CS 2601 Linear and Convex Optimization

6. Gradient descent (part 1)

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Unconstrained optimization problems

Consider an unconstrained, smooth convex optimization problem

$$\min_{\boldsymbol{x}} \; f(\boldsymbol{x})$$

where f is convex and differentiable on $\mathbb{R}^n$.

The optimal solution satisfies the first-order optimality condition

$$\nabla f(\boldsymbol{x}^*) = \boldsymbol{0}$$

In some rare cases, this yields closed-form solutions, e.g.

$$\min_{\boldsymbol{w}} \; \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2$$

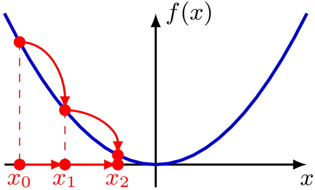
has closed-form solution

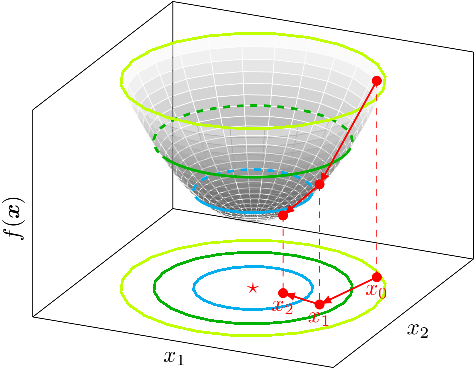
$$\boldsymbol{w}^* = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

But in most cases we need numerical algorithms.

Descent method

choose initial point $\boldsymbol{x}_0 \in \mathbb{R}^n$
repeat
  choose descent direction $\boldsymbol{d}_k \in \mathbb{R}^n$ and step size $t_k > 0$
  $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + t_k \boldsymbol{d}_k \quad$ s.t. $\quad f(\boldsymbol{x}_{k+1}) < f(\boldsymbol{x}_k)$
until stopping criterion is satisfied





Questions

- How to choose $\boldsymbol{d}_k$ and t_k?
- Does $\boldsymbol{x}_k$ converge to $\boldsymbol{x}^*$?

Descent direction

$\boldsymbol{d}_k$ is a descent direction at $\boldsymbol{x}_k$ if for all small enough $t > 0$

$$g(t) \triangleq f(\boldsymbol{x}_k + t\boldsymbol{d}_k) < f(\boldsymbol{x}_k) = g(0)$$

For differentiable f (not necessarily convex),

- if $\boldsymbol{d}_k$ is a descent direction, then $g'(0) = \boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k) \leq 0$;
- if $g'(0) = \boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k) < 0$, then $\boldsymbol{d}_k$ is a descent direction.

For convex f, by the first-order condition for convexity,

$$f(\boldsymbol{x}_k) > f(\boldsymbol{x}_k + t\boldsymbol{d}_k) \geq f(\boldsymbol{x}_k) + t\boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k).$$

$\boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k) < 0$ is also necessary for $\boldsymbol{d}_k$ to be a descent direction.

For convex differentiable f,

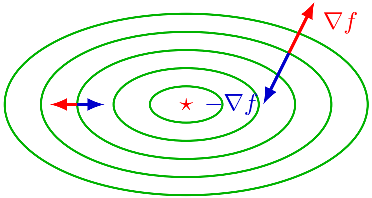
$$\boldsymbol{d}_k \text{ is a descent direction} \iff \boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k) < 0$$

Gradient descent

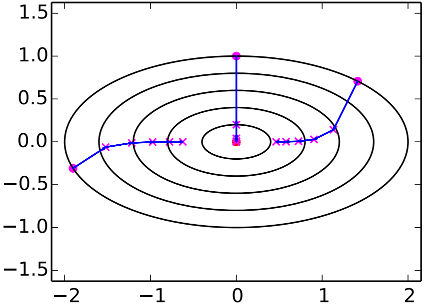
Choose $\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k)$, $\boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k) = -\|\nabla f(\boldsymbol{x}_k)\|_2^2 < 0$ unless $\nabla f(\boldsymbol{x}_k) = 0$.

Updating rule

$$\boxed{\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - t_k \nabla f(\boldsymbol{x}_k)}$$



level curves of $f(x_1, x_2) = \frac{x_1^2}{4} + x_2^2$



Question. What happens if $\nabla f(\boldsymbol{x}_k) = \mathbf{0}$?

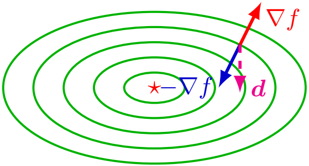
Max-rate descending direction

$-\nabla f(\boldsymbol{x}_k)$ is the direction of fastest rate of decrease of f at $\boldsymbol{x}_k$

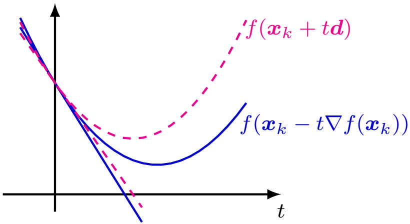
- If $\|\boldsymbol{d}_k\|_2 = 1$,

$$\lim_{t \downarrow 0} \frac{f(\boldsymbol{x}_k) - f(\boldsymbol{x}_k + t\boldsymbol{d}_k)}{t} = -\boldsymbol{d}_k^T \nabla f(\boldsymbol{x}_k) \leq \|\nabla f(\boldsymbol{x}_k)\|_2$$

with equality iff $\boldsymbol{d}_k = -\nabla f(\boldsymbol{x}_k)/\|\nabla f(\boldsymbol{x}_k)\|_2$



level curves of $f(x_1, x_2) = \frac{x_1^2}{4} + x_2^2$



Gradient descent algorithm

initialization $\boldsymbol{x} \leftarrow \boldsymbol{x}_0 \in \mathbb{R}^n$
while $\|\nabla f(\boldsymbol{x})\| > \delta$ **do**
    $\boldsymbol{x} \leftarrow \boldsymbol{x} - t\nabla f(\boldsymbol{x})$
end while
return $\boldsymbol{x}$

Step size (aka learning rate in machine learning)

- the above algorithm uses constant step size t for all iterations
- there are other methods for choosing t for each iteration, e.g. exact line search, backtracking line search

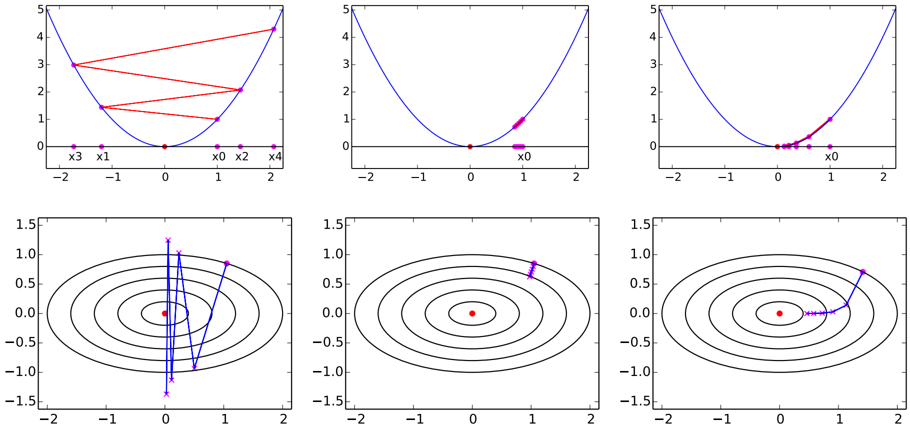
Stopping criterion

- ideally, stop if $\nabla f(\boldsymbol{x}) = 0$ (optimality condition), but impractical
- more practical: stop when $\|\nabla f(\boldsymbol{x})\| \leq \delta$ for some small δ
- other criteria: $|f(\boldsymbol{x}_{\text{new}}) - f(\boldsymbol{x}_{\text{old}})| \leq \delta$, $\frac{|f(\boldsymbol{x}_{\text{new}}) - f(\boldsymbol{x}_{\text{old}})|}{|f(\boldsymbol{x}_{\text{old}})|} \leq \delta$, ...
- in practice, also stop if maximum # of iterations is reached

Large vs. small step size

Consider constant step size. How large should the step size be?

- Too large: may oscillate and diverge
- Too small: may be too slow
- “Just right”: fast convergence



1D example

Consider $f(x) = \frac{1}{2}ax^2$, where $a > 0$.

- gradient step

$$x_{k+1} = x_k - tf'(x_k) = (1 - at)x_k$$

- descent condition

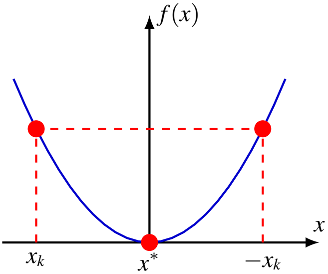
$$f(x_{k+1}) < f(x_k) \iff |1 - at| < 1 \iff 0 < t < \frac{2}{a}$$

- $x_k = (1 - at)^k x_0 \to x^* = 0$ geometrically for such t

Note f satisfies

- $|f'(x) - f'(y)| = a|x - y|$
- $f''(x) = a$

f' is so-called Lipschitz continuous and t is roughly the order of $\frac{1}{a}$.



Lipschitz continuity

A function $f : \mathbb{R}^n \to \mathbb{R}^m$ is Lipschitz continuous with Lipschitz constant $L > 0$, or simply L-Lipschitz, if

$$\|f(\boldsymbol{x}) - f(\boldsymbol{y})\| \leq L\|\boldsymbol{x} - \boldsymbol{y}\|, \quad \forall \boldsymbol{x}, \boldsymbol{y}$$

Note. Lipschitz continuity can be defined with respect to any norms. But we will assume the norms in the above definition are the 2-norms in $\mathbb{R}^n$ and $\mathbb{R}^m$, respectively, unless stated otherwise.

Note. Lipschitz continuity implies uniform continuity.

Example. $f(x) = ax$ is $|a|$-Lipschitz, $|f(x) - f(y)| = |a| \cdot |x - y|$

Example. $f(x) = |x|$ is 1-Lipschitz, $|f(x) - f(y)| = \big||x| - |y|\big| \leq |x - y|$

Example. $f(\boldsymbol{x}) = \boldsymbol{a}^T\boldsymbol{x}$ is $\|\boldsymbol{a}\|$-Lipschitz, $|\boldsymbol{a}^T\boldsymbol{x} - \boldsymbol{a}^T\boldsymbol{y}| \leq \|\boldsymbol{a}\| \cdot \|\boldsymbol{x} - \boldsymbol{y}\|$ by the Cauchy-Schwarz inequality.

Lipschitz continuity (cont'd)

Example. Let $\boldsymbol{Q} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$. $f(\boldsymbol{x}) = \boldsymbol{Q}\boldsymbol{x} = (x_1, 2x_2)^T$ is 2-Lipschitz.

$$f(\boldsymbol{x}) - f(\boldsymbol{y}) = (x_1 - y_1, 2x_2 - 2y_2)^T = (d_1, 2d_2)^T$$

$$\|f(\boldsymbol{x}) - f(\boldsymbol{y})\| = \sqrt{d_1^2 + 4d_2^2} \le 2\sqrt{d_1^2 + d_2^2} = 2\|\boldsymbol{x} - \boldsymbol{y}\|$$

More generally, $f(\boldsymbol{x}) = \boldsymbol{Q}\boldsymbol{x}$ with $\boldsymbol{Q} \succeq \boldsymbol{O}$ is $\lambda_{\max}(\boldsymbol{Q})$-Lipschitz, where $\lambda_{\max}(\boldsymbol{Q})$ is the largest eigenvalue of $\boldsymbol{Q}$[1].

Proof. Let $\boldsymbol{d} = \boldsymbol{x} - \boldsymbol{y}$. By slide 32 of §2,

$$\|f(\boldsymbol{x}) - f(\boldsymbol{y})\| = \|\boldsymbol{Q}\boldsymbol{d}\| = \sqrt{\boldsymbol{d}^T\boldsymbol{Q}^2\boldsymbol{d}} \le \sqrt{\lambda_{\max}(\boldsymbol{Q}^2)\|\boldsymbol{d}\|^2} = \lambda_{\max}(\boldsymbol{Q})\|\boldsymbol{x} - \boldsymbol{y}\|$$

The last equality uses the fact $\lambda_{\max}(\boldsymbol{Q}^2) = \lambda_{\max}^2(\boldsymbol{Q})$.

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[1] For general $\boldsymbol{Q}$, $f(\boldsymbol{x}) = \boldsymbol{Q}\boldsymbol{x}$ is $\sigma_{\max}(\boldsymbol{Q})$-Lipschitz, where $\sigma_{\max}(\boldsymbol{Q}) = \sqrt{\lambda_{\max}(\boldsymbol{Q}^T\boldsymbol{Q})}$ is the largest singular value of $\boldsymbol{Q}$.

L-smoothness

A function is L-smooth if it is differentiable and its gradient is L-Lipschitz, i.e.

$$\|\nabla f(\boldsymbol{x}) - \nabla f(\boldsymbol{y})\| \leq L\|\boldsymbol{x} - \boldsymbol{y}\|, \quad \forall \boldsymbol{x}, \boldsymbol{y}$$

Note. L upper bounds the rate of change of ∇f

Example. $f(x) = \frac{1}{2}ax^2$ is $|a|$-smooth, since $f'(x) = ax$ is $|a|$-Lipschitz

Example. $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x}$ with $\boldsymbol{Q} \succeq \boldsymbol{O}$ is $\lambda_{\max}(\boldsymbol{Q})$-smooth, since $\nabla f(\boldsymbol{x}) = \boldsymbol{Q}\boldsymbol{x}$ is $\lambda_{\max}(\boldsymbol{Q})$-Lipschitz.

With $\boldsymbol{Q} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$, we obtain $f(\boldsymbol{x}) = \frac{1}{2}x_1^2 + x_2^2$ is 2-smooth.

Lemma. A twice continuously differentiable convex $f : \mathbb{R}^n \to \mathbb{R}$ is L-smooth iff $\nabla^2 f(\boldsymbol{x}) \preceq L\boldsymbol{I}$, meaning $L\boldsymbol{I} - \nabla^2 f(\boldsymbol{x}) \succeq \boldsymbol{O}$, or equivalently $\lambda_{\max}(\nabla^2 f(\boldsymbol{x})) \leq L$.

如果不是凸函数这要加个绝对值

Appendix: Second-order condition for L-smoothness

Lemma. A twice continuously differentiable $f : \mathbb{R}^n \to \mathbb{R}$ is L-smooth iff for any $\boldsymbol{x}$, $-L\boldsymbol{I} \preceq \nabla^2 f(\boldsymbol{x}) \preceq L\boldsymbol{I}$, or equivalently $|\lambda| \leq L$ for all eigenvalues λ of $\nabla^2 f(\boldsymbol{x})$.

Proof. "$\Leftarrow$". Assume $-L\boldsymbol{I} \preceq \nabla^2 f(\boldsymbol{x}) \preceq L\boldsymbol{I}$ for all $\boldsymbol{x}$. By the Mean Value Theorem and slide 30 of §2,

$$\|\nabla f(\boldsymbol{x}) - \nabla f(\boldsymbol{y})\| = \|\nabla^2 f(\boldsymbol{z})(\boldsymbol{x} - \boldsymbol{y})\| \leq L\|\boldsymbol{x} - \boldsymbol{y}\|$$

"$\Rightarrow$". Assume f is L-smooth. Let $\boldsymbol{d}$ be an eigenvector of $\nabla^2 f(\boldsymbol{x})$ with associated eigenvalue λ. By L-smoothness,

$$\|\nabla f(\boldsymbol{x} + t\boldsymbol{d}) - \nabla f(\boldsymbol{x})\| \leq L\|t\boldsymbol{d}\| = tL\|\boldsymbol{d}\|$$

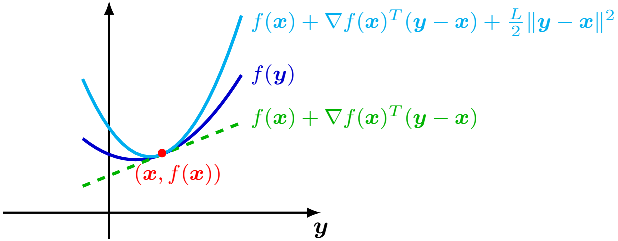
Dividing both sides by t and letting $t \to 0$,

$$|\lambda| \cdot \|\boldsymbol{d}\| = \|\nabla^2 f(\boldsymbol{x})\boldsymbol{d}\| \leq L\|\boldsymbol{d}\| \implies |\lambda| \leq L$$

Quadratic upper bound

Lemma. If f is L-smooth, then

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



Note. The upper bound does not assume the convexity of f.

If $\nabla^2 f(\boldsymbol{x}) \preceq L\boldsymbol{I}$, this is intuitive from the second-order Taylor expansion

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

for some $\boldsymbol{z}$ on the line segment between $\boldsymbol{x}$ and $\boldsymbol{y}$. (Check $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x}$)

Proof

First prove the 1D case. Let $g(t)$ be L_g-smooth, $|g'(t) - g'(s)| \leq L_g|t - s|$.

$$\begin{aligned} g(1) &= g(0) + \int_0^1 g'(t)dt \\ &= g(0) + g'(0) + \int_0^1 [g'(t) - g'(0)]dt \\ &\leq g(0) + g'(0) + \int_0^1 L_g t dt \quad \text{since } |g'(t) - g'(0)| \leq L_g t \\ &= g(0) + g'(0) + \frac{1}{2}L_g \end{aligned}$$

For the general case, apply the above to $g(t) = f(\boldsymbol{x} + t\boldsymbol{d})$ with $\boldsymbol{d} = \boldsymbol{y} - \boldsymbol{x}$ and $L_g = L\|\boldsymbol{d}\|^2$. By the Cauchy-Schwarz inequality

$$\begin{aligned} |g'(t) - g'(s)| &= \left|[\nabla f(\boldsymbol{x} + t\boldsymbol{d}) - \nabla f(\boldsymbol{x} + s\boldsymbol{d})]^T \boldsymbol{d}\right| \\ &\leq \|\nabla f(\boldsymbol{x} + t\boldsymbol{d}) - \nabla f(\boldsymbol{x} + s\boldsymbol{d})\| \cdot \|\boldsymbol{d}\| \quad \text{Cauchy-Schwarz} \\ &\leq (t - s)L\|\boldsymbol{d}\|^2 \quad f \text{ is } L\text{-smooth} \end{aligned}$$

Consequence of quadratic upper bound

For L-smooth f, the sequence $\{\boldsymbol{x}_k\}$ produced by gradient descent satisfies

$$f(\boldsymbol{x}_{k+1}) \leq f(\boldsymbol{x}_k) - t\left(1 - \frac{Lt}{2}\right)\|\nabla f(\boldsymbol{x}_k)\|^2$$

Proof. Plugging in $\boldsymbol{x} = \boldsymbol{x}_k$ and $\boldsymbol{y} = \boldsymbol{x}_{k+1} = \boldsymbol{x}_k - t\nabla f(\boldsymbol{x}_k)$ in the quadratic upper bound,

$$\begin{aligned} f(\boldsymbol{x}_{k+1}) &\leq f(\boldsymbol{x}_k) - t\|\nabla f(\boldsymbol{x}_k)\|^2 + \frac{L}{2}t^2\|\nabla f(\boldsymbol{x}_k)\|^2 \\ &= f(\boldsymbol{x}_k) - t\left(1 - \frac{Lt}{2}\right)\|\nabla f(\boldsymbol{x}_k)\|^2 \end{aligned}$$

Note. If $\nabla f(\boldsymbol{x}_k) \neq 0$ and $0 < t < \frac{2}{L}$, then $f(\boldsymbol{x}_{k+1}) < f(\boldsymbol{x}_k)$, so gradient descent with step size $t \in (0, 2/L)$ is indeed a descent method.

Note. We can lower bound the decrease in function value in each step. In particular, for $0 < t \leq \frac{1}{L}$,

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1}) \geq \frac{t}{2}\|\nabla f(\boldsymbol{x}_k)\|^2$$

Convergence analysis

Theorem. If f is convex and L-smooth, and $\boldsymbol{x}^*$ is a minimum of f, then for step size $t \in (0, \frac{1}{L}]$, the sequence $\{\boldsymbol{x}_k\}$ produced by the gradient descent algorithm satisfies

$$f(\boldsymbol{x}_k) - f(\boldsymbol{x}^*) \leq \frac{\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|^2}{2tk}$$

Notes.

- $f(\boldsymbol{x}_k) \downarrow f^*$ as $k \to \infty$.
- Any limiting point of $\boldsymbol{x}_k$ is an optimal solution.
- The rate of convergence is $O(1/k)$, i.e. # of iterations to guarantee $f(\boldsymbol{x}_k) - f(\boldsymbol{x}^*) \leq \epsilon$ is $O(1/\epsilon)$. For $\epsilon = 10^{-p}$, $k = O(10^p)$, exponential in the number of significant digits!
- Faster convergence with larger t; best $t = \frac{1}{L}$, but L is unknown.
- Good initial guess helps.

Proof

不要求

1. By the basic gradient step $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - t\nabla f(\boldsymbol{x}_k)$,

$$\begin{aligned}\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|^2 &= \|\boldsymbol{x}_k - t\nabla f(\boldsymbol{x}_k) - \boldsymbol{x}^*\|^2 \\ &= \|\boldsymbol{x}_k - \boldsymbol{x}^*\|^2 + t^2\|\nabla f(\boldsymbol{x}_k)\|^2 + 2t\nabla f(\boldsymbol{x}_k)^T(\boldsymbol{x}^* - \boldsymbol{x}_k)\end{aligned}$$

2. By the last inequality on slide 15, the second term is upper bounded by

$$t^2\|\nabla f(\boldsymbol{x}_k)\|^2 \le 2t[f(\boldsymbol{x}_k) - f(\boldsymbol{x}_{k+1})]$$

3. By the first-order condition for convexity, the third term is upper bounded by

$$2t\nabla f(\boldsymbol{x}_k)^T(\boldsymbol{x}^* - \boldsymbol{x}_k) \le 2t[f(\boldsymbol{x}^*) - f(\boldsymbol{x}_k)]$$

4. Plugging 2 and 3 into 1,

$$\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|^2 \le \|\boldsymbol{x}_k - \boldsymbol{x}^*\|^2 + 2t[f(\boldsymbol{x}^*) - f(\boldsymbol{x}_{k+1})]$$

Proof (cont'd)

5. Rearranging and using the descent property $f(\boldsymbol{x}_{k+1}) \leq f(\boldsymbol{x}_k)$, the suboptimality gap is upper bounded by

$$f(\boldsymbol{x}_N) - f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}_{k+1}) - f(\boldsymbol{x}^*) \leq \frac{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^2 - \|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|^2}{2t}$$

   for $k \leq N - 1$.

6. Summing over k from 0 to $N - 1$,

$$N[f(\boldsymbol{x}_N) - f(\boldsymbol{x}^*)] \leq \frac{\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|^2 - \|\boldsymbol{x}_N - \boldsymbol{x}^*\|^2}{2t} \leq \frac{\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|^2}{2t}$$

   so

$$f(\boldsymbol{x}_N) - f(\boldsymbol{x}^*) \leq \frac{\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|^2}{2Nt}$$