TD - Gradient descent : solution

Let $f : \mathbb{R}^n \to \mathbb{R}$ *be a differentiable function whose gradient is* L*-Lipschitz continuous* i.e. $\|\nabla f(y) - \nabla f(x)\| \leq L\|y - x\|$ *for all* x*,* y*.*

1. *Prove that for all* x, y*,* $\langle \nabla f(y) - \nabla f(x), y - x\rangle \leq L\|y - x\|^2$*.*

   ▶ We are using Cauchy-Schwartz inequality :

$$\begin{aligned}\langle \nabla f(y) - \nabla f(x), y - x\rangle &\leq |\langle \nabla f(y) - \nabla f(x), y - x\rangle| \leq \|\nabla f(y) - \nabla f(x)\| . \|y - x\| \\ &\leq L\,\|y - x\|^2\end{aligned}$$

2. *Set* $\varphi(t) = f(x + t(y - x))$ *for all* $t \in [0, 1]$*. Prove that*

$$f(y) - f(x) - \langle \nabla f(x), y - x\rangle = \varphi(1) - \varphi(0) - \varphi'(0)\,.$$

   ▶ It is clear that $\varphi(0) = f(x)$ and $\varphi(1) = f(y)$. Note that $\varphi(t) = f(g(t))$ where $g(t) = x + t(y - x)$. By the theorem of derivation of composite functions,

$$\varphi'(t) = \langle \nabla f(g(t)), g'(t)\rangle = \langle \nabla f(x + t(y - x)), y - x\rangle \tag{1}$$

   So $\varphi'(0) = \langle \nabla f(x), y - x\rangle$. Combining the three equalities yields

$$\varphi(1) - \varphi(0) - \varphi'(0) = f(y) - f(x) - \langle \nabla f(x), y - x\rangle\,.$$

3. *Deduce that*

$$f(y) - f(x) - \langle \nabla f(x), y - x\rangle = \int_0^1 \langle \nabla f(x + t(y - x)) - \nabla f(x), y - x\rangle dt$$

   ▶ As φ is a primitive of φ',

$$\varphi(1) = \varphi(0) + \int_0^1 \varphi'(t)dt.$$

   Hence, using (1)

$$\begin{aligned}f(y) - f(x) - \langle \nabla f(x), y - x\rangle = \varphi(1) - \varphi(0) - \varphi'(0) &= \int_0^1 \varphi'(t)dt - \varphi'(0) \\ &= \int_0^1 \langle \nabla f(x + t(y - x)), y - x\rangle dt - \int_0^1 \langle \nabla f(x), y - x\rangle dt \\ &= \int_0^1 \langle \nabla f(x + t(y - x)) - \nabla f(x), y - x\rangle dt\end{aligned}$$

4. *Using the first question, conclude that*

$$f(y) \leq f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2}\|y - x\|^2 .$$

▶ We know that for all x, z, $\langle \nabla f(z) - \nabla f(x), z - x \rangle \leq L\|z - x\|^2$. We use this inequality with $z = x + t(y-x)$: $\langle \nabla f(x+t(y-x)) - \nabla f(x), t(y-x) \rangle \leq L\|t(y-x)\|^2$. Dividing by t and integrating between 0 and 1, we get

$$\int_0^1 \langle \nabla f(x+t(y-x)) - \nabla f(x), y-x \rangle dt \leq \int_0^1 tL \|y-x\|^2 dt = \left[\frac{t^2}{2}\right]_0^1 L \|y-x\|^2 = \frac{L}{2} \|y-x\|^2$$

We conclude using Question 3.

Consider the gradient algorithm i.e., *the sequence* (x_k) *defined by* $x_{k+1} = x_k - \gamma \nabla f(x_k)$ *where* $\gamma > 0$ *is a constant step size.*

5. *Show that*

$$f(x_{k+1}) \leq f(x_k) - \gamma(1 - \frac{\gamma L}{2})\|\nabla f(x_k)\|^2 . \tag{2}$$

▶ We use the result of Question 4 :

$$f(x_{k+1}) \leq f(x_k) + \langle \nabla f(x_k), x_{k+1} - x_k \rangle + \frac{L}{2}\|x_{k+1} - x_k\|^2$$

But $x_{k+1} = x_k - \gamma \nabla f(x_k)$ so

$$f(x_{k+1}) \leq f(x_k) - \gamma \langle \nabla f(x_k), \nabla f(x_k) \rangle + \frac{L}{2} \|\gamma \nabla f(x_k)\|^2 = f(x_k) - \gamma(1 - \frac{\gamma L}{2})\|\nabla f(x_k)\|^2$$

6. *Provide a condition on* γ *which ensures that* $f(x_{k+1}) \leq f(x_k)$.
▶ If $\gamma(1 - \frac{\gamma L}{2})\|\nabla f(x_k)\|^2 \geq 0$, then $f(x_{k+1}) \leq f(x_k) - \gamma(1 - \frac{\gamma L}{2})\|\nabla f(x_k)\|^2 \leq f(x_k)$. Now $\gamma(1 - \frac{\gamma L}{2})\|\nabla f(x_k)\|^2 \geq 0 \Leftrightarrow \gamma(1 - \frac{\gamma L}{2}) \geq 0 \Leftrightarrow \gamma \leq \frac{2}{L}$ since $\gamma > 0$.

7. *Based on Eq. (2), what value of* γ *would you suggest to choose ?*
▶ There are two possible answers for this question.

   – First answer : we may want to choose γ the largest possible that ensures a strict decrease of the objective value. Hence, we will take $\gamma = \frac{2}{L} - \epsilon$ where $\epsilon > 0$ is small. Taking long stepsizes helps obtaining an algorithm that goes faster to the minimum.

   – Second answer : we may want to choose γ such that the bound we found is the smallest possible. Hence, we will take $\gamma = \frac{1}{L}$. Minimizing the bound helps guaranteeing a better decrease in the objective function.

   For the rest of the exercise, we will take $\gamma = \frac{1}{L}$ because the expressions are easier to manipulate.

From now on, we set γ *equal to the value suggested above. Consider an arbitrary* $y \in \mathbb{R}^n$.

8. *Prove that*

$$\langle \nabla f(x_k), y - x_k \rangle + \frac{L}{2}\|x_k - y\|^2 - \frac{L}{2}\|x_{k+1} - y\|^2 = -\frac{1}{2L}\|\nabla f(x_k)\|^2 .$$

▶
$$\begin{aligned} \frac{L}{2}\|x_{k+1} - y\|^2 &= \frac{L}{2}\|x_k - \gamma \nabla f(x_k) - y\|^2 \\ &= \frac{L}{2}\left\|x_k - y\right\|^2 - L\gamma\langle x_k - y, \nabla f(x_k)\rangle + \frac{L}{2}\gamma^2\left\|\nabla f(x_k)\right\|^2 \end{aligned}$$

Rearranging and simplifying $\gamma L = 1$, we get the expected result.

9. *Deduce that*

$$f(x_{k+1}) \le f(x_k) + \langle \nabla f(x_k), y - x_k \rangle + \frac{L}{2}\|x_k - y\|^2 - \frac{L}{2}\|x_{k+1} - y\|^2 . \qquad (3)$$

▶ $f(x_{k+1}) \le f(x_k) - \gamma(1 - \frac{\gamma L}{2})\|\nabla f(x_k)\|^2 = f(x_k) - \frac{1}{2L}\|\nabla f(x_k)\|^2$
$= f(x_k) + \langle \nabla f(x_k), y - x_k \rangle + \frac{L}{2}\|x_k - y\|^2 - \frac{L}{2}\|x_{k+1} - y\|^2$

We assume from now on that f is convex and admits (at least) one minimizer $x^\star$.

10. *Show that*

$$f(x_{k+1}) \le f(x^\star) + \frac{L}{2}\|x_k - x^\star\|^2 - \frac{L}{2}\|x_{k+1} - x^\star\|^2 .$$

▶ As f is convex, $f(x^*) \ge f(x_k) + \langle \nabla f(x_k), x^* - x_k \rangle$. Combining this inequality with (3) applied with $y = x^*$, we get :

$$\begin{aligned} f(x_{k+1}) &\le f(x_k) + \langle \nabla f(x_k), x^* - x_k \rangle + \frac{L}{2}\|x_k - x*\|^2 - \frac{L}{2}\|x_{k+1} - x*\|^2 \\ &\le f(x^*) + \frac{L}{2}\|x_k - x*\|^2 - \frac{L}{2}\|x_{k+1} - x*\|^2 \end{aligned}$$

11. *Deduce that for all $k \ge 1$,*

$$\sum_{i=1}^{k} f(x_i) \le k f(x^\star) + \frac{L}{2}\|x_0 - x^\star\|^2 .$$

▶ We sum the inequality in Question 10 for i between 0 and $k-1$:

$$\sum_{i=0}^{k-1} f(x_{i+1}) \le k f(x^\star) + \sum_{i=0}^{k-1}\left(\frac{L}{2}\|x_i - x^\star\|^2 - \frac{L}{2}\|x_{i+1} - x^\star\|^2\right)$$

We recognise a telescoping sum. We also make a change of variable $i \leftarrow i+1$ in the first sum.

$$\sum_{i=1}^{k} f(x_i) \le k f(x^\star) + \frac{L}{2}\|x_0 - x^\star\|^2 - \frac{L}{2}\|x_k - x^\star\|^2 \le k f(x^\star) + \frac{L}{2}\|x_0 - x^\star\|^2$$

12. *Show that*

$$f(x_k) - f(x^\star) \le \frac{L\|x_0 - x^\star\|^2}{2k}\,.$$

▶ Recall that $f(x_k) \le f(x_{k-1})$ for all k. So

$$f(x_k) - f(x^*) \le \sum_{i=1}^{k} \frac{1}{k}\big(f(x_i) - f(x^*)\big) \le \frac{L\,\|x_0 - x^*\|^2}{2k}$$

We assume from now on that f is μ-strongly convex. Recall that a function f is said μ-strongly convex if $f - \frac{\mu}{2}\|\,.\,\|^2$ is convex.

13. *Prove that for any x, y,*

$$f(y) \ge f(x) + \langle \nabla f(x), y - x\rangle + \frac{\mu}{2}\|y - x\|^2\,.$$

▶ The function $g = f - \frac{\mu}{2}\|\,.\,\|^2$ is convex so for all x, y,

$$\begin{aligned} &g(y) \ge g(x) + \langle \nabla g(x), y - x\rangle \\ &f(y) - \frac{\mu}{2}\,\|y\|^2 \ge f(x) - \frac{\mu}{2}\,\|x\|^2 + \langle \nabla f(x) - \mu x, y - x\rangle \end{aligned}$$

We get the result since $-\,\|x\|^2 - 2\langle x, y - x\rangle + \|y\|^2 = \|x\|^2 - 2\langle x, y\rangle + \|y\|^2 = \|y - x\|^2$.

14. *Using Eq. (3), prove that*

$$f(x_{k+1}) \le f(x^\star) + \frac{L-\mu}{2}\|x_k - x^\star\|^2 - \frac{L}{2}\|x_{k+1} - x^\star\|^2\,.$$

▶ As f is μ-strongly convex, $f(x^*) \ge f(x_k) + \langle \nabla f(x_k), x^* - x_k\rangle + \frac{\mu}{2}\,\|x^* - x\|^2$. Combining this inequality with (3) applied with $y = x^*$, we get :

$$\begin{aligned} f(x_{k+1}) &\le f(x_k) + \langle \nabla f(x_k), x^* - x_k\rangle + \frac{L}{2}\|x_k - x*\|^2 - \frac{L}{2}\|x_{k+1} - x*\|^2 \\ &\le f(x^*) + \frac{L-\mu}{2}\|x_k - x*\|^2 - \frac{L}{2}\|x_{k+1} - x*\|^2 \end{aligned}$$

15. *Define $\Delta_{k+1} = f(x_{k+1}) - f(x^\star) + \frac{L}{2}\|x_{k+1} - x^\star\|^2$. Show that*

$$\Delta_{k+1} \le \left(1 - \frac{\mu}{L}\right)\Delta_k\,.$$

▶ Using Question 14 and the fact that $f(x_k) \ge f(x^*)$, we get

$$\begin{aligned} \Delta_{k+1} &= f(x_{k+1}) - f(x^\star) + \frac{L}{2}\|x_{k+1} - x^\star\|^2 \le \frac{L-\mu}{2}\,\|x_k - x^*\|^2 \\ &\le \frac{L-\mu}{L}\Big(f(x_k) - f(x^*) + \frac{L}{2}\,\|x_k - x^*\|^2\Big) = \Big(1 - \frac{\mu}{L}\Big)\Delta_k \end{aligned}$$

16. *Conclude that*

$$f(x_k) - f(x^\star) \leq \left(1 - \frac{\mu}{L}\right)^k \Delta_0$$
$$\|x_k - x^\star\|^2 \leq \left(1 - \frac{\mu}{L}\right)^k \frac{2\Delta_0}{L}.$$

▶ Iterating the relation $\Delta_k \leq \left(1 - \frac{\mu}{L}\right)\Delta_{k-1}$, we get that $\Delta_k \leq \left(1 - \frac{\mu}{L}\right)^k \Delta_0$. As Δ_k is the sum of two nonnegative quantities, this means that $f(x_k) - f(x^*) \leq (1 - \frac{\mu}{L})^k \Delta_0$ and $\frac{2}{L}\|x_k - x^*\|^2 \leq (1 - \frac{\mu}{L})^k \Delta_0$.

17. *The ratio $Q = L/\mu$ is called the* condition number *of f. Discuss the influence of Q on the convergence rate.*

▶ The smaller the condition number the faster the convergence. If the problem is ill-conditioned, there will be a slow convergence.

Application : From now on, we define $f(x) = \frac{1}{2}x^T Hx + c^T x$ where H is positive semidefinite $n \times n$ matrix. We denote by λ_{max} and λ_{min} the largest and smallest eigenvalues of H respectively.

18. *What is the Hessian matrix of f ? Deduce that f is convex.*

▶ The Hessian matrix at x of f is H for all x. As it is positive semi-definite, f is convex.

19. *Justify briefly that ∇f is λ_{max}-Lipschitz continuous.*

▶ $\|\nabla f(x) - \nabla f(y)\| = \|Hx - Hy\| \leq \|H\| \|x - y\| = \lambda_{\max} \|y - x\|$.

20. *Prove that f is λ_{min}-strongly convex.*

▶ The Hessian matrix of $f - \frac{\lambda_{\min}}{2}\|\cdot\|^2$ is equal to $H - \lambda_{\min} I$, which is positive semi-definite by definition of $\lambda_{\min}$. Note that if $\lambda_{\min} = 0$, then f is not strongly convex.

21. *Write the condition number Q of f. What kind of matrix H yields the smallest condition number ?*

▶ $Q = \lambda_{\max}/\lambda_{\min}$. The smallest condition number is for $H = \alpha I$, $\alpha > 0$. In this case $Q = 1$.

22. *Characterize the set of minimizers of f.*

▶ As f is convex and differentiable, x is a minimizer of f if and only if $\nabla f(x) = 0$. This means $Hx = -c$ and so we have three cases.

- If H is invertible, then $x = H^{-1}c$ is the unique solution.
- If H is not invertible and $-c \in \text{Range}(H)$, then the set of solution is $H^{-1}(\{-c\})$, the pre-image of $\{-c\}$ by H. It is a linear subspace of $\mathbb{R}^m$.
- If H is not invertible and $-c \notin \text{Range}(H)$, then there is no solution.