Labs

Optimization for Machine Learning Spring 2021

EPFL

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github.com/epfml/OptML_course

Problem Set 7 — Solutions (Non-Convex Optimization and Newton's Method)

Non-Convex Optimization

Non-convex

Exercise 35. Prove Lemma 6.3 (gradient descent does not overshoot on smooth functions).

Solution: On the one hand, we have sufficient decrease, since f is also smooth with parameter L' > L:

$$f(\mathbf{x}') \le f(\mathbf{x}) - \frac{1}{2L'} \|\nabla f(\mathbf{x})\|^2$$
.

Now assume for contradiction that \mathbf{x}' is a critical point, meaning that $\nabla f(\mathbf{x}') = \mathbf{0}$. Then, by smoothness with parameter L, and because $\mathbf{x}' = \mathbf{x} - \gamma \nabla f(\mathbf{x})$, we get that

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

$$= f(\mathbf{x}') + \frac{L}{2} \|\mathbf{x} - \mathbf{x}'\|^{2}$$

$$= f(\mathbf{x}') + \frac{L}{2} \frac{1}{(L')^{2}} \|\nabla f(\mathbf{x})\|^{2} < f(\mathbf{x}') + \frac{L'}{2} \frac{1}{(L')^{2}} \|\nabla f(\mathbf{x})\|^{2}$$

$$= f(\mathbf{x}') + \frac{1}{2L'} \|\nabla f(\mathbf{x})\|^{2},$$

where the strict inequality in the second-to-last line uses $\nabla f(\mathbf{x}) \neq \mathbf{0}$. Hence,

$$f(\mathbf{x}') > f(\mathbf{x}) - \frac{1}{2L'} \|\nabla f(\mathbf{x})\|^2,$$

which contradicts sufficient decrease.

Exercise 36. Consider the function $f(\mathbf{x}) = \frac{1}{2} \left(\prod_{k=1}^d x_k - 1 \right)^2$. Prove that for any starting point $\mathbf{x}_0 \in X = \{ \mathbf{x} \in \mathbb{R}^d : \mathbf{x} > \mathbf{0}, \prod_k \mathbf{x}_k \ge 1 \}$ and any $\varepsilon > 0$, gradient descent attains $f(\mathbf{x}_T) \le \varepsilon$ for some iteration T.

Solution: We first prove smoothness along the trajectory. With C being the maximum value of $\prod_{k\neq I}(\mathbf{x}_0)_k$ over all sets I of size at most 2, we bound the squared Frobeinus norm of the Hessian by bounding each of the d^2 entries:

$$\|\nabla^2 f(\mathbf{x}_0)\|_F^2 = \sum_{i,j} |\nabla^2 f(\mathbf{x}_0)_{i,j}|^2 \le 9d^2C^4$$
,

where we used that the diagonal term are smaller than $C \leq 3C^2$ and the off-diagonal terms are smaller than $3C^2$ by the triangle inequality. Note that if we start from $\mathbf{x} \in X$, then each gradient descent step can only decrease the values x_k as long as we do not overshoot. We therefore get as in Lemma 6.7 that $\|\nabla^2 f(\mathbf{x})\| \leq \|\nabla^2 f(\mathbf{x})\|_F \leq 3dC^2$ along the trajectory. Up to the first point of overshooting, f is therefore smooth with parameter $3dC^2$ over the trajectory (Lemma 6.1), and then the smooth step size $1/3dC^2$ guarantees that we actually never overshoot (Lemma 6.3). Hence, Lemma 2.6 yields sufficient decrease:

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

We still need a lower bound for

$$\|\nabla f(\mathbf{x})\|^2 = 2f(\mathbf{x}) \sum_{i=1}^d \left(\prod_{k \neq i} x_k\right)^2,$$

for $x \in X$. We claim that for some i,

$$\prod_{k \neq i} x_k \ge 1.$$

If not, we would have

$$1 > \prod_{i=1}^{d} \prod_{k \neq i} x_k = \left(\prod_{k} x_k\right)^{d-1},$$

which would mean that $\prod_k x_k < 1$, contradiction. Hence, we have

$$\|\nabla f(\mathbf{x}_t)\|^2 \ge 2f(\mathbf{x}_t),$$

and hence

$$f(\mathbf{x}_{t+1}) \le f(\mathbf{x}_t) - \frac{1}{3dC^2} f(\mathbf{x}_t) = \left(1 - \frac{1}{3dC^2}\right) f(\mathbf{x}_t).$$

Convergence follows.

Exercise 37. Consider the function $f(\mathbf{x}) = \frac{1}{2} \left(\prod_{k=1}^{d} x_k - 1 \right)^2$. Prove that for even dimension $d \geq 2$, there is a point \mathbf{x}_0 (not a critical point) such that gradient descent does not converge to a global minimum when started at \mathbf{x}_0 , regardless of step size(s).

Solution: Throughout, let \mathbf{x}_0 be such that all entries have the same absolute value. We first prove that gradient descent maintains this property in all iterations. Recall that with $\Delta := -\gamma(\prod_k x_k - 1)(\prod_k x_k)$, the gradient descent step is

$$x'_{k} = x_{k} + \frac{\Delta}{x_{k}}, \quad k = 1, \dots, d.$$

Suppose that $|x_k| = \alpha$ for all k. Then $x_k' \in \{\alpha + \Delta/\alpha, -\alpha - \Delta/\alpha\}$, hence $|x_k'| = |\alpha + \Delta/\alpha|$ for all k. We also see that either all entries in \mathbf{x}' have the *same* sign as in \mathbf{x} (if $\alpha + \Delta/\alpha > 0$), or all entries in \mathbf{x}' have the *opposite* sign as in \mathbf{x} (if $\alpha + \Delta/\alpha < 0$). (The special case where $\alpha + \Delta/\alpha = 0$ leads to $\mathbf{x}' = \mathbf{0}$ in which case we have already converged to a saddle point, so we do not consider this case further.)

If d is even, any starting point with an odd number of negative signs will lead to all iterates having an odd number of negative signs. This means that – regardless of stepsize – we will always have $\prod_k x_k \leq 0$, so we can never converge to an optimal point where $\prod_k x_k = 1$.

Newton's Method

Exercise 43. Prove Lemma 7.6!

Solution: We use that for any two matrices, $||AB|| \le ||A|| \, ||B||$. Indeed,

$$||AB|| = \max_{\mathbf{v} \neq \mathbf{0}} \frac{||AB\mathbf{v}||}{||\mathbf{v}||} \le \max_{\mathbf{v} \neq \mathbf{0}} \frac{||A|| ||B\mathbf{v}||}{||\mathbf{v}||} = ||A|| ||B||.$$

Hence,

$$1 = \left\| \nabla^2 f(\mathbf{x}^\star) \nabla^2 f(\mathbf{x}^\star)^{-1} \right\| \leq \left\| \nabla^2 f(\mathbf{x}^\star) \right\| \left\| \nabla^2 f(\mathbf{x}^\star)^{-1} \right\| \leq \left\| \nabla^2 f(\mathbf{x}^\star) \right\| \frac{1}{\mu},$$

so, $\|\nabla^2 f(\mathbf{x}^*)\| \ge \mu$.

Now, by the Lipschitz assumption and Corollary 7.5,

$$\|\nabla^2 f(\mathbf{x}_T) - \nabla^2 f(\mathbf{x}^*)\| \le B \|\mathbf{x}_T - \mathbf{x}^*\| \le \mu \left(\frac{1}{2}\right)^{2^T - 1}.$$

Together with $\|\nabla^2 f(\mathbf{x}^*)\| \ge \mu$, the statement follows.

Exercise 45. Let $\delta > 0$ be any real number. Find an example of a convex function $f : \mathbb{R} \to \mathbb{R}$ such that (i) the unique global minimum x^* has a vanishing second derivative $f''(x^*) = 0$, and (ii) Newton's method satisfies

$$|x_{t+1} - x^*| \ge (1 - \delta)|x_t - x^*|,$$

for all $x_t \neq x^*$.

Solution: We take $f(x) = x^k$ for some even natural number k satisfying $k \ge 4$ and $1/(k-1) \le \delta$. We have

$$f'(x) = kx^{k-1},$$

 $f''(x) = k(k-1)x^{k-2} \ge 0,$

hence f is convex by the second-order characterization (??), and we have $x^* = 0$ as well as $f''(x^*) = 0$. Suppose w.l.o.g. that $x_t > 0$. The Newton step (7.1) is

$$x_{t+1} = x_t - \frac{f'(x_t)}{f''(x_t)} = x_t - \frac{kx_t^{k-1}}{k(k-1)x_t^{k-2}} = x_t - \frac{1}{k-1}x_t \ge (1-\delta)x_t.$$

Quasi-Newton Methods

Exercise 48. Consider a step of the secant method:

$$x_{t+1} = x_t - f(x_t) \frac{x_t - x_{t-1}}{f(x_t) - f(x_{t-1})}, \quad t \ge 1.$$

Assuming that $x_t \neq x_{t-1}$ and $f(x_t) \neq f(x_{t-1})$, prove that the line through the two points $(x_{t-1}, f(x_{t-1}))$ and $(x_t, f(x_t))$ intersects the x-axis at the point $x = x_{t+1}$.

Solution: Let the line be y = ax + b. Then we have

$$f(x_t) = ax_t + b,$$

$$f(x_{t-1}) = ax_{t-1} + b.$$

Subtracting the two equations yields

$$a = \frac{f(x_t) - f(x_{t-1})}{x_t - x_{t-1}}.$$

To compute the intersection with the x-axis, we need to solve

$$0 = ax + b.$$

Subtracting from this the first of the previous two equations yields

$$-f(x_t) = a(x - x_t) \quad \Leftrightarrow \quad x = x_t - f(x_t)a^{-1} = x_t - f(x_t)\frac{x_t - x_{t-1}}{f(x_t) - f(x_{t-1})}.$$

By definition of the secant method, $x = x_{t+1}$.

Fixed Point Iteration

Solutions are provided in solution/.