ORIE 7391: Faster: Algorithmic Ideas for Speeding Up Optimization

Convex Optimization

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Quiz

- ► A strongly convex function always satisfies the Polyak-Lojasiewiczcondition
 - A. true
 - B. false
- Suppose $f: \mathbf{R} \to \mathbf{R}$ has an L-Lipschitz derivative and satisfies the Polyak-Lojasiewiczcondition. Then any stationary point $\nabla f(x) = 0$ of f is a global optimum: $f(x) = \operatorname{argmin}_{V} f(y) =: f^{*}$.
 - A. true
 - B. false
- Suppose $f: \mathbf{R} \to \mathbf{R}$ has an L-Lipschitz derivative and satisfies the Polyak-Lojasiewiczcondition. Then gradient descent on f converges linearly from any starting point.
 - A. true
 - B. false

Outline

Convexity

Gradient descent

Classical analysis of GD

Polyak-Lojasiewiczcondition

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$$\theta w + (1 - \theta)v \in S$$

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- ▶ A differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ is convex iff it satisfies the first order condition

$$f(v) - f(w) \ge \nabla f(w)^{\top} (v - w) \qquad \forall w, v \in \mathbf{R}^n$$

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$$f(v) - f(w) \ge \nabla f(w)^{\top} (v - w) \qquad \forall w, v \in \mathbf{R}^n$$

▶ A twice differentiable function $f : \mathbf{R}^n \to \mathbf{R}$ is convex iff its Hessian is always **positive semidefinite**: $\lambda_{\min}(\nabla^2 f) \geq 0$

Convexity examples

Q: Which of these functions are convex?

Quadratic approximation

Suppose $f : \mathbf{R} \to \mathbf{R}$ is differentiable. For any $x \in \mathbf{R}$, write its second order expansion about x:

$$f(y) \approx f(x) + \nabla f(x)^{T} (y - x) + \frac{1}{2} (y - x)^{T} \nabla^{2} f(x) (y - x).$$

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Quadratic approximations are useful because quadratics are easy to minimize:

$$y^* = \operatorname*{argmin}_{y} f(x) + \nabla f(x)^T (y - x) + \frac{1}{2} (y - x)^T (y - x)^T (y - x) + \frac{1}{2} (y - x)^T (y - x) +$$

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$$y^* = \operatorname*{argmin}_{y} f(x) + \nabla f(x)^{T} (y - x) + \frac{1}{2} (y - x)$$
$$\nabla f(x) + H(y - x) = 0$$

$$y^* = x + H^{-1}(-\nabla f(x)).$$

If we approximate the Hessian of f by $H = \frac{1}{t}I$ for some t > 0 and choose x^+ to minimize the quadratic approximation, we obtain the **gradient descent** update with step size t:

$$x^+ = x + -t\nabla f(x)$$

A function $f: \mathbf{R} \to \mathbf{R}$ is *L*-smooth if

$$f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{L}{2} ||y - x||^2.$$

Equivalently, the operator $\frac{1}{L}\nabla f$ is *L*-**Lipschitz continuous**:

$$\|\nabla f(y) - \nabla f(x)\| \le L\|y - x\|$$

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Q: For $A \succeq 0$, the quadratic function $f(x) = \frac{1}{2}x^T Ax$ is ?-smooth and ?-strongly convex

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Unconstrained minimization

minimize f(x)

- ▶ $f : \mathbf{R}^n \to \mathbf{R}$ convex, ctsly differentiable (hence **dom** f open)
- ▶ assume optimal value $f^* = \inf_x f(x)$ is attained (and finite)
- ▶ assume a starting point $x^{(0)}$ such that $x^{(0)} \in \operatorname{dom} f$ is known

unconstrained minimization methods

▶ produce sequence of points $x^{(k)} \in \operatorname{dom} f$, k = 0, 1, ... with

$$f(x^{(k)}) \to f^*$$

 can be seen as iterative methods for solving optimality condition

$$\nabla f(x^*) = 0$$

Rates of convergence

linear convergence:

$$f(x^{(k)}) - f^* \le c^k (f(x^{(0)}) - f^*)$$

- looks like a line on a semi-log plot
- example: gradient descent on smooth strongly convex function
- sublinear convergence
 - looks slower than a line (curves up) on a semi-log plot
 - example: gradient descent on smooth convex function
 - example: stochastic gradient descent

Gradient descent

minimize
$$f(x)$$

idea: go downhill to get to a (the?) minimum!

Algorithm Gradient descent

Given: $f : \mathbb{R}^d \to \mathbb{R}$, stepsize t, maxiters **Initialize:** x = 0 (or anything you'd like)

For: $k = 1, \ldots, maxiters$

update x:

$$x \leftarrow x - t \nabla f(x)$$

Gradient descent: choosing a step-size

- **constant step-size.** $t^{(k)} = t$ (constant)
- **b** decreasing step-size. $t^{(k)} = 1/k$
- ▶ **line search.** try different possibilities for $t^{(k)}$ until objective at new iterate

$$f(x^{(k)}) = f(x^{(k-1)} - t^{(k)} \nabla f(x^{(k-1)}))$$

decreases enough.

tradeoff: evaluating f(x) takes O(nd) flops each time . . .

define
$$x^+ = x - t\nabla f(x)$$

- ightharpoonup exact line search: find t to minimize $f(x^+)$
- the Armijo rule requires t to satisfy

$$f(x^+) \le f(x) - ct \|\nabla f(x)\|^2$$

for some $c \in (0,1)$, *e.g.*, c = .01.

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a simple backtracking line search algorithm:

- \triangleright set t=1
- \triangleright if step decreases objective value sufficiently, accept x^+ :

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a simple backtracking line search algorithm:

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 \mathbf{Q} : can we can always satisfy the Armijo rule for some t?

A: yes! see gradient descent demo

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Quadratic upper and lower bounds

what problem does the gradient descent step $x := x + t\nabla f(x)$ solve?

Quadratic upper and lower bounds

what problem does the gradient descent step $x := x + t\nabla f(x)$ solve? answer:

minimize_y
$$f(x) + \nabla f(x)^{T} (y - x) + \frac{1}{2t} ||x - y||^{2}$$

So gradient descent will work best if Hessian is "almost" scaled multiple of the identity.

Formally, find $\alpha \in \mathbf{R}$ and $\beta \in \mathbf{R}$ so that for all x, $y \in \operatorname{dom} f$,

$$f(x) + \nabla f(x)^T (y - x) + \frac{\alpha}{2} ||x - y||^2 \le f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{\beta}{2} ||x - y||^2$$

- lower bound is called **strong convexity** (with parameter α)
- upper bound is called **smoothness** (with parameter β)
- ightharpoonup clearly $\alpha \leq \beta$

Example I: quadratic

$$f(x) + \nabla f(x)^T (y - x) + \frac{\alpha}{2} ||x - y||^2 \le f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{\beta}{2} ||x - y||^2$$

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- strongly convex, with parameter $lpha=\lambda_{\min}(A)$ (if $\lambda_{\min}(A)>0$)
- ightharpoonup smooth, with parameter $\beta = \lambda_{\max}(A)$

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suppose $A \in \mathbf{S}_{+}^{n}$, and consider $f(x) = \frac{1}{2}x^{T}Ax$. is f smooth and strongly convex?

- strongly convex, with parameter $\alpha = \lambda_{\min}(A)$ (if $\lambda_{\min}(A) > 0$)
- lacktriangle smooth, with parameter $eta=\lambda_{\max}(A)$

proof:

$$\frac{1}{2}y^{T}Ay = \frac{1}{2}(x + (y - x))^{T}A(x + (y - x))$$
$$= \frac{1}{2}x^{T}x + (Ax)^{T}(y - x) + \frac{1}{2}(y - x)^{T}A(y - x)$$

Example II: smoothed absolute value

$$f(x) + \nabla f(x)^T (y - x) + \frac{\alpha}{2} ||x - y||^2 \le f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{\beta}{2} ||x - y||^2$$

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- upper bound is called **smoothness** (with parameter β)

consider

huber(x) =
$$\begin{cases} \frac{1}{2}x^2 & x^2 \le 1\\ |x| - \frac{1}{2} & \text{otherwise} \end{cases}$$

is huber smooth and strongly convex?

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is huber smooth and strongly convex?

- not strongly convex
- ightharpoonup smooth, with parameter $\beta = 1$

Example III: regularized absolute value

$$f(x) + \nabla f(x)^T (y - x) + \frac{\alpha}{2} ||x - y||^2 \le f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{\beta}{2} ||x - y||^2$$

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consider $f(x) = |x| + x^2$. is f smooth and strongly convex?

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consider $f(x) = |x| + x^2$. is f smooth and strongly convex?

- ightharpoonup strongly convex, with parameter $\alpha=1$
- not smooth

Roadmap

we'll analyze gradient descent for a few cases:

- \blacktriangleright is f α -strongly convex, or not?
- ightharpoonup is f β -smooth, or not?
- ▶ is f Lipschitz differentiable, or not?
- do we use a fixed step size, or line-search?

a question: are these rates "the best possible"? how could we tell? compared to what?

we'll do the β -smooth case first, then work up to the others

Monotone gradient

first, another convexity condition:

▶ a differentiable function $f : \mathbf{R}^n \to \mathbf{R}$ is convex iff for all x, $y \in \operatorname{dom} f$,

$$(\nabla f(x) - \nabla f(y))^T (x - y) \ge 0$$

- ightharpoonup
 abla f is called a monotone mapping
- ► strict inequality ⇒ strictly monotone mapping

Monotone gradient: proof

if f is differentiable and convex, then

$$f(y) \ge f(x) + \nabla f(x)^T (y - x)$$
 $f(x) \ge f(y) + \nabla f(y)^T (x - y)$ add these to get

$$0 \ge (\nabla f(x) - \nabla f(y))^T (y - x)$$

▶ if ∇f is monotone, then for any x, $y \in \operatorname{dom} f$, let g(t) = f(x + t(y - x)). for $t \ge 0$,

$$g'(t) = \nabla f(x + t(y - x))^T (y - x) \ge g'(0).$$

SO

$$f(y) = g(1) = g(0) + \int_0^1 g'(t)dt \ge g(0) + g'(0)$$

= $f(x) + \nabla f(x)(y - x)$

Smoothness: equivalent definitions

for convex $f : \mathbf{R}^n \to \mathbf{R}$, the following properties are all equivalent:

- 1. $\frac{\beta}{2}x^Tx f(x)$ is convex
- 2. \bar{f} is β -smooth: for all $x, y \in \text{dom } f$,

$$f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{\beta}{2} ||x - y||^2$$

- 3. (if f is twice differentiable) $\nabla^2 f(x) \leq \beta I$
- 4. ∇f is **Lipschitz continuous** with parameter β : $\forall x, y \in \operatorname{dom} f$,

$$\|\nabla f(x) - \nabla f(y)\| \le \beta \|x - y\|$$

5. ∇f is **co-coercive** with parameter $\frac{1}{\beta}$: for all x, $y \in \operatorname{dom} f$,

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- 3. (if f is twice differentiable) $\nabla^2 f(x) \prec \beta I$
- 4. ∇f is **Lipschitz continuous** with parameter β : $\forall x, y \in \operatorname{dom} f$,

$$\|\nabla f(x) - \nabla f(y)\| < \beta \|x - y\|$$

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$$(\nabla f(x) - \nabla f(y))^T(x - y) \ge \frac{1}{\beta} ||\nabla f(x) - \nabla f(y)||^2$$

proof: 2) is first order condition for convexity of 1); 3) is second order condition for convexity of 1); 4) \implies 2) by integration; 5)

Smoothness: proofs of equivalence

1. f is β -smooth: for all $x, y \in \text{dom } f$,

$$f(y) \le f(x) + \nabla f(x)^T (y - x) + \frac{\beta}{2} ||x - y||^2$$

2. ∇f is **Lipschitz continuous** with parameter β : for all x, $y \in \operatorname{dom} f$,

$$\|\nabla f(x) - \nabla f(y)\| \le \beta \|x - y\|$$

proof. integrate and use Lipschitz ∇f (last line) to prove smoothness:

$$f(y) - f(x) - \nabla f(x)^{T}(y - x)$$

$$= \int_{0}^{1} \nabla f(x + t(y - x))^{T}(y - x) dt - \nabla f(x)^{T}(y - x)$$

$$= \int_{0}^{1} (\nabla f(x + t(y - x)) - \nabla f(x))^{T}(y - x) dt$$

$$\leq \int_{0}^{1} \|\nabla f(x + t(y - x)) - \nabla f(x)\|_{2} \|(y - x)\|_{2} dt$$

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$$(\nabla f(x) - \nabla f(y))^T(x - y) \ge \frac{1}{\beta} ||\nabla f(x) - \nabla f(y)||^2$$

proof. use Cauchy-Shwarz (first ineq) and co-coercivity (second)

$$\|\nabla f(x) - \nabla f(y)\|\|(x - y)\| \ge (\nabla f(x) - \nabla f(y))^T (x - y)$$

$$\ge \frac{1}{\beta} \|\nabla f(x) - \nabla f(y)\|^2$$

$$\|(x - y)\| \ge \frac{1}{\beta} \|\nabla f(x) - \nabla f(y)\|$$

to get Lipschitz continuity

three assumptions for analysis:

- $f: \mathbb{R}^n \to \mathbb{R}$ convex and differentiable with **dom** $f = \mathbb{R}^n$
- f is smooth with parameter $\beta > 0$
- optimal value $f^* = \inf_x f(x)$ finite and attained at x^*

Algorithm: GD with constant step size.

pick constant step size $0 < t \le \frac{1}{\beta}$, and repeat

$$x^{(k+1)} = x^{(k)} - t\nabla f(x^{(k)})$$

(nb: not implementable without guess for β)

use quadratic upper bound with $y = x^+ = x - t\nabla f(x)$:

$$f(x^{+}) \leq f(x) + \nabla f(x)(x^{+} - x) + \frac{\beta}{2} ||x^{+} - x||^{2}$$
$$= f(x) - t ||\nabla f(x)||^{2} + t^{2} \frac{\beta}{2} ||\nabla f(x)||^{2}$$

if constant step size $0 < t \le \frac{1}{\beta}$,

$$f(x^{+}) \leq f(x) - \frac{t}{2} \|\nabla f(x)\|^{2}$$

$$\leq f(x^{*}) - \nabla f(x)^{T} (x - x^{*}) - \frac{t}{2} \|\nabla f(x)\|^{2}$$

$$= f^{*} + \frac{1}{2t} (\|x - x^{*}\|^{2} - \|x - x^{*} - t\nabla f(x)\|^{2})$$

$$= f^{*} + \frac{1}{2t} (\|x - x^{*}\|^{2} - \|x^{+} - x^{*}\|^{2})$$

(second line uses first order convexity condition)

take average over iteration counter i = 1, ..., k:

$$\frac{1}{k} \sum_{i=1}^{k} f(x^{(i)}) - f^* \leq \frac{1}{k} \sum_{i=1}^{k} \frac{1}{2t} (\|x^{(i)} - x^*\|^2 - \|x^{(i+1)} - x^*\|^2) \\
\leq \frac{1}{2tk} (\|x^{(0)} - x^*\|^2 - \|x^{(k+1)} - x^*\|^2) \\
\leq \frac{1}{2tk} \|x^{(0)} - x^*\|^2$$

since $f(x^{(k)})$ is non-increasing,

$$f(x^{(k)}) - f^* \le \frac{1}{2tk} ||x^{(0)} - x^*||^2$$

so number of iterations k to reach $f(x^{(k)}) - f^* \le \epsilon$ is $\mathcal{O}(1/\epsilon)$

now, with line search!

▶ t chosen by line search w/params $(a, b) = (\frac{1}{2}, \frac{1}{2})$ (to simplify proofs), so $x^+ = x - t\nabla f(x)$ satisfies

$$f(x^+) < f(x) - \frac{t}{2} \|\nabla f(x)\|^2$$
.

- from smoothness of f, we know $t = \frac{1}{\beta}$ would work
- **>** so linesearch returns $t \geq \frac{b}{\beta} = \frac{1}{2\beta}$

Algorithm: GD with line search.

pick line search parameters $(a,b)=(\frac{1}{2},\frac{1}{2})$ and $x^{(0)}\in \mathbf{R}^n$, and repeat

- 1. compute $\nabla f(x^{(k)})$
- 2. find $t^{(k)}$ by line search
- 3. update

$$x^{(k+1)} = x^{(k)} - t\nabla f(x^{(k)})$$

using line search condition,

$$f(x^{+}) \leq f(x) - \frac{t}{2} \|\nabla f(x)\|^{2}$$

$$\leq f(x^{*}) - \nabla f(x)^{T} (x - x^{*}) - \frac{t}{2} \|\nabla f(x)\|^{2}$$

$$= f^{*} + \frac{1}{2t} (\|x - x^{*}\|^{2} - \|x - x^{*} - t\nabla f(x)\|^{2})$$

$$= f^{*} + \frac{1}{2t} (\|x - x^{*}\|^{2} - \|x^{+} - x^{*}\|^{2})$$

$$\leq f^{*} + \beta (\|x - x^{*}\|^{2} - \|x^{+} - x^{*}\|^{2})$$

second line uses first order convexity condition, last line uses $\frac{1}{t} \leq \frac{\beta}{b} = 2\beta$

take average over iteration counter i = 1, ..., k:

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

since $f(x^{(k)})$ is non-increasing,

$$f(x^{(k)}) - f^* \le \frac{\beta}{k} ||x^{(0)} - x^*||^2$$

so number of iterations k to reach $f(x^{(k)}) - f^* \le \epsilon$ is $\mathcal{O}(1/\epsilon)$

Strong convexity: equivalent definitions

for convex $f : \mathbf{R}^n \to \mathbf{R}$, the following properties are all equivalent:

- 1. $f(x) \frac{\alpha}{2}x^Tx$ is convex
- 2. f is α -strongly convex: for all $x, y \in \text{dom } f$,

$$f(y) \ge f(x) + \nabla f(x)^{T} (y - x) + \frac{\alpha}{2} ||x - y||^{2}$$

- 3. (if f is twice differentiable) $\nabla^2 f(x) \succeq \alpha I$
- 4. ∇f is **coercive** with parameter α : for all x, $y \in \operatorname{dom} f$,

$$(\nabla f(x) - \nabla f(y))^T (x - y) \ge \alpha ||x - y||^2$$

proof: 2) is first order condition for convexity of 1); 3) is second order condition for convexity of 1); 4) is monotone gradient condition for 1)

Strong convexity + smoothness

if f is α -strongly convex and β -smooth, then $h(x) = f(x) - \alpha/2||x||^2$ is convex and $(\beta - \alpha)$ -smooth:

$$(\nabla h(x) - \nabla h(y))^T(x - y) \ge \frac{1}{\beta - \alpha} \|\nabla h(x) - \nabla h(y)\|^2$$

expand h to show

$$(\nabla f(x) - \nabla f(y))^T(x - y) \ge \frac{\alpha \beta}{\alpha + \beta} ||x - y||^2 + \frac{1}{\alpha + \beta} ||\nabla f(x) - \nabla f(y)||^2$$

assumptions for analysis:

- $ightharpoonup f: \mathbf{R}^n \to \mathbf{R}$ convex and differentiable with $\operatorname{\mathbf{dom}} f = \mathbf{R}^n$
- f is smooth with parameter $\beta > 0$
- f is strongly convex with parameter $\alpha > 0$
- optimal value $f^* = \inf_x f(x)$ finite and attained at x^*

Algorithm: GD with constant step size.

pick constant step size $0 < t \leq \frac{2}{\alpha + \beta}$, and repeat

$$x^{(k+1)} = x^{(k)} - t\nabla f(x^{(k)})$$

note $\alpha < \beta \implies \frac{1}{\beta} < \frac{2}{\alpha + \beta}$, so SSC allows larger step sizes than just smoothness

$$||x^{+} - x^{*}||^{2} = ||x - t\nabla f(x) - x^{*}||^{2}$$

$$= ||x - x^{*}||^{2} + t^{2}||\nabla f(x)||^{2} - 2t\nabla f(x)^{T}(x - x^{*})$$

$$\leq ||x - x^{*}||^{2} + t^{2}||\nabla f(x)||^{2}$$

$$-2t\left(\frac{\alpha\beta}{\alpha + \beta}||x - x^{*}||^{2} + \frac{1}{\alpha + \beta}||\nabla f(x)||^{2}\right)$$

$$= \left(1 - t\left(\frac{2\alpha\beta}{\alpha + \beta}\right)\right)||x - x^{*}||^{2} + t\left(t - \frac{2}{\alpha + \beta}\right)||\nabla f(x)||^{2}$$

$$\leq \left(1 - t\left(\frac{2\alpha\beta}{\alpha + \beta}\right)\right)||x - x^{*}||^{2}$$

(first inequality uses coercivity + co-coercivity, last uses $t \leq \frac{2}{\alpha + \beta}$)

lacktriangle distance to optimum decreases by $c=1-t(rac{2lphaeta}{lpha+eta})$ every iteration

$$||x^{(k)} - x^*||^2 \le c^k ||x^{(0)} - x^*||^2$$

i.e., "linear convergence"

- if $t = \frac{2}{\alpha + \beta}$, $c = (\frac{\kappa 1}{\kappa + 1})^2$, where $\kappa = \frac{\beta}{\alpha} \ge 1$ is condition number
- using quadratic upper bound, get bound on function value

$$f(x^{(k)}) - f^* \le \frac{\beta}{2} ||x^{(k)} - x^*||^2 \le \frac{\beta c^k}{2} ||x^{(0)} - x^*||^2$$

▶ so number of iterations k to reach $f(x^{(k)}) - f^* \le \epsilon$ is $\mathcal{O}(\log(1/\epsilon))$

Conclusion

we showed that the gradient method with appropriate step sizes converges, and guarantees

 \blacktriangleright for f convex and β -smooth,

$$f(x^{(k)}) - f^* \le \frac{\beta}{2k} ||x^{(0)} - x^*||^2$$

• for f convex, β -smooth, and α -strongly convex,

$$f(x^{(k)}) - f^* \le \frac{\beta c^k}{2} ||x^{(0)} - x^*||^2,$$

where $c=(\frac{\kappa-1}{\kappa+1})^2$, $\kappa=\frac{\beta}{\alpha}\geq 1$ is condition number

References

- ▶ Lieven Vandenberghe, UCLA EE236C: Gradient methods
- Sebastian Bubeck, Convex Optimization: Algorithms and Complexity

Outline

Convexity

Gradient descent

Classical analysis of GD

Polyak-Lojasiewiczcondition

The Polyak-Lojasiewiczcondition

A function $f : \mathbf{R} \to \mathbf{R}$ satisfies the **Polyak-Lojasiewiczcondition** if

$$\frac{1}{2}\|\nabla f(x)\|^2 \ge \mu(f(x) - f^*)$$

The Polyak-Lojasiewiczcondition

A function $f : \mathbf{R} \to \mathbf{R}$ satisfies the **Polyak-Lojasiewiczcondition** if

$$\frac{1}{2}\|\nabla f(x)\|^2 \ge \mu(f(x) - f^*)$$

proof: plug the points (x, x^*) into the strong convexity condition:

$$f(x) - f^* \le \nabla f(x)^T (x - x^*) - \frac{\mu}{2} ||x - x^*||^2$$

since $f(x) - f^* \ge 0$, we can establish μ -coercivity of ∇f :

$$\nabla f(x)^{T}(x - x^{*}) \geq \frac{\mu}{2} \|x - x^{*}\|^{2}$$
$$\|\nabla f(x)\| \|x - x^{*}\| \geq \frac{\mu}{2} \|x - x^{*}\|^{2}$$
$$\|\nabla f(x)\| \geq \frac{\mu}{2} \|x - x^{*}\|$$

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