

3. Optimal gradient methods

- lower complexity bounds
- estimate sequence
- optimal gradient methods

Lower complexity bound for smooth convex optimization

computational model

- problem formulation: minimize $_{x \in \mathbf{R}^n} f(x)$
- problem class: f is convex and $\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$
- oracle: first-order local black box
- approximate solution: find \bar{x} such that $f(\bar{x}) - f^* \leq \epsilon$

assumption: iterative algorithm generates a sequence $\{x^{(k)}\}$ such that

$$x^{(k)} \in x^{(0)} + \text{span} \left\{ \nabla f(x^{(0)}), \nabla f(x^{(1)}), \dots, \nabla f(x^{(k-1)}) \right\}$$

theorem (Nesterov): for any integer $k \leq (n - 1)/2$ and any $x^{(0)}$, there exists a function in the problem class such that

$$f(x^{(k)}) - f^* \geq \frac{3L\|x^{(0)} - x^*\|_2^2}{32(k + 1)^2}$$

proof: consider the quadratic function

$$f(x) = \frac{L}{4} \left(\frac{1}{2} \left(x_1^2 + \sum_{i=1}^{n-1} (x_i - x_{i+1})^2 + x_n^2 \right) - x_1 \right)$$

which can be expressed as $f(x) = \frac{L}{4} \left(\frac{1}{2} x^T A x - e_1^T x \right)$, where

$$A = \begin{bmatrix} 2 & -1 & 0 & & & & \\ -1 & 2 & -1 & 0 & & & \\ 0 & -1 & 2 & -1 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 & \\ & & & 0 & -1 & 2 & \end{bmatrix}, \quad e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$$

- $0 \preceq \nabla^2 f(x) \preceq L \implies f$ is convex and $\nabla f(x)$ is L -Lipschitz continuous
- optimal solution $x_i^* = 1 - \frac{i}{n+1}$ for $i = 1, \dots, n$ (by solving $Ax^* = e_1$)

$$\|x^*\|_2^2 = \frac{1}{(n+1)^2} (n^2 + \dots + 1^2) \leq \frac{1}{3} (n+1)$$

- optimal value: $f(x^*) = \frac{L}{4} \left(\frac{1}{2} x^{*T} A x^* - e_1^T x^* \right) = -\frac{L}{8} e_1^T x^* = -\frac{L}{8} \frac{n}{(n+1)}$

without loss of generality, let $x^{(0)} = 0$; by the tri-diagonal form of A ,

$$\begin{aligned}\nabla f(x^{(0)}) &= -\frac{L}{4}e_1 \implies x^{(1)} \in \text{span}\{e_1\} \\ \implies \nabla f(x^{(1)}) &\in \text{span}\{e_1, e_2\} \implies x^{(2)} \in \text{span}\{e_1, e_2\} \\ &\dots \implies x^{(k)} \in \text{span}\{e_1, \dots, e_k\}\end{aligned}$$

therefore

$$f(x^{(k)}) \geq \inf_{x^{(k+1)}=\dots=x^{(n)}=0} f(x) = -\frac{L}{8} \frac{k}{(k+1)}$$

for $k \approx n/2$ or $n = 2k + 1$

$$f(x^{(k)}) - f^* \geq -\frac{L}{8} \frac{k}{(k+1)} + \frac{L}{8} \frac{n}{(n+1)} \geq \frac{L}{16(k+1)}$$

finally

$$\frac{f(x^{(k)}) - f^*}{\|x^{(0)} - x^*\|_2^2} \geq \frac{L}{16(k+1)} \bigg/ \frac{2k+2}{3} = \frac{3L}{32(k+1)^2}$$

Lower complexity bound for $\mathcal{S}_{\mu,L}(\mathbf{R}^\infty)$

computational model

- formulation: minimize $f(x)$, where $\ell_2 = \{x \in \mathbf{R}^\infty \mid \sum_{i=1}^\infty x_i^2 \leq \infty\}$
- problem class: f is μ -strongly convex & $\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2$
- oracle: first-order local black box
- approximate solution: find \bar{x} such that $f(\bar{x}) - f^* \leq \epsilon$

assumption: iterative algorithm generates a sequence $\{x^{(k)}\}$ such that

$$x^{(k)} \in x^{(0)} + \text{span} \left\{ \nabla f(x^{(0)}), \nabla f(x^{(1)}), \dots, \nabla f(x^{(k-1)}) \right\}$$

theorem (Nesterov): for any constants $\mu > 0$ and $\kappa \triangleq L/\mu > 1$, and any $x^{(0)} \in \ell_2$, there exist a function in the problem class such that

$$f(x^{(k)}) - f^* \geq \frac{\mu}{2} \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^{2k} \|x^{(0)} - x^*\|_2^2$$

proof: consider the quadratic function

$$f(x) = \frac{\mu(\kappa - 1)}{4} \left(\frac{1}{2} \left(x_1^2 + \sum_{i=1}^{\infty} (x_i - x_{i+1})^2 \right) - x_1 \right) + \frac{\mu}{2} \|x\|^2$$

which can be expressed as $f(x) = \frac{\mu(\kappa-1)}{4} \left(\frac{1}{2} x^T A x - e_1^T x \right) + \frac{\mu}{2} \|x\|^2$, where

$$A = \begin{bmatrix} 2 & -1 & 0 & & \\ -1 & 2 & -1 & 0 & \\ 0 & -1 & 2 & -1 & 0 \\ & \ddots & \ddots & \ddots & \ddots \end{bmatrix}, \quad e_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}$$

- $0 \preceq A \preceq 4I \implies \mu I \preceq \nabla^2 f(x) \preceq LI$
- first-order optimality condition: $\nabla f(x^*) = 0 \implies \left(A + \frac{4}{\kappa-1} \right) x^* = e_1$

$$x_i^* = q^i, \quad i = 1, 2, \dots \quad \text{where} \quad q = \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}$$

therefore

$$\|x^*\|^2 = \sum_{i=1}^{\infty} x_i^{*2} = \sum_{i=1}^{\infty} q^{2i} = \frac{q^2}{1 - q^2}$$

without loss of generality, let $x^{(0)} = 0$; by the tri-diagonal form of A ,

$$\begin{aligned}\nabla f(x^{(0)}) &= -\frac{L}{4}e_1 \implies x^{(1)} \in \text{span}\{e_1\} \\ \implies \nabla f(x^{(1)}) &\in \text{span}\{e_1, e_2\} \implies x^{(2)} \in \text{span}\{e_1, e_2\} \\ \dots &\implies x^{(k)} \in \text{span}\{e_1, \dots, e_k\}\end{aligned}$$

therefore

$$\|x^{(k)} - x^*\|^2 \geq \sum_{i=k+1}^{\infty} x_i^{*2} = \sum_{i=k+1}^{\infty} q^{2i} = \frac{q^{2(k+1)}}{1 - q^2} = q^{2k} \|x^{(0)} - x^*\|^2$$

by strong convexity with parameter μ ,

$$f(x^{(k)}) - f^* \geq \frac{\mu}{2} \|x^{(k)} - x^*\|^2 \geq \frac{\mu}{2} q^{2k} \|x^{(0)} - x^*\|^2$$

Complexity of the gradient method

gradient method does not match the lower bound

- for smooth convex functions (L -Lipshichz gradient)

$$f(x^{(k)}) - f^* \leq \frac{L}{2k} \|x^{(0)} - x^*\|_2^2$$

- for strongly convex and smooth functions

$$f(x^{(k)}) - f^* \leq \frac{L}{2} \left(\frac{L - \mu}{L + \mu} \right)^{2k} \|x^{(0)} - x^*\|_2^2$$

Nesterov's comments:

- gradient method relied on decreasing objective values (“relaxation”):

$$f(x^{(k+1)}) \leq f(x^{(k)})$$

- optimal methods: don't rely on relaxation (too “*microscopic*” of a property); use some *global* properties of convex functions

Estimate sequence (Nesterov)

a pair of sequences $\{\lambda_k, \phi_k(x)\}_{k=0}^{\infty}$ is called *estimate sequence* of $f(x)$ if

- $\lambda_k \rightarrow 0$
- $\phi_k(x) \leq (1 - \lambda_k)f(x) + \lambda_k\phi_0(x)$ for any $x \in \mathbf{R}^n$ and all $k > 0$

lemma: if a sequence $\{x^{(k)}\}$ satisfies $f(x^{(k)}) \leq \min_{x \in \mathbf{R}^n} \phi_k(x)$, then

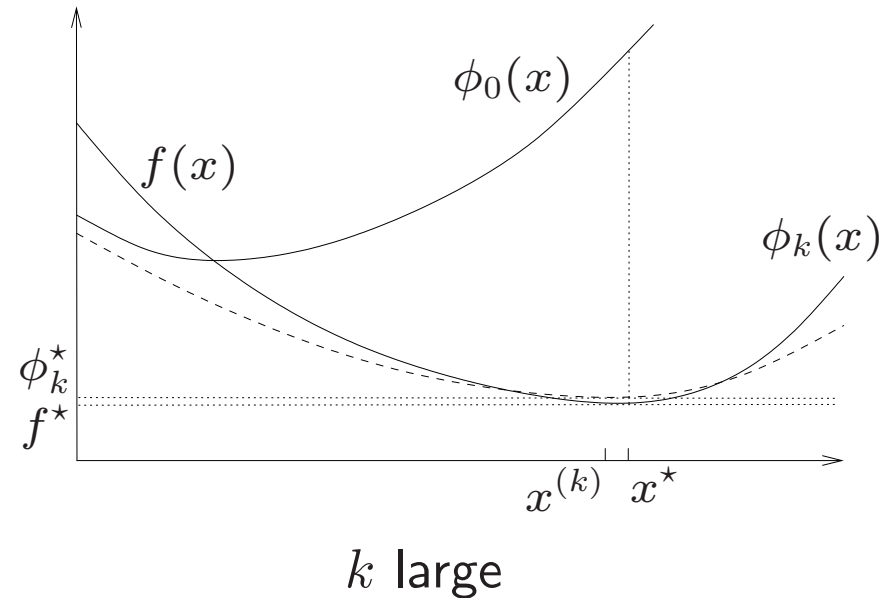
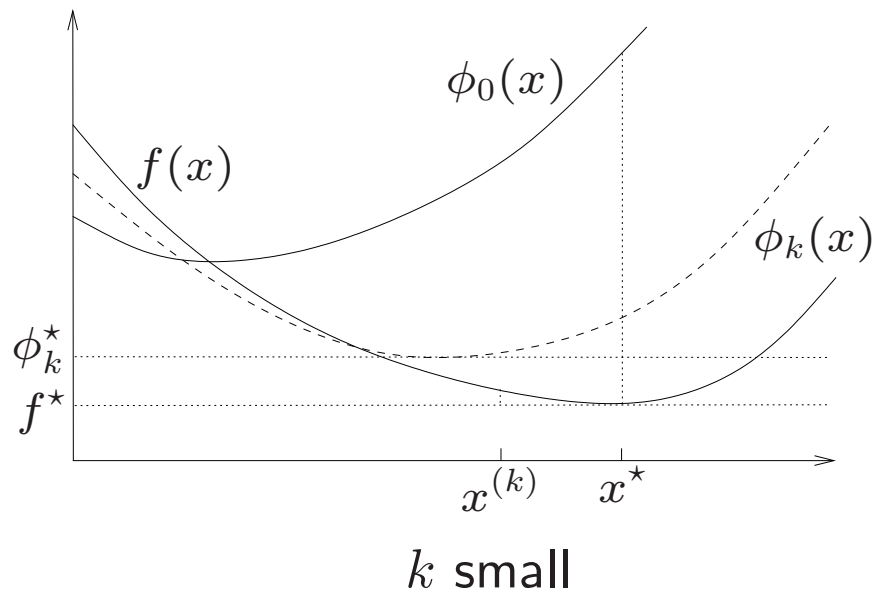
$$f(x^{(k)}) - f^* \leq \lambda_k (\phi_0(x^*) - f^*) \rightarrow 0$$

proof:

$$\begin{aligned} f(x^{(k)}) &\leq \min_{x \in \mathbf{R}^n} \phi_k(x) \leq \min_{x \in \mathbf{R}^n} \{(1 - \lambda_k)f(x) + \lambda_k\phi_0(x)\} \\ &\leq (1 - \lambda_k)f(x^*) + \lambda_k\phi_0(x^*) \\ &= f(x^*) + \lambda_k (\phi_0(x^*) - f(x^*)) \end{aligned}$$

estimate sequence: pair of sequences $\{\lambda_k, \phi_k(x)\}_{k=0}^{\infty}$ such that

- $\lambda_k \rightarrow 0$
- $\phi_k(x) \leq (1 - \lambda_k)f(x) + \lambda_k\phi_0(x)$ for any $x \in \mathbf{R}^n$ and all $k > 0$



questions:

- how to form the estimate sequence?
- how can we ensure $f(x^{(k)}) \leq \phi_k^* \triangleq \min_{x \in \mathbf{R}^n} \phi_k(x)$?

lemma: suppose $f \in \mathcal{S}_{\mu,L}(\mathbf{R}^n)$, then for any function $\phi_0(x)$, any sequence $\{y^{(k)}\}_{k=1}^{\infty}$, and $\{\alpha_k\}_{k=0}^{\infty}$ that satisfies

$$\alpha_k \in (0, 1), \quad \sum_{k=1}^{\infty} \alpha_k = \infty$$

the following pair is an estimate sequence

$$\lambda_{k+1} = (1 - \alpha_k)\lambda_k, \quad \text{with } \lambda_0 = 1$$

$$\phi_{k+1}(x) = (1 - \alpha_k)\phi_k(x) + \alpha_k \left(f(y^{(k)}) + \left\langle \nabla f(y^{(k)}), x - y^{(k)} \right\rangle + \frac{\mu}{2} \|x - y^{(k)}\|^2 \right)$$

proof: note $\phi_0(x) \leq (1 - \lambda_0)f(x) + \lambda_0\phi_0(x) = \phi_0(x)$; use induction

$$\begin{aligned} \phi_{k+1}(x) &\leq (1 - \alpha_k)\phi_k(x) + \alpha_k f(x) \\ &= (1 - (1 - \alpha_k)\lambda_k)f(x) + (1 - \alpha_k)(\phi_k(x) - (1 - \lambda_k)f(x)) \\ &\leq (1 - (1 - \alpha_k)\lambda_k)f(x) + (1 - \alpha_k)\lambda_k\phi_0(x) \\ &= (1 - \lambda_{k+1})f(x) + \lambda_{k+1}\phi_0(x) \end{aligned}$$

$\lambda_k = \lambda_0 \prod_{i=0}^k (1 - \alpha_i) \rightarrow 0$ due to the fact

$$\alpha_k \in (0, 1), \quad \sum_{k=1}^{\infty} \alpha_k = \infty \quad \implies \quad \prod_{k=0}^{\infty} (1 - \alpha_k) \rightarrow 0$$

proof:

- $\{\lambda_k\}_{k=0}^{\infty}$ monotone decreasing and bounded below, so has limit
- suppose $\lambda_k \rightarrow c > 0$
- rewrite iteration as $\lambda_k - \lambda_{k+1} = \alpha_k \lambda_k$, and sum over $k = 0, \dots, N$

$$\lambda_0 - \lambda_{N+1} = \sum_{k=1}^N \alpha_k \lambda_k \geq c \sum_{k=1}^N \alpha_k$$

contradiction when $N \rightarrow \infty$, so need to have $c = 0$

Update quadratic approximations

let $\phi_0(x) = \phi_0^* + \frac{\gamma_0}{2}\|x - v_0\|^2$, then $\{\phi_k(x)\}$ on page 3–11 can be written as

$$\phi_k(x) = \phi_k^* + \frac{\gamma_k}{2}\|x - v^{(k)}\|^2,$$

where

$$\begin{aligned}\gamma_{k+1} &= (1 - \alpha_k)\gamma_k + \alpha_k\mu \\ v^{(k+1)} &= \frac{1}{\gamma_{k+1}}\left((1 - \alpha_k)\gamma_k v^{(k)} + \alpha_k\mu y^{(k)} - \alpha_k \nabla f(y^{(k)})\right) \\ \phi_{k+1}^* &= (1 - \alpha_k)\phi_k^* + \alpha_k f(y^{(k)}) - \frac{\alpha_k^2}{2\gamma_{k+1}}\|\nabla f(y^{(k)})\|^2 \\ &\quad + \frac{\alpha_k(1 - \alpha_k)\gamma_k}{\gamma_{k+1}}\left(\langle \nabla f(y^{(k)}), v^{(k)} - y^{(k)} \rangle + \frac{\mu}{2}\|y^{(k)} - v^{(k)}\|^2\right)\end{aligned}$$

(manipulations of simple quadratic functions)

assume we already have $\phi_k^* \geq f(x^{(k)})$, then

$$\begin{aligned}\phi_{k+1}^* &\geq (1 - \alpha_k)f(x^{(k)}) + \alpha_k f(y^{(k)}) - \frac{\alpha_k^2}{2\gamma_{k+1}} \|\nabla f(y^{(k)})\|^2 \\ &\quad + \frac{\alpha_k(1 - \alpha_k)\gamma_k}{\gamma_{k+1}} \langle \nabla f(y^{(k)}), v^{(k)} - y^{(k)} \rangle\end{aligned}$$

by convexity, $f(x^{(k)}) \geq f(y^{(k)}) + \langle \nabla f(y^{(k)}), x^{(k)} - y^{(k)} \rangle$,

$$\begin{aligned}\phi_{k+1}^* &\geq f(y^{(k)}) - \frac{\alpha_k^2}{2\gamma_{k+1}} \|\nabla f(y^{(k)})\|^2 \\ &\quad + (1 - \alpha_k) \left\langle \nabla f(y^{(k)}), \frac{\alpha_k \gamma_k}{\gamma_{k+1}} (v^{(k)} - y^{(k)}) + x^{(k)} - y^{(k)} \right\rangle\end{aligned}$$

finally, in order to make $\phi_{k+1}^* \geq f(x^{(k+1)})$,

- choose $x^{(k+1)}$ such that $f(x^{(k+1)}) \leq f(y^{(k)}) - \frac{\alpha_k^2}{2\gamma_{k+1}} \|\nabla f(y^{(k)})\|^2$
- choose $y^{(k)}$ so that $\frac{\alpha_k \gamma_k}{\gamma_{k+1}} (v^{(k)} - y^{(k)}) + x^{(k)} - y^{(k)} = 0$

Choose $\{y^{(k)}\}$ and $\{x^{(k+1)}\}$

- choose $y^{(k)}$ to eliminate inner-product term

$$y^{(k)} = \frac{1}{\gamma_k + \alpha_k \mu} (\alpha_k \gamma_k v^{(k)} + \gamma_{k+1} x^{(k)})$$

- recall from quadratic upper bound (page 2-6):

$$f\left(y - \frac{1}{L} \nabla f(y)\right) \leq f(y) - \frac{1}{2L} \|\nabla f(y)\|_2^2$$

so we can let

$$x^{(k+1)} = y^{(k)} - \frac{1}{L} \nabla f(y^{(k)})$$

and solve for α_k from the equation $\frac{\alpha_k^2}{\gamma_{k+1}} = \frac{1}{L}$, that is,

$$L\alpha_k^2 = (1 - \alpha_k)\gamma_k + \alpha_k \mu$$

General scheme of optimal method (Nesterov)

- choose $x_0 \in \mathbf{R}^n$ and $\gamma_0 > 0$, and set $v_0 = x_0$
- for $k = 0, 1, 2, \dots$, repeat

1. find $\alpha_k \in (0, 1)$ that satisfies the equation

$$L\alpha_k^2 = (1 - \alpha_k)\gamma_k + \alpha_k\mu$$

and let $\gamma_{k+1} = (1 - \alpha_k)\gamma_k + \alpha_k\mu$

2. choose

$$y^{(k)} = \frac{1}{\gamma_k + \alpha_k\mu}(\alpha_k\gamma_kv^{(k)} + \gamma_{k+1}x^{(k)})$$

and compute $f(y^{(k)})$ and $\nabla f(y^{(k)})$

3. find $x^{(k+1)}$ such that $f(x^{(k+1)}) \leq f(y^{(k)}) - \frac{1}{2L}\|\nabla f(y^{(k)})\|^2$

4. set

$$v^{(k+1)} = \frac{1}{\gamma_{k+1}}\left((1 - \alpha_k)\gamma_kv^{(k)} + \alpha_k\mu y^{(k)} - \alpha_k\nabla f(y^{(k)})\right)$$

Bounding λ_k

lemma: if $\gamma_0 \geq \mu$ in the optimal scheme on page 3–16, then

$$\lambda_k = \prod_{i=0}^{k-1} (1 - \alpha_i) \leq \min \left\{ \left(1 - \sqrt{\frac{\mu}{L}} \right)^k, \frac{4L}{(2\sqrt{L} + k\sqrt{\gamma_0})^2} \right\}$$

proof:

- $\gamma_k \geq \mu$ and $\alpha_k \geq \sqrt{\mu/L}$ for all $k \geq 0$ because

$$\gamma_{k+1} = L\alpha_k^2 = (1 - \alpha_k)\gamma_k + \alpha_k\mu \geq \mu$$

- $\gamma_k \geq \gamma_0\lambda_k$ for all $k \geq 0$, since $\gamma_0 \geq \gamma_0\lambda_0$ and

$$\gamma_{k+1} \geq (1 - \alpha_k)\gamma_k \geq (1 - \alpha_k)\gamma_0\lambda_k = \gamma_0\lambda_{k+1}$$

- let $a_k = \frac{1}{\sqrt{\lambda_k}}$, then $a_k \geq 1 + \frac{k}{2}\sqrt{\frac{\gamma_0}{L}}$ because

$$\begin{aligned} a_{k+1} - a_k &= \frac{\sqrt{\lambda_k} - \sqrt{\lambda_{k+1}}}{\sqrt{\lambda_k}\sqrt{\lambda_{k+1}}} = \frac{\lambda_k - \lambda_{k+1}}{\sqrt{\lambda_k}\sqrt{\lambda_{k+1}}(\sqrt{\lambda_k} + \sqrt{\lambda_{k+1}})} \\ &\geq \frac{\lambda_k - \lambda_{k+1}}{2\lambda_k\sqrt{\lambda_{k+1}}} = \frac{\alpha_k\lambda_k}{2\lambda_k\sqrt{\lambda_{k+1}}} = \frac{\alpha_k}{2\sqrt{\lambda_{k+1}}} \geq \frac{1}{2}\sqrt{\frac{\gamma_0}{L}} \end{aligned}$$

Rate of convergence

theorem: let $\gamma_0 = L$, then the method on page 3–16 generates $\{x^{(k)}\}_{k=0}^{\infty}$ such that

$$f(x^{(k)}) - f^* \leq \min \left\{ \left(1 - \sqrt{\frac{\mu}{L}}\right)^k, \frac{4}{(k+2)^2} \right\} L \|x_0 - x^*\|^2$$

this means the method is *optimal* for functions from class $\mathcal{S}_{\mu,L}(\mathbf{R}^n)$

proof: by lemma on page 3–9,

$$f(x^{(k)}) - f^* \leq \lambda_k \left(f(x^{(0)}) - f^* + \frac{\gamma_0}{2} \|x^{(0)} - x^*\|^2 \right)$$

then use $\gamma_0 = L$ and quadratic upper bound $f(x^{(0)}) - f^* \leq \frac{L}{2} \|x^{(0)} - x^*\|_2^2$

Variant of optimal method

eliminate $\{v^{(k)}\}$ and $\{\gamma_k\}$, and use constant step size $t = 1/L$

- choose $x^{(0)} \in \mathbf{R}^n$ and $\alpha_0 \in [\sqrt{\frac{\mu}{L}}, 1)$, set $y^{(0)} = x^{(0)}$ and $q = \mu/L$
- for $k = 0, 1, 2, \dots$, repeat
 1. compute $f(y^{(k)})$ and $\nabla f(y^{(k)})$, use gradient step update in step 3 in page 3-16, i.e.,

$$x^{(k+1)} = y^{(k)} - \frac{1}{L} \nabla f(y^{(k)})$$

2. compute $\alpha_{k+1} \in (0, 1)$ from equation

$$\alpha_{k+1}^2 = (1 - \alpha_{k+1})\alpha_k^2 + q\alpha_{k+1}$$

and set $\beta_k = \frac{\alpha_k(1-\alpha_k)}{\alpha_k^2 + \alpha_{k+1}}$ and

$$y^{(k+1)} = x^{(k+1)} + \beta_k(x^{(k+1)} - x^{(k)})$$

A simpler variant

choose $\alpha_0 = \sqrt{\frac{\mu}{L}}$, then

$$\alpha_k = \sqrt{\frac{\mu}{L}}, \quad \beta_k = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$$

- choose $y^{(0)} = x^{(0)} \in \mathbf{R}^n$
- for $k = 0, 1, 2, \dots$, repeat

$$\begin{aligned} x^{(k+1)} &= y^{(k)} - \frac{1}{L} \nabla f(y^{(k)}) \\ y^{(k+1)} &= x^{(k+1)} + \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}} (x^{(k+1)} - x^{(k)}) \end{aligned}$$

however, this scheme does not work for $\mu = 0$

A simple variant when $\mu = 0$

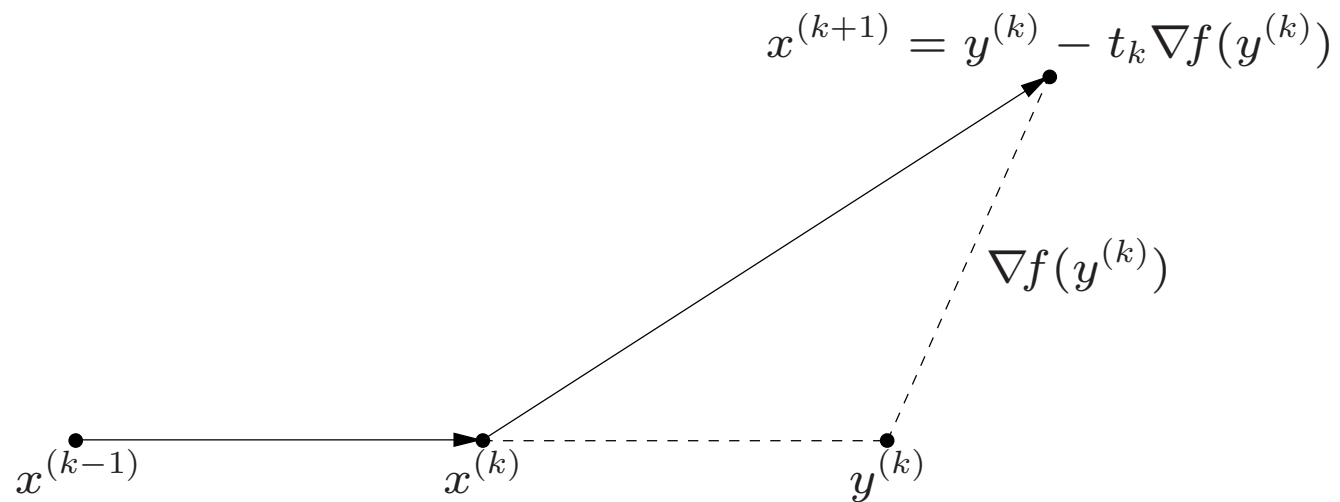
- choose $y^{(0)} = x^{(0)} \in \mathbf{R}^n$
- for $k = 0, 1, 2, \dots$, repeat

$$\begin{aligned}x^{(k+1)} &= y^{(k)} - \frac{1}{L} \nabla f(y^{(k)}) \\ y^{(k+1)} &= x^{(k+1)} + \frac{k}{k+3} (x^{(k+1)} - x^{(k)})\end{aligned}$$

when L is unknown, can replace first equation with line search

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

Interpretation

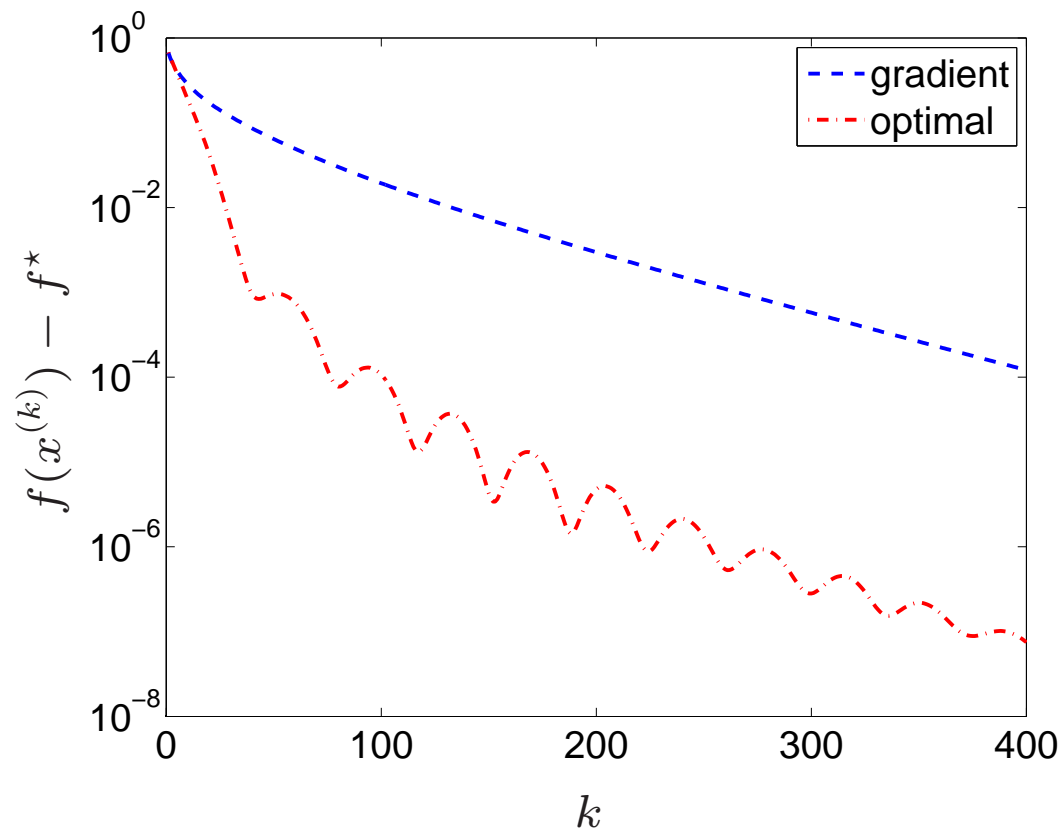


keep the momentum!

Example

$$\text{minimize} \quad \log \left(\sum_{i=1}^m \exp(a_i^T x + b_i) \right)$$

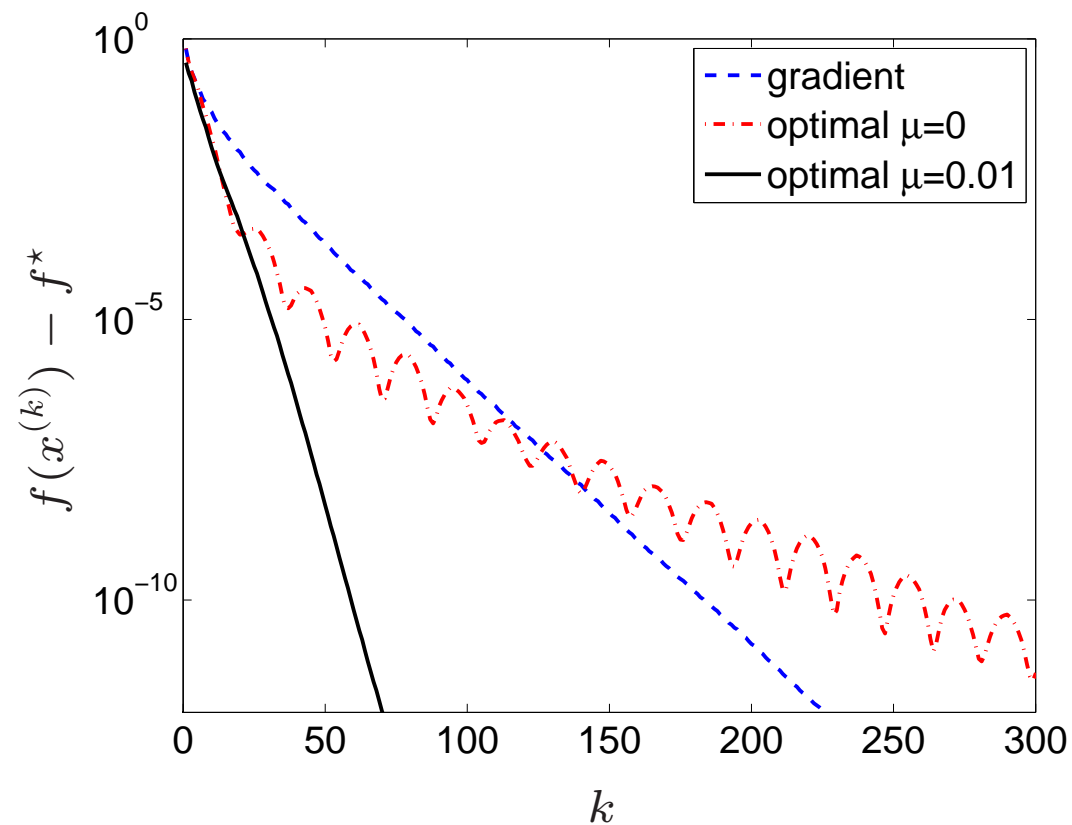
randomly generated data with $m = 500$ and $n = 200$, same fixed step size



Example

$$\text{minimize} \quad \log \left(\sum_{i=1}^m \exp(a_i^T x + b_i) \right)$$

randomly generated data with $m = 500$, $n = 200$, backtracking line search



References

- Yu. Nesterov, *Introductory Lectures on Convex Optimization. A Basic Course* (2004), Section 2.2.
- P. Tseng, *On accelerated proximal gradient methods for convex-concave optimization* (2008).
- L. Vandenberghe, *Lecture notes for EE236C - Optimization Methods for Large-Scale Systems* (Spring 2011), UCLA.

almost all materials of this lecture are taken from Nesterov's book (2004)
(except the numerical examples)