MATH 6490. NONLINEAR OPTIMIZATION IN MACHINE LEARNING. ASSIGNMENT 2.

There are 3 problems, each problem is worth 5 points, total is 15 points.

1. Let $f: \mathbb{R}^n \to \mathbb{R}$ be a twice continuously differentiable function, show that f is m-strongly convex in the sense of (2.4) in the Lecture Notes, i.e, for any $x, y \in \mathbb{R}^n$

$$f((1-\alpha)x + \alpha y) \le (1-\alpha)f(x) + \alpha f(y) - \frac{1}{2}m\alpha(1-\alpha)\|x - y\|_2^2, \qquad (0.1)$$

if and only if $\nabla^2 f(x) \succeq mI$ for all x, i.e., the eigenvalues $\lambda_1, ..., \lambda_n$ of $\nabla^2 f(x)$ satisfy $\min_{1 \le i \le n} \lambda_i \ge m$. You can make use of the following fact: Let A be a symmetric nonnegative definite $n \times n$ matrix. Then the eigenvalues $\lambda_1, ..., \lambda_n$ of A satisfy $\min_{1 \le i \le n} \lambda_i \ge m$ if and only if for any $u \in \mathbb{R}^n$ we have $u^T A u \ge m \|u\|^2$.

(Hint: Suppose that the function f is strongly—m convex with the standard inequality (0.1) above for m-convexity. Set $z_{\alpha} = (1 - \alpha)x + \alpha y$. Then by (0.1) we have

$$\alpha f(y) - \alpha f(x) \ge f(z_{\alpha}) - f(x) + \frac{1}{2} m\alpha (1 - \alpha) ||x - y||^2$$
.

Making use of Taylor's expansion

$$\alpha f(y) - \alpha f(x) \ge (\nabla f(x))^T (z_{\alpha} - x) + O(\|z_{\alpha} - x\|^2) + \frac{1}{2} m\alpha (1 - \alpha) \|x - y\|^2.$$

Since $z_{\alpha} \to x$ as $\alpha \to 0$, and $z_{\alpha} - x = \alpha(y - x)$, we can set $\alpha \to 0$ to get from above that for any $x, y \in \mathbb{R}^n$

$$f(y) \ge f(x) + (\nabla f(x))^T (y - x) + \frac{m}{2} ||y - x||^2 . \tag{0.2}$$

Set $u \in \mathbb{R}^n$ and $\alpha > 0$, then we consider the Taylor's expansion

$$f(x + \alpha u) = f(x) + \alpha \nabla f(x)^T u + \frac{1}{2} \alpha^2 u^T \nabla^2 f(x + t\alpha u) u$$
 (0.3)

for some $0 \le t \le 1$. We apply (0.2) with $y = x + \alpha u$ so that

$$f(x + \alpha u) \ge f(x) + \alpha (\nabla f(x))^T u + \frac{m}{2} \alpha^2 ||u||^2$$
 (0.4)

Comparing (0.3) and (0.4) we see that for arbitrary choice of $u \in \mathbb{R}^n$ we have

$$u^T \nabla^2 f(x + t\alpha u) u \ge m ||u||^2.$$

This implies that $\nabla^2 f(x) \succeq mI$ as claimed. This shows the "only if" part.

For the "if" part, we assume that $\nabla^2 f(x) \succeq mI$. Then for any $z \in \mathbb{R}^n$ we have that $(x-z)^T \nabla^2 f(z+t(x-z))(x-z) \geq m\|x-z\|^2$. Thus

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

$$\geq f(z) + (\nabla f(z))^{T} (x - z) + \frac{m}{2} ||x - z||^{2}.$$
(0.5)

Similarly

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

$$\geq f(z) + (\nabla f(z))^{T} (y - z) + \frac{m}{2} ||y - z||^{2}.$$
(0.6)

We consider $(1-\alpha)(0.5)+\alpha(0.6)$ and we set $z=(1-\alpha)x+\alpha y$. This gives

$$(1 - \alpha)f(x) + \alpha f(y)$$

$$\geq (\alpha + (1 - \alpha))f(z) + (\nabla f(z))^{T}((1 - \alpha)(x - z) + \alpha(y - z)) + \frac{m}{2} ((1 - \alpha)\|x - z\|^{2} + \alpha\|y - z\|^{2})$$

$$= f(z) + (\nabla f(z))^{T}((1 - \alpha)(x - z) + \alpha(y - z)) + \frac{m}{2} ((1 - \alpha)\|x - z\|^{2} + \alpha\|y - z\|^{2}) .$$

$$(0.7)$$

Since $x-z=\alpha(x-y)$ and $y-z=(1-\alpha)(y-x)$, we see that $((1-\alpha)(x-z)+\alpha(y-z))=0$. Moreover, this means that

$$(1-\alpha)\|x-z\|^2 + \alpha\|y-z\|^2 = \left[(1-\alpha)\alpha^2 + \alpha(1-\alpha)^2 \right] \|x-y\|^2 = \alpha(1-\alpha)\|x-y\|^2.$$

From these we see that (0.7) is the same as saying

$$(1-\alpha)f(x) + \alpha f(y) \ge f((1-\alpha)x + \alpha y) + \frac{m}{2}\alpha(1-\alpha)\|x-y\|^2$$
,

which is (0.1).)

2. Consider the fully connected-neural network via the recursive relation

$$a^{[1]} = x, z^{[l]} = W^{[l]}a^{[l]} + b^{[l]}, a^{[l]} = \sigma(z^{[l-1]})$$
 for $l = 2, 3, ..., L$,

in which l stands for the number of layers in the neural network, and $W=(W^{[1]},...,W^{[L]})$ and $b=(b^{[1]},...,b^{[L]})$ are the weight matrices and bias vectors. We can view the neural network function as a chain with $a^{[1]}=x$ and $a^{[L]}=g(x;\omega)$. Let the training data be one point (x,y). Then the loss function is given by

$$C = C(W, b) = \frac{1}{2} ||y - a^{[L]}||^2$$
.

Set the error in the j-th neuron at layer l to be $\delta^{[l]} = (\delta^{[l]}_j)_j$ (viewed as a column vector) with $\delta^{[l]}_j = \frac{\partial C}{\partial z^{[l]}_i}$. Prove the back-propagation relation

$$\delta^{[l]} = \sigma'(z^{[l]}) \circ (W^{[l+1]})^T \delta^{[l+1]} , \text{ for } 2 \le l \le L-1 ,$$

where for $x, y \in \mathbb{R}^n$, we let $x \circ y \in \mathbb{R}^n$ to be the Hadamard product defined by $(x \circ y)_i = x_i y_i$.

(Hint: Let the l-th layer contain n_l neurons. We can directly calculate that

$$\delta_j^{[l]} = \frac{\partial C}{\partial z_j^{[l]}} = \sum_{k=1}^{n_{l+1}} \frac{\partial C}{\partial z_k^{[l+1]}} \frac{\partial z_k^{[l+1]}}{\partial z_j^{[l]}} = \sum_{k=1}^{n_{l+1}} \delta_k^{[l+1]} \frac{\partial z_k^{[l+1]}}{\partial z_j^{[l]}} \;.$$

Since we have

$$z^{[l+1]} = W^{[l+1]}\sigma(z^{[l]}) + b^{[l+1]}$$

we see that we can further have

$$\frac{\partial z_k^{[l+1]}}{\partial z_j^{[l]}} = \frac{\partial [W^{[l+1]}\sigma(z^{[l]})]_k}{\partial z_j^{[l]}} = \left(W^{[l+1]}\frac{\partial \sigma(z^{[l]})}{\partial z_j^{[l]}}\right)_k \;,$$

Notice that $\frac{\partial \sigma(z^{[l]})}{\partial z_j^{[l]}} = (0, ..., 0, \sigma'(z_j^{[l]}), 0, ..., 0)^T$ where the $\sigma'(z_j^{[l]})$ term lies on the j-th position, we have $W^{[l+1]} \frac{\partial \sigma(z^{[l]})}{\partial z_j^{[l]}} = \sigma'(z_j^{[l]}) W_j^{[l+1]}$, where $W^{[l+1]} = (W_j^{[l+1]})$. This gives us $\left(W^{[l+1]} \frac{\partial \sigma(z^{[l]})}{\partial z_j^{[l]}}\right)_k = \sigma'(z_j^{[l]}) W_{jk}^{[l+1]}$, where W_{jk} is the element at the j-th column and k-th row of W. So we finally get

$$\delta_j^{[l]} = \sum_{k=1}^{n_{l+1}} \delta_k^{[l+1]} \sigma'(z_j^{[l]}) W_{jk}^{[l+1]} = \sigma'(z_j^{[l]}) [(W^{[l+1]})^T \delta^{[l+1]}]_j ,$$

which leads to what we wanted to prove.)

3. Consider solving an optimization problem $\min_{x \in \mathbb{R}^n} f(x)$ via a line search method of the form $x^{k+1} = x^k + \alpha d^k$ where the stepsize $\alpha > 0$ and the descent direction $d^k \in \mathbb{R}^n$. Assume one can obtain an inequality of the form

$$f(x^{k+1}) \le f(x^k) - C \|\nabla f(x^k)\|^2$$

for some constant C > 0. Assume that the objective function f is bounded from below and its gradient ∇f is L-Lipschitz. Suppose there is a subsequence $x_{n_k} \to \bar{x}$ as $k \to \infty$, show that $\nabla f(\bar{x}) = 0$. In particular, if the function f is convex, this implies that \bar{x} is a solution to the optimization problem.

(Hint: Rewrite the inequality into $\|\nabla f(x^k)\|^2 \leq \frac{f(x^k) - f(x^{k+1})}{C}$ and use the fact that $\{f(x^k)\}_{k\geq 1}$ is a monotonically decreasing sequence that is bounded from below. This indicates that $\lim_{k\to\infty} [f(x^k) - f(x^{k+1})] = 0$, which implies that $\lim_{k\to\infty} \|\nabla f(x^k)\| = 0$. As we have $x^{n_k} \to \bar{x}$ as $k \to \infty$, by the continuity of $\nabla f(x)$ we have $\nabla f(\bar{x}) = \lim_{k\to\infty} \nabla f(x^{n_k}) = 0$, as claimed.)