SYS 6003: Optimization

Lecture 14

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Last time we introduced a class of functions which has Lipschitz continuous gradient, and its property.

Lemma 1 Let a function f has L-Lipschitz continuous gradient over dom f, then for any $\mathbf{x}, \mathbf{y} \in \mathbf{dom} f$, we have

$$|f(\mathbf{x}) - f(\mathbf{y}) - \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y})| \le \frac{L}{2} \|\mathbf{x} - \mathbf{y}\|_2^2.$$

Proof: Let $g(t) \equiv f(\mathbf{y} + t(\mathbf{x} - \mathbf{y}))$. From calculus (the Fundamental Theorem of Calculus) we know that

$$\int_0^1 g'(t)dt = g(1) - g(0) = f(\mathbf{x}) - f(\mathbf{y}).$$

It then follows that

$$\begin{aligned} |f(\mathbf{x}) - f(\mathbf{y}) - \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y})| \\ &= \Big| \int_{0}^{1} \nabla f(\mathbf{y} + t(\mathbf{x} - \mathbf{y}))^{\top} (\mathbf{x} - \mathbf{y}) dt - \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y}) \Big| \\ &= \Big| \int_{0}^{1} \left(\nabla f(\mathbf{y} + t(\mathbf{x} - \mathbf{y})) - \nabla f(\mathbf{y}) \right)^{\top} (\mathbf{x} - \mathbf{y}) dt \Big| \\ &\leq \Big| \int_{0}^{1} \left\| \nabla f(\mathbf{y} + t(\mathbf{x} - \mathbf{y})) - \nabla f(\mathbf{y}) \right\|_{2} \cdot \left\| \mathbf{x} - \mathbf{y} \right\|_{2} dt \Big|, \end{aligned}$$

where the inequality follows from the Cauchy-Schwartz inequality. Since f has L-Lipschitz continuous gradient, we then have

$$|f(\mathbf{x}) - f(\mathbf{y}) - \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y})| \leq \left| L \|\mathbf{x} - \mathbf{y}\|_{2}^{2} \int_{0}^{1} t dt \right|$$
$$= \frac{L}{2} \|\mathbf{x} - \mathbf{y}\|_{2}^{2}.$$

Now, we introduce a new class of functions, which is L-smooth. Although L-smooth is a weaker condition than L-Lipschitz continuous gradient, it can be implied by L-Lipschitz continuous gradient when a function is convex.

Definition 1 (L-smooth) A function f is L-smooth if for any $\mathbf{x}, \mathbf{y} \in \mathbf{dom} f$, it holds that

$$f(\mathbf{x}) \le f(\mathbf{y}) + \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y}) + \frac{L}{2} \|\mathbf{x} - \mathbf{y}\|_2^2.$$

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Remark 1 If f is twice differentiable, then there is an equivalent, and perhaps easier, definition of smoothness: f is smooth if there exists a constant L > 0 such that $\nabla^2 f(x) \preceq L\mathbf{I}$, where \mathbf{I} is an identity matrix. In other words, the largest eigenvalue of the Hessian of f is uniformly upper bounded by L everywhere.

Then, we turn to an important property of L-smooth functions.

Lemma 2 If a function f is L-smooth and convex, then for any $\mathbf{x}, \mathbf{y} \in \mathbf{dom} f$, we have

$$f(\mathbf{x}) \ge f(\mathbf{y}) + \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y}) + \frac{1}{2L} \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_{2}^{2}.$$

Proof: Define a function $g_{\mathbf{y}}(\mathbf{x}) \equiv f(\mathbf{x}) - f(\mathbf{y}) - \nabla f(\mathbf{y})^{\top}(\mathbf{x} - \mathbf{y})$. Since $f(\mathbf{x})$ is convex, $g_{\mathbf{y}}(\mathbf{x}) \geq 0$. In particular, $g_{\mathbf{y}}(\mathbf{y}) = 0$. Thus, we have

$$g_{\mathbf{y}}(\mathbf{y}) = \min_{\mathbf{x}} g_{\mathbf{y}}(\mathbf{x}) \text{ and } \nabla g_{\mathbf{y}}(\mathbf{y}) = 0.$$

From the optimality of **y**, it then follows that

$$g_{\mathbf{y}}(\mathbf{y}) \leq \min_{\eta} g_{\mathbf{y}}(\mathbf{x} - \eta \nabla g_{\mathbf{y}}(\mathbf{x})) = \min_{\eta} f\left(\mathbf{x} - \eta \nabla g_{\mathbf{y}}(\mathbf{x})\right) - f(\mathbf{y}) - \nabla f(\mathbf{y})^{\top} \left(\mathbf{x} - \eta \nabla g_{\mathbf{y}}(\mathbf{x}) - \mathbf{y}\right).$$
(1)

By definition of *L*-smooth, we have

$$f(\mathbf{x} - \eta \nabla g_{\mathbf{y}}(\mathbf{x})) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} \left(-\eta \nabla g_{\mathbf{y}}(\mathbf{x})\right) + \frac{L}{2} \|\eta \nabla g_{\mathbf{y}}(\mathbf{x})\|_{2}^{2}.$$

It then follows from (1) that

$$g_{\mathbf{y}}(\mathbf{y}) \leq \min_{\eta} f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} \left(-\eta \nabla g_{\mathbf{y}}(\mathbf{x}) \right) + \frac{L}{2} \|\eta \nabla g_{\mathbf{y}}(\mathbf{x})\|_{2}^{2} - f(\mathbf{y}) - \nabla f(\mathbf{y})^{\top} \left(\mathbf{x} - \mathbf{y} - \eta \nabla g_{\mathbf{y}}(\mathbf{x})\right) = \min_{\eta} g_{\mathbf{y}}(\mathbf{x}) + \frac{L}{2} \|\eta \nabla g_{\mathbf{y}}(\mathbf{x})\|_{2}^{2} - \eta \nabla g_{\mathbf{y}}(\mathbf{x})^{\top} \left(\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\right) = \min_{\eta} g_{\mathbf{y}}(\mathbf{x}) + \frac{L}{2} \eta^{2} \|\nabla g_{\mathbf{y}}(\mathbf{x})\|_{2}^{2} - \eta \|\nabla g_{\mathbf{y}}(\mathbf{x})\|_{2}^{2}.$$

It is easy to show that the minimum solution η to the above quadratic function minimization problem is $g_{\mathbf{y}}(\mathbf{x}) - \|\nabla g_{\mathbf{y}}(\mathbf{x})\|_2^2/2L$. Thus, from our definition of $g_{\mathbf{y}}(\mathbf{x})$, it immediately follows

$$0 \le f(\mathbf{x}) - f(\mathbf{y}) - \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y}) - \frac{1}{2L} \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_{2}^{2}$$

Now, let's go back to the gradient descent algorithm. We will show that if a function is L-smooth and convex, then we have faster convergence rate when we apply the gradient descent algorithm to optimize the function.

Theorem 1 If a function f is L-smooth and convex, then the gradient descent algorithm with $0 \le \eta \le 1/L$ satisfies

$$f(\mathbf{x}_{t+1}) - f(\mathbf{x}^*) \le \frac{\|\mathbf{x}_1 - \mathbf{x}^*\|_2^2}{2\eta t}$$

Proof: Let $\mathbf{x}^+ \equiv \mathbf{x}_{t+1}$ and $\mathbf{x} \equiv \mathbf{x}_t$. Since f is L-smooth, we have

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

Note that $\mathbf{x}^+ = \mathbf{x} - \eta \nabla f(\mathbf{x})$, it then follows that

$$f(\mathbf{x}^{+}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} \left(-\eta \nabla f(\mathbf{x})\right) + \frac{L}{2} \|-\eta \nabla f(\mathbf{x})\|_{2}^{2}$$
$$= f(\mathbf{x}) - \left(1 - \frac{L\eta}{2}\right) \eta \|\nabla f(\mathbf{x})\|_{2}^{2}$$
$$\leq f(\mathbf{x}) - \frac{1}{2} \eta \|\nabla f(\mathbf{x})\|_{2}^{2}, \tag{2}$$

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where the last inequality follows from $0 \le \eta \le 1/L$. Note that (2) implies that the function value is monotonically decreasing.

In addition, since $f(\mathbf{x})$ is convex,

$$f(\mathbf{x}^*) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{x}^* - \mathbf{x}).$$
(3)

Combining (2) and (3), we get

$$f(\mathbf{x}^{+}) \leq f(\mathbf{x}^{*}) - \nabla f(\mathbf{x})^{\top} (\mathbf{x}^{*} - \mathbf{x}) - \frac{1}{2} \eta \|\nabla f(\mathbf{x})\|_{2}^{2}$$

Substituting $\nabla f(\mathbf{x})$ in the above inequality with $\frac{1}{\eta}(\mathbf{x} - \mathbf{x}^+)$, we have

$$\begin{split} f(\mathbf{x}^{+}) &\leq f(\mathbf{x}^{*}) - \frac{1}{\eta} (\mathbf{x} - \mathbf{x}^{+})^{\top} (\mathbf{x}^{*} - \mathbf{x}) - \frac{1}{2} \eta \big\| \frac{1}{\eta} (\mathbf{x} - \mathbf{x}^{+}) \big\|_{2}^{2} \\ &= f(\mathbf{x}^{*}) - \frac{1}{\eta} (\mathbf{x} - \mathbf{x}^{+})^{\top} (\mathbf{x}^{*} - \mathbf{x}) - \frac{1}{2\eta} \big\| (\mathbf{x} - \mathbf{x}^{+}) \big\|_{2}^{2}. \end{split}$$

Recall that $-2\mathbf{a}^{\top}\mathbf{b} = \|\mathbf{a}\|_2^2 + \|\mathbf{b}\|_2^2 - \|\mathbf{a} + \mathbf{b}\|_2^2$. Then, setting $\mathbf{a} = (\mathbf{x} - \mathbf{x}^+)$ and $\mathbf{b} = (\mathbf{x}^* - \mathbf{x})$ gives

$$\begin{aligned} f(\mathbf{x}^{+}) &\leq f(\mathbf{x}^{*}) + \frac{1}{2\eta} \Big(\|\mathbf{x} - \mathbf{x}^{+}\|_{2}^{2} + \|\mathbf{x}^{*} - \mathbf{x}\|_{2}^{2} - \|\mathbf{x}^{+} - \mathbf{x}^{*}\|_{2}^{2} \Big) - \frac{1}{2\eta} \Big\| (\mathbf{x} - \mathbf{x}^{+}) \Big\|_{2}^{2} \\ &= f(\mathbf{x}^{*}) + \frac{1}{2\eta} \Big(\|\mathbf{x} - \mathbf{x}^{*}\|_{2}^{2} - \|\mathbf{x}^{+} - \mathbf{x}^{*}\|_{2}^{2} \Big). \end{aligned}$$

Note that this inequality holds for any positive integer t. Specifically, we have

$$f(\mathbf{x}_{t+1}) - f(\mathbf{x}^*) \leq \frac{1}{2\eta} \Big(\|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \Big),$$

...
$$f(\mathbf{x}_2) - f(\mathbf{x}^*) \leq \frac{1}{2\eta} \Big(\|\mathbf{x}_1 - \mathbf{x}^*\|_2^2 - \|\mathbf{x}_2 - \mathbf{x}^*\|_2^2 \Big).$$

Adding these inequalities gives

$$\sum_{i=2}^{t+1} f(\mathbf{x}_i) - tf(\mathbf{x}^*) \le \frac{1}{2\eta} \Big(\|\mathbf{x}_1 - \mathbf{x}^*\|_2^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \Big) \le \frac{1}{2\eta} \Big(\|\mathbf{x}_1 - \mathbf{x}^*\|_2^2 \Big).$$

Recall from (2) we have proven that the function value is monotonically decreasing, so $tf(\mathbf{x}_{t+1}) \leq \sum_{i=2}^{t+1} f(\mathbf{x}_i)$. Therefore, the inequality above leads to

$$tf(\mathbf{x}_{t+1}) - tf(\mathbf{x}^*) \le \frac{\|\mathbf{x}_1 - \mathbf{x}^*\|_2^2}{2\eta}$$

Dividing both sides of this inequality by t completes the proof.