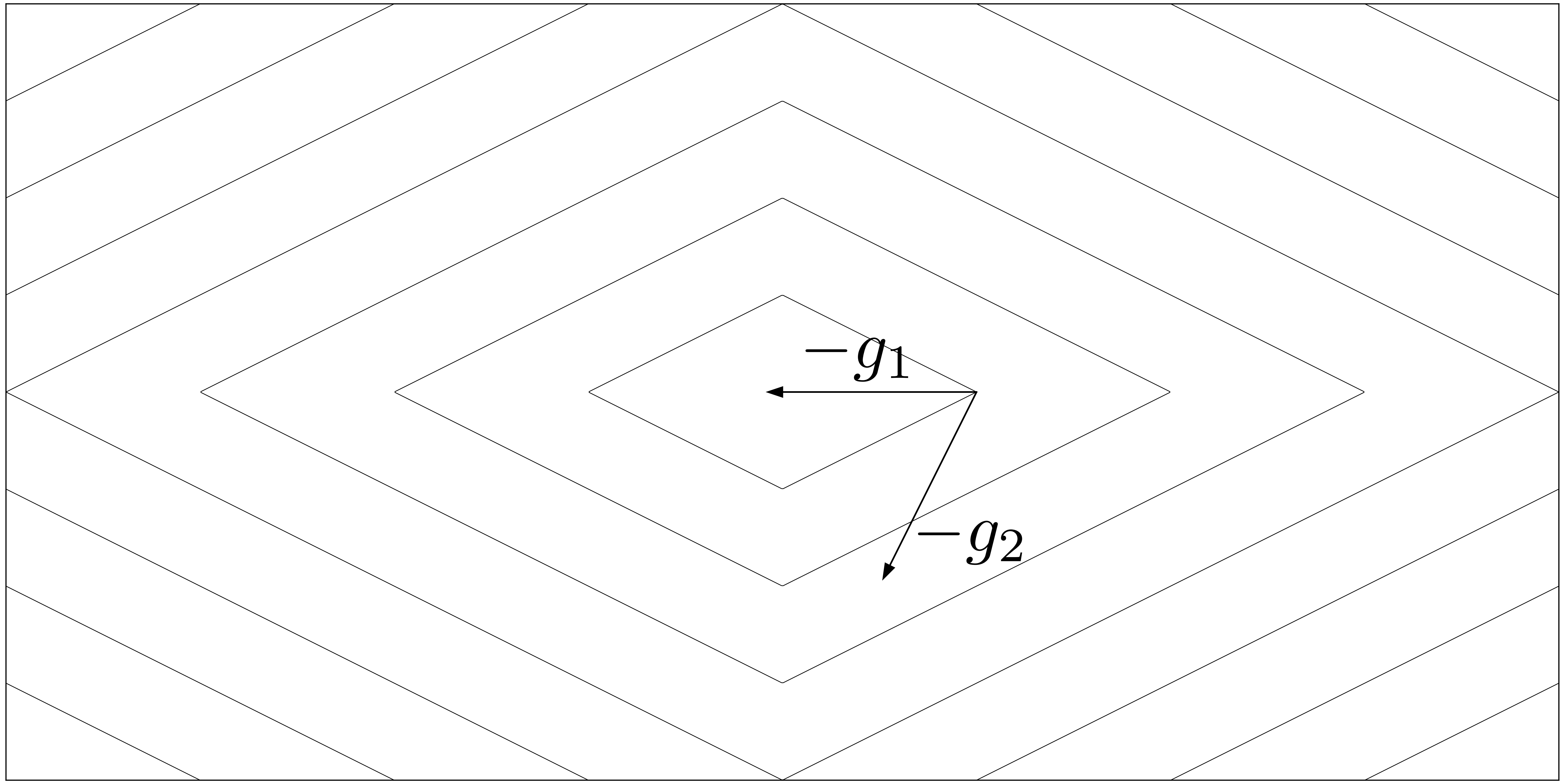
$$\begin{array}{ll} \text{maximize} & b^T\lambda \\ \text{subject to} & A^T\lambda = 0 \\ & \lambda \geq 0, \quad \mathbf{1}^T\lambda = 1 \end{array}$$

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 $\quad f(x) \qquad$ (optimal cost $f^\star$)

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 $k = 0, \ldots$

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

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

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

Convergence

Assumptions

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

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

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

Convergence

Lipschitz continuity equivalence

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

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

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

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,

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

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

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

$$f(y) \geq f(x) + g^T(y - x) = f(x) + \|g\|_2 > f(x) + G \qquad \blacksquare$$

Convergence

Theorem

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

$$f_{\mathrm{best}}^k - f^\star \leq \frac{R^2 + G^2 \sum_{i=0}^k t_i^2}{2 \sum_{i=0}^k t_i}$$

where $\|x^0 - x^\star\|_2 \leq R$

Convergence

Proof

Key quantity: euclidean distance to optimal set
(not function value since it can go up and down)

$$\begin{aligned}
\|x^{k+1} - x^\star\|_2^2 &= \|x^k - t_k g^k - x^\star\|_2^2 \\
&= \|x^k - x^\star\|_2^2 - 2t_k (g^k)^T (x^k - x^\star) + t_k^2 \|g^k\|_2^2 \\
&\le \|x^k - x^\star\|_2^2 - 2t_k (f(x^k) - f^\star) + t_k^2 \|g^k\|_2^2
\end{aligned}$$

using subgradient definition $f^\star = f(x^\star) \ge f(x^k) + (g^k)^T (x^\star - x^k)$

Convergence

Proof (continued)

Combine inequalities for $i = 0, \ldots, k$

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

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

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

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

Convergence

Proof (continued)

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

Combine it with

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

to get

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

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Implications for step size rules

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

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

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

May be suboptimal

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

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

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

Optimal step size and convergence rate

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

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

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

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

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

Convergence rate

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

Iterations required

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

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

Stopping criterion

Terminating when

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

is really, really slow.

Bad news

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

Optimal step size when $f^\star$ is known

Polyak step size

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

Motivation: minimize righthand side of

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

Obtaining $(f(x^k) - f^\star)^2 \leq \left(\|x^{k+1} - x^\star\|_2^2 - \|x^k - x^\star\|_2^2\right) G^2$

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

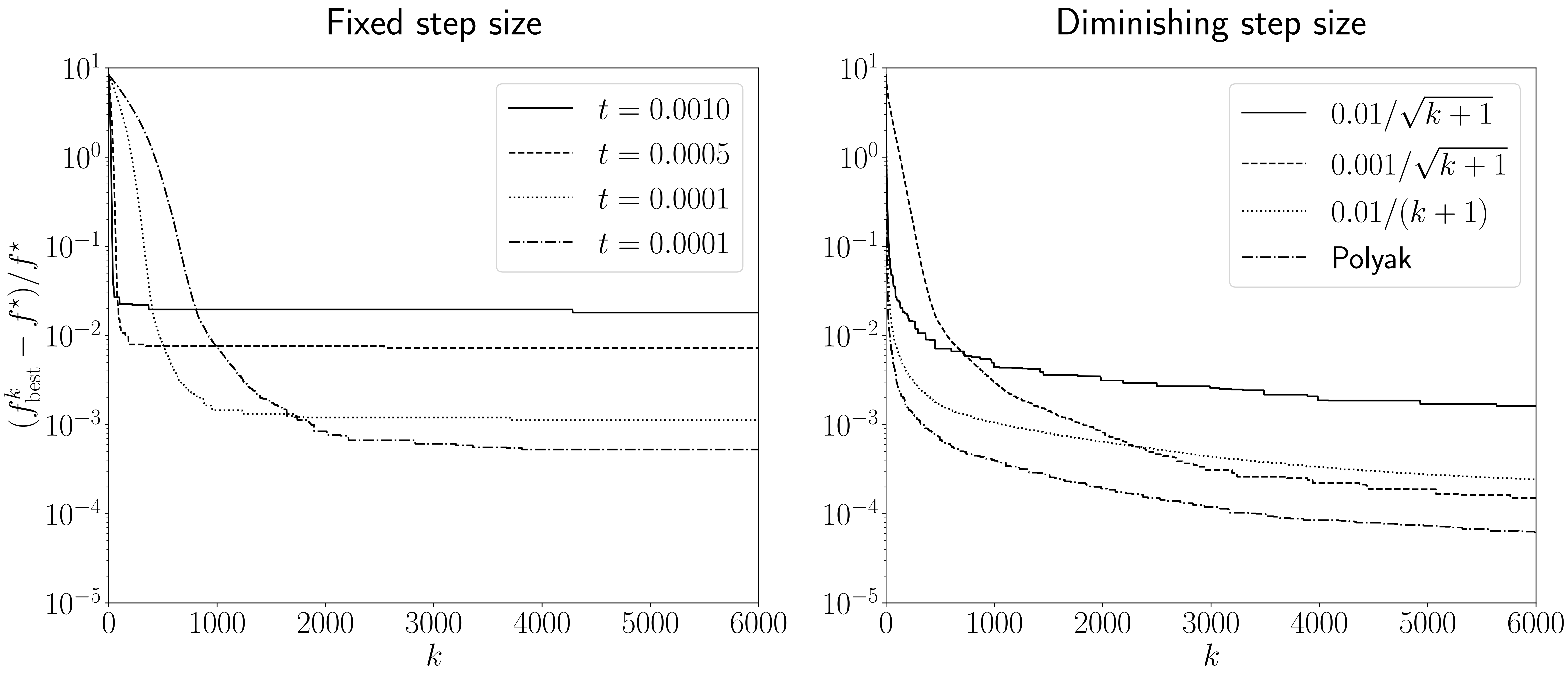
Iterations required

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

still slow

Example: 1-norm minimization

minimize $\quad f(x) = \|Ax - b\|_1 \qquad\qquad g = A^T \,\mathbf{sign}(Ax - b) \in \partial f(x)$



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