Optimization for Machine Learning
CS-439

Lecture 6: Non-convex optimization; Accelerated Gradient Descent

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Trajectory Analysis

Even if the “landscape” (graph) of a nonconvex function has local minima, saddle points, and flat parts, gradient descent may avoid them and still converge to a global minimum.

For this, one needs a good starting point and some theoretical understanding of what happens when we start there—this is **trajectory analysis**.

2018: trajectory analysis for training deep linear linear neural networks, under suitable conditions [ACGH18].

Here: vastly simplified setting that allows us to show the main ideas (and limitations).

Linear models with several outputs

Recall: Learning linear models

- n inputs $\mathbf{x}_1, \ldots, \mathbf{x}_n$, where each input $\mathbf{x}_i \in \mathbb{R}^d$
- n outputs $y_1, \ldots, y_n \in \mathbb{R}$
- Hypothesis (after centering):

$$y_i \approx \mathbf{w}^\top x_i,$$

  for a weight vector $\mathbf{w} = (w_1, \ldots, w_d) \in \mathbb{R}^d$ to be learned.

Now more than one output value:

- n outputs $\mathbf{y}_1, \ldots, \mathbf{y}_n$, where each output $\mathbf{y}_i \in \mathbb{R}^m$
- Hypothesis:

$$\mathbf{y}_i \approx W\mathbf{x}_i,$$

  for a weight matrix $W \in \mathbb{R}^{m \times d}$ to be learned.

Minimizing the least squares error

Compute

$$W^\star = \operatorname*{argmin}_{W \in \mathbb{R}^{m \times d}} \sum_{i=1}^{n} \|W\mathbf{x}_i - \mathbf{y}_i\|^2 .$$

- $X \in \mathbb{R}^{d \times n}$: matrix whose columns are the $\mathbf{x}_i$
- $Y \in \mathbb{R}^{m \times n}$: matrix whose columns are the $\mathbf{y}_i$

Then

$$W^\star = \operatorname*{argmin}_{W \in \mathbb{R}^{m \times d}} \|WX - Y\|_F^2,$$

where $\|A\|_F = \sqrt{\sum_{i,j} a_{ij}^2}$ is the Frobenius norm of a matrix A.

Frobenius norm of A = Euclidean norm of $\mathrm{vec}(A)$ ("flattening" of A)

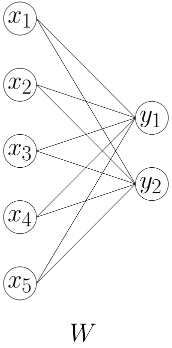
Minimizing the least squares error II

$$W^\star = \underset{W \in \mathbb{R}^{m \times d}}{\operatorname{argmin}} \|WX - Y\|_F^2$$

is the global minimum of a convex quadratic function $f(W)$.

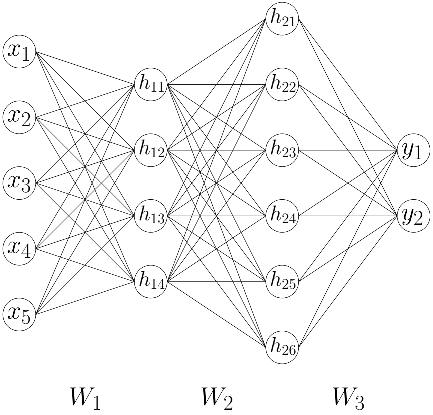
To find $W^\star$, solve $\nabla f(W) = \mathbf{0}$ (system of linear equations).

$\Leftrightarrow$ training a **linear neural network with one layer** under least squares error.



$$\mathbf{x} \mapsto \mathbf{y} = W\mathbf{x}$$

Deep linear neural networks



$$\mathbf{x} \mapsto \mathbf{y} = W_3 W_2 W_1 \mathbf{x}$$

Not more expressive:

$$\mathbf{x} \mapsto \mathbf{y} = W_3 W_2 W_1 \mathbf{x} \quad \Leftrightarrow \quad \mathbf{x} \mapsto \mathbf{y} = W\mathbf{x},\ W := W_3 W_2 W_1.$$

Training deep linear neural networks

With ℓ layers:

$$W^\star = \operatorname*{argmin}_{W_1, W_2, \ldots, W_\ell} \|W_\ell W_{\ell-1} \cdots W_1 X - Y\|_F^2,$$

Nonconvex function for $\ell > 1$.

Simple playground in which we can try to understand why training deep neural networks with gradient descent works.

Here: all matrices are 1×1, $W_i = x_i, X = 1, Y = 1, \ell = d \quad \Rightarrow f : \mathbb{R}^d \to \mathbb{R}$,

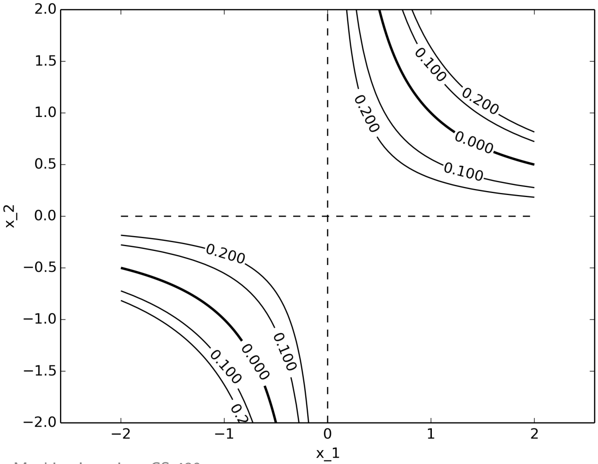
$$f(\mathbf{x}) := \frac{1}{2} \left(\prod_{k=1}^{d} x_k - 1 \right)^2 .$$

Toy example in our simple playground.

But analysis of gradient descent on f has similar ingredients as the one on general deep linear neural networks [ACGH18].

A simple nonconvex function

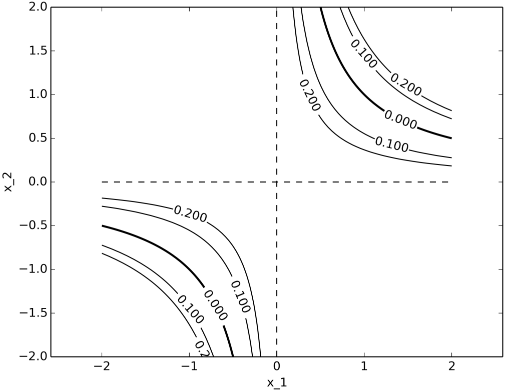
As d is fixed, abbreviate $\prod_{k=1}^{d} x_k$ by $\prod_k x_k$: $f(\mathbf{x}) = \frac{1}{2}\left(\prod_k x_k - 1\right)^2$



Level set plot

The gradient

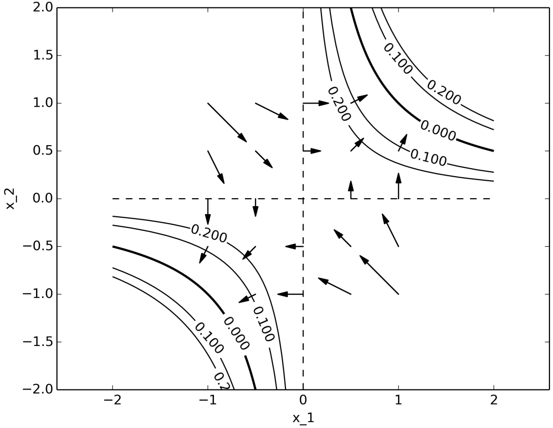
$$\nabla f(\mathbf{x}) = \left(\prod_k x_k - 1\right)\left(\prod_{k\neq 1} x_k, \ldots, \prod_{k\neq d} x_k\right).$$



Critical points ($\nabla f(\mathbf{x}) = \mathbf{0}$):

- $\prod_k x_k = 1$ (global minima)
  - $d = 2$: the hyperbola $\{(x_1, x_2) : x_1 x_2 = 1\}$
- at least two of the x_k are zero (saddle points)
  - $d = 2$: the origin $(x_1, x_2) = (0, 0)$

Negative gradient directions (followed by gradient descent)



Difficult to avoid convergence to a global minimum, but it is possible (Exercise 37).

Convergence analysis: Overview

Want to show that for any $d > 1$, and from anywhere in $X = \{\mathbf{x} : \mathbf{x} > \mathbf{0}, \prod_k \mathbf{x}_k \leq 1\}$, gradient descent will converge to a global minimum.

f is not smooth over X. We show that f is smooth along the trajectory of gradient descent for suitable L, so that we get sufficient decrease

$$f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \frac{1}{2L}\|\nabla f(\mathbf{x}_t)\|^2, \quad t \geq 0.$$

Then, we cannot converge to a saddle point: all these have (at least two) zero entries and therefore function value $1/2$. But for starting point $\mathbf{x}_0 \in X$, we have $f(\mathbf{x}_0) < 1/2$, so we can never reach a saddle while decreasing f.

Doesn't this imply converge to a global mimimum? No!

- Sublevel sets are unbounded, so we could in principle run off to infinity.
- Other bad things might happen (we haven't characterized what can go wrong).

Convergence analysis: Overview II

For $\mathbf{x} > \mathbf{0}, \prod_k \mathbf{x}_k \geq 1$, we also get convergence (Exercise 36).

$\Rightarrow$ convergence from anywhere in the interior of the positive orthant $\{\mathbf{x} : \mathbf{x} > \mathbf{0}\}$.

But there are also starting points from which gradient descent will not converge to a global minimum (Exercise 37).

Main tool: Balanced iterates

Definition

Let $\mathbf{x} > \mathbf{0}$ (componentwise), and let $c \geq 1$ be a real number. $\mathbf{x}$ is called c-balanced if $x_i \leq c x_j$ for all $1 \leq i, j \leq d$.

Any initial iterate $\mathbf{x}_0 > \mathbf{0}$ is c-balanced for some (possibly large) c.

Lemma

Let $\mathbf{x} > \mathbf{0}$ be c-balanced with $\prod_k x_k \leq 1$. Then for any stepsize $\gamma > 0$, $\mathbf{x}' := \mathbf{x} - \gamma \nabla f(\mathbf{x})$ satisfies $\mathbf{x}' \geq \mathbf{x}$ (componentwise) and is also c-balanced.

Proof.

$\Delta := -\gamma(\prod_k x_k - 1)(\prod_k x_k) \geq 0. \qquad \nabla f(\mathbf{x}) = (\prod_k x_k - 1)\left(\prod_{k \neq 1} x_k, \ldots, \prod_{k \neq d} x_k\right).$

Gradient descent step:

$$x'_k = x_k + \frac{\Delta}{x_k} \geq x_k, \quad k = 1, \ldots, d.$$

For i, j, we have $x_i \leq c x_j$ and $x_j \leq c x_i$ ($\Leftrightarrow 1/x_i \leq c/x_j$). We therefore get

$$x'_i = x_i + \frac{\Delta}{x_i} \leq c x_j + \frac{\Delta c}{x_j} = c x'_j.$$

□

Bounded Hessians along the trajectory

Compute $\nabla^2 f(\mathbf{x})$:

$\nabla^2 f(\mathbf{x})_{ij}$ is the j-th partial derivative of the i-th entry of $\nabla f(\mathbf{x})$.

$$(\nabla f)_i = \left(\prod_k x_k - 1\right) \prod_{k \neq i} x_k$$

$$\nabla^2 f(\mathbf{x})_{ij} = \begin{cases} \left(\prod_{k \neq i} x_k\right)^2, & j = i \\ 2 \prod_{k \neq i} x_k \prod_{k \neq j} x_k - \prod_{k \neq i,j} x_k, & j \neq i \end{cases}$$

Need to bound $\prod_{k \neq i} x_k, \quad \prod_{k \neq j} x_k, \quad \prod_{k \neq i,j} x_k$!

Bounded Hessians along the trajectory II

Lemma

Suppose that $\mathbf{x} > \mathbf{0}$ *is* c*-balanced. Then for any* $I \subseteq \{1, \ldots, d\}$, *we have*

$$\left(\frac{1}{c}\right)^{|I|} \left(\prod_k x_k\right)^{1-|I|/d} \leq \prod_{k \notin I} x_k \leq c^{|I|} \left(\prod_k x_k\right)^{1-|I|/d}.$$

Proof.

For any i, we have $x_i^d \geq (1/c)^d \prod_k x_k$ by balancedness, hence $x_i \geq (1/c)(\prod_k x_k)^{1/d}$.It follows that

$$\prod_{k \notin I} x_k = \frac{\prod_k x_k}{\prod_{i \in I} x_i} \leq \frac{\prod_k x_k}{(1/c)^{|I|}(\prod_k x_k)^{|I|/d}} = c^{|I|} \left(\prod_k x_k\right)^{1-|I|/d}.$$

The lower bound follows in the same way from $x_i^d \leq c^d \prod_k x_k$. □

Bounded Hessians along the trajectory III

Lemma

Let $\mathbf{x} > \mathbf{0}$ *be* c*-balanced with* $\prod_k x_k \leq 1$. *Then*

$$\left\|\nabla^2 f(\mathbf{x})\right\| \leq \left\|\nabla^2 f(\mathbf{x})\right\|_F \leq 3dc^2.$$

where $\|A\|_F$ *is the Frobenius norm and* $\|A\|$ *the spectral norm.*

Proof.

$\|A\| \leq \|A\|_F$: Exercise 38. Now use previous lemma and $\prod_k x_k \leq 1$:

$$\left|\nabla^2 f(\mathbf{x})_{ii}\right| = |(\prod_{k\neq i} x_k)^2| \leq c^2$$

$$\left|\nabla^2 f(\mathbf{x})_{ij}\right| \leq |2\prod_{k\neq i} x_k \prod_{k\neq j} x_k| + |\prod_{k\neq i,j} x_k| \leq 3c^2.$$

Hence, $\left\|\nabla^2 f(\mathbf{x})\right\|_F^2 \leq 9d^2c^4$. Taking square roots, the statement follows. □

Smoothness along the trajectory

Lemma

Let $\mathbf{x} > \mathbf{0}$ be c-balanced with $\prod_k x_k < 1$, $L = 3dc^2$. Let $\gamma := 1/L$. Then for all $0 \leq \nu \leq \gamma$,

$$\mathbf{x}' := \mathbf{x} - \nu \nabla f(\mathbf{x}) \geq \mathbf{x}$$

is c-balanced with $\prod_k x'_k \leq 1$, and f is smooth with parameter L over the line segment connecting $\mathbf{x}$ and $\mathbf{x} - \gamma \nabla f(\mathbf{x})$.

Proof.

- $\mathbf{x}' \geq \mathbf{x} > \mathbf{0}$ is c-balanced by Lemma 6.5.
- $\nabla f(\mathbf{x}) \neq \mathbf{0}$ (due to $\mathbf{x}' > \mathbf{0}, \prod_k x_k < 1$, we can't be at a critical point).
- No overshooting: we can't reach $\prod_k x'_k = 1$ (global minimum) for $\nu < \gamma$, as f is smooth with parameter L between $\mathbf{x}$ and $\mathbf{x}'$ (using previous bound on Hessians in Lemma 6.1).
- By continutity, $\prod_k x'_k \leq 1$ for all $\nu \leq \gamma$.
- f is smooth with parameter L between $\mathbf{x}$ and $\mathbf{x}'$ for $\nu = \gamma$.

Convergence

Theorem

Let $c \geq 1$ and $\delta > 0$ such that $\mathbf{x}_0 > \mathbf{0}$ is c-balanced with $\delta \leq \prod_k (\mathbf{x}_0)_k < 1$. Choosing stepsize

$$\gamma = \frac{1}{3dc^2},$$

gradient descent satisfies

$$f(\mathbf{x}_T) \leq \left(1 - \frac{\delta^2}{3c^4}\right)^T f(\mathbf{x}_0), \quad T \geq 0.$$

- Error converges to 0 exponentially fast.
- Exercise 39: iterates themselves converge (to an optimal solution).

Convergence: Proof

Proof.

- For $t \geq 0$, f is smooth between $\mathbf{x}_t$ and $\mathbf{x}_{t+1}$ with parameter $L = 3dc^2$.
- Sufficient decrease:

$$f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \frac{1}{6dc^2} \left\|\nabla f(\mathbf{x}_t)\right\|^2.$$

For every c-balanced $\mathbf{x}$ with $\delta \leq \prod_k x_k \leq 1$, $\left\|\nabla f(\mathbf{x})\right\|^2$ equals

$$2f(\mathbf{x}) \sum_{i=1}^{d} \left(\prod_{k \neq i} x_k\right)^2 \geq 2f(\mathbf{x}) \frac{d}{c^2} \left(\prod_k x_k\right)^{2-2/d} \geq 2f(\mathbf{x}) \frac{d}{c^2} \left(\prod_k x_k\right)^2 \geq 2f(\mathbf{x}) \frac{d}{c^2} \delta^2.$$

- Hence, $f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t) - \frac{1}{6dc^2} 2f(\mathbf{x}_t) \frac{d}{c^2} \delta^2 = f(\mathbf{x}_t) \left(1 - \frac{\delta^2}{3c^4}\right)$.

Discussion

Fast convergence as for strongly convex functions!

But there is a catch...

Consider starting point $\mathbf{x}_0 = (1/2, \ldots, 1/2)$.

$\delta \leq \prod_k (\mathbf{x}_0)_k = 2^{-d}$.

Decrease in function value by a factor of

$$\left(1 - \frac{1}{3 \cdot 4^d}\right),$$

per step.

Need $T \approx 4^d$ to reduce the initial error by a constant factor not depending on d.

Problem: gradients are exponentially small in the beginning, extremely slow progress.

For polynomial runtime, must start at distance $O(1/\sqrt{d})$ from optimality.

Chapter 7

Accelerated Gradient Descent

Smooth convex functions: less than $\mathcal{O}(1/\varepsilon)$ steps?

Fixing L and $R = \|\mathbf{x}_0 - \mathbf{x}^\star\|$, the error of gradient descent after T steps is $O(1/T)$.

Lee and Wright [LW19]:

- A better upper bound of $o(1/T)$ holds.
- A lower bound of $\Omega(1/T^{1+\delta})$ also holds, for any fixed $\delta > 0$.

So, gradient descent is slightly faster on smooth functions than what we proved, but not significantly.

First-order methods: less than $\mathcal{O}(1/\varepsilon)$ steps?

Maybe gradient descent is not the best possible algorithm?

After all, it is just some algorithm that uses gradient information.

First-order method:

- An algorithm that gains access to f only via an oracle that is able to return values of f and ∇f at arbitrary points.
- Gradient descent is a specific first-order method.

What is the best first-order method for smooth convex functions, the one with the smallest upper bound on the number of oracle calls in the worst case?

Nemirovski and Yudin 1979 [NY83]: every first-order method needs in the worst case $\Omega(1/\sqrt{\varepsilon})$ steps (gradient evaluations) in order to achieve an additive error of ε on smooth functions.

There is a gap between $O(1/\varepsilon)$ (gradient descent) and the lower bound!

Acceleration for smooth convex functions: $\mathcal{O}(1/\sqrt{\varepsilon})$ steps

Nesterov 1983 [Nes83, Nes18]: There is a first-order method that needs only $O(1/\sqrt{\varepsilon})$ steps on smooth convex functions, and by the lower bound of Nemirovski and Yudin, this is a best possible algorithm!

The algorithm is known as (Nesterov's) accelerated gradient descent.

A number of (similar) optimal algorithms with other proofs of the $\mathcal{O}(1/\sqrt{\varepsilon})$ upper bound are known, but there is no well-established "simplest proof".

Here: a recent proof based on potential functions [BG17]. Proof is simple but not very instructive (it works, but it's not clear why).

Nesterov's accelerated gradient descent

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex, differentiable, and smooth with parameter L. Choose $\mathbf{z}_0 = \mathbf{y}_0 = \mathbf{x}_0$ arbitrary. For $t \geq 0$, set

$$\begin{aligned} \mathbf{y}_{t+1} &:= \mathbf{x}_t - \frac{1}{L}\nabla f(\mathbf{x}_t) \\ \mathbf{z}_{t+1} &:= \mathbf{z}_t - \frac{t+1}{2L}\nabla f(\mathbf{x}_t) \\ \mathbf{x}_{t+1} &:= \frac{t+1}{t+3}\mathbf{y}_{t+1} + \frac{2}{t+3}\mathbf{z}_{t+1}. \end{aligned}$$

- Perform a "smooth step" from $\mathbf{x}_t$ to $\mathbf{y}_{t+1}$.
- Perform a more aggressive step from $\mathbf{z}_t$ to $\mathbf{z}_{t+1}$.
- Next iterate $\mathbf{x}_{t+1}$ is a weighted average of $\mathbf{y}_{t+1}$ and $\mathbf{z}_{t+1}$, where we compensate for the more aggressive step by giving $\mathbf{z}_{t+1}$ a relatively low weight.

Why should this work??

Nesterov's accelerated gradient descent: Error bound

Theorem

Let $f : \mathbb{R}^d \to \mathbb{R}$ be convex and differentiable with a global minimum $\mathbf{x}^\star$; furthermore, suppose that f is smooth with parameter L. Accelerated gradient descent yields

$$f(\mathbf{y}_T) - f(\mathbf{x}^\star) \leq \frac{2L \left\|\mathbf{z}_0 - \mathbf{x}^\star\right\|^2}{T(T+1)}, \quad T > 0.$$

To reach error at most ε, accelerated gradient descent therefore only needs $O(1/\sqrt{\varepsilon})$ steps instead of $O(1/\varepsilon)$.

Recall the bound for gradient descent:

$$f(\mathbf{x}_T) - f(\mathbf{x}^\star) \leq \frac{L}{2T}\|\mathbf{x}_0 - \mathbf{x}^\star\|^2, \quad T > 0.$$

Nesterov's accelerated gradient descent: The potential function

Idea: assign a potential $\Phi(t)$ to each time t and show that $\Phi(t+1) \leq \Phi(t)$.

Out of the blue: let's define the potential as

$$\Phi(t) := t(t+1)\left(f(\mathbf{y}_t) - f(\mathbf{x}^\star)\right) + 2L\left\|\mathbf{z}_t - \mathbf{x}^\star\right\|^2.$$

If we can show that the potential always decreases, we get

$$\underbrace{T(T+1)\left(f(\mathbf{y}_T) - f(\mathbf{x}^\star)\right) + 2L\left\|\mathbf{z}_T - \mathbf{x}^\star\right\|^2}_{\Phi(T)} \leq \underbrace{2L\left\|\mathbf{z}_0 - \mathbf{x}^\star\right\|^2}_{\Phi(0)}.$$

Rewriting this, we get the claimed error bound.

Potential function decrease: Three Ingredients

Sufficient decrease for the smooth step from $\mathbf{x}_t$ to $\mathbf{y}_{t+1}$:

$$f(\mathbf{y}_{t+1}) \leq f(\mathbf{x}_t) - \frac{1}{2L}\|\nabla f(\mathbf{x}_t)\|^2; \tag{1}$$

Vanilla analysis for the more aggressive step from $\mathbf{z}_t$ to $\mathbf{z}_{t+1}$: ($\gamma = \frac{t+1}{2L}$, $\mathbf{g}_t = \nabla f(\mathbf{x}_t)$):

$$\mathbf{g}_t^\top(\mathbf{z}_t - \mathbf{x}^\star) = \frac{t+1}{4L}\|\mathbf{g}_t\|^2 + \frac{L}{t+1}\left(\|\mathbf{z}_t - \mathbf{x}^\star\|^2 - \|\mathbf{z}_{t+1} - \mathbf{x}^\star\|^2\right); \tag{2}$$

Convexity (graph of f is above the tangent hyperplane at $\mathbf{x}_t$):

$$f(\mathbf{x}_t) - f(\mathbf{w}) \leq \mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{w}), \quad \mathbf{w} \in \mathbb{R}^d. \tag{3}$$

Potential function decrease: Proof

By definition of potential,

$$\begin{aligned}\Phi(t+1) &= t(t+1)\left(f(\mathbf{y}_{t+1}) - f(\mathbf{x}^\star)\right) + 2(t+1)\left(f(\mathbf{y}_{t+1}) - f(\mathbf{x}^\star)\right) + 2L\left\|\mathbf{z}_{t+1} - \mathbf{x}^\star\right\|^2, \\ \Phi(t) &= t(t+1)\left(f(\mathbf{y}_t) - f(\mathbf{x}^\star)\right) + 2L\left\|\mathbf{z}_t - \mathbf{x}^\star\right\|^2.\end{aligned}$$

Now, prove that $\Delta := (\Phi(t+1) - \Phi(t))/(t+1) \leq 0$:

$$\begin{aligned}\Delta &= t\left(f(\mathbf{y}_{t+1}) - f(\mathbf{y}_t)\right) + 2\left(f(\mathbf{y}_{t+1}) - f(\mathbf{x}^\star)\right) + \frac{2L}{t+1}\left(\left\|\mathbf{z}_{t+1} - \mathbf{x}^\star\right\|^2 - \left\|\mathbf{z}_t - \mathbf{x}^\star\right\|^2\right) \\ &\overset{(2)}{=} t\left(f(\mathbf{y}_{t+1}) - f(\mathbf{y}_t)\right) + 2\left(f(\mathbf{y}_{t+1}) - f(\mathbf{x}^\star)\right) + \frac{t+1}{2L}\|\mathbf{g}_t\|^2 - 2\mathbf{g}_t^\top(\mathbf{z}_t - \mathbf{x}^\star) \\ &\overset{(1)}{\leq} t\left(f(\mathbf{x}_t) - f(\mathbf{y}_t)\right) + 2\left(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\right) - \frac{1}{2L}\|\mathbf{g}_t\|^2 - 2\mathbf{g}_t^\top(\mathbf{z}_t - \mathbf{x}^\star) \\ &\leq t\left(f(\mathbf{x}_t) - f(\mathbf{y}_t)\right) + 2\left(f(\mathbf{x}_t) - f(\mathbf{x}^\star)\right) - 2\mathbf{g}_t^\top(\mathbf{z}_t - \mathbf{x}^\star) \\ &\overset{(3)}{\leq} t\mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{y}_t) + 2\mathbf{g}_t^\top(\mathbf{x}_t - \mathbf{x}^\star) - 2\mathbf{g}_t^\top(\mathbf{z}_t - \mathbf{x}^\star) \\ &= \mathbf{g}_t^\top\left((t+2)\mathbf{x}_t - t\mathbf{y}_t - 2\mathbf{z}_t\right) \overset{\text{(algo)}}{=} \mathbf{g}_t^\top\mathbf{0} = 0. \quad \square\end{aligned}$$

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