HUT , Institute of mathematics Mat-1.196 Mathematics of neural networks Exercise 9 12.3–21.3.2002

1. Assume that $\mathbf{x} \in \mathbb{R}^d$. Calculate the gradient of the function

$$f(\mathbf{w}) = \frac{1}{2} |\mathbf{x} - (\mathbf{w} \cdot \mathbf{x})\mathbf{w}|^2, \quad \mathbf{w} \in \mathbb{R}^d,$$

at a point where $|\mathbf{w}| = 1$.

Solution: We have

$$f(\mathbf{w}) = \frac{1}{2} \|\mathbf{x}\|^2 - (\mathbf{w} \cdot \mathbf{x})^2 + \frac{1}{2} (\mathbf{w} \cdot \mathbf{x})^2 \|\mathbf{w}\|^2.$$

If $1 \leq j \leq d$ then a straightforward calculation shows that

$$\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}(j)} = -2(\mathbf{w} \cdot \mathbf{x})\mathbf{x}(j) + (\mathbf{w} \cdot \mathbf{x})\mathbf{x}(j) \|\mathbf{w}\|^2 + (\mathbf{w} \cdot \mathbf{x})^2\mathbf{w}(j) = -(\mathbf{w} \cdot \mathbf{x})\mathbf{x}(j) + (\mathbf{w} \cdot \mathbf{x})^2\mathbf{w}(j),$$

where we used the fact that $|\mathbf{w}| = 1$. Thus the gradient of f is

$$f'(\mathbf{w}) = -(\mathbf{w} \cdot \mathbf{x})\mathbf{x} + (\mathbf{w} \cdot \mathbf{x})^2 \mathbf{w}.$$

Note that if we want to minimize f for a given fixed \mathbf{x} we choose, of course, $\mathbf{w} = \frac{1}{|\mathbf{x}|}\mathbf{x}$, but if \mathbf{x} is not fixed but a random vector, this is not a good idea. However, if we are given a sequence of samples of this random vector, we can at each step change \mathbf{w} a small step in the direction of the negative gradient, and then we get the updating formula

$$\mathbf{w}_{n+1} = \mathbf{w}_n + \gamma_n ((\mathbf{w}_n \cdot \mathbf{x}_n) \mathbf{x}_n - (\mathbf{w}_n \cdot \mathbf{x}_n)^2 \mathbf{w}_n).$$

2. Assume that $\mathbf{w} \in \mathbb{R}^d$ is such that $|\mathbf{w}| = 1$. If $\mathbf{x} \in \mathbb{R}^d$, define

$$\mathbf{w}^* = \frac{1}{|\mathbf{w} + \eta(\mathbf{w} \cdot \mathbf{x})\mathbf{x}|} (\mathbf{w} + \eta(\mathbf{w} \cdot \mathbf{x})\mathbf{x}),$$

so that $|\mathbf{w}^*| = 1$. Show that

$$\mathbf{w}^* = \mathbf{w} + \eta(\mathbf{w} \cdot \mathbf{x})(\mathbf{x} - (\mathbf{w} \cdot \mathbf{x})\mathbf{w}) + O(\eta^2).$$

Solution: Because $|\mathbf{w}| = 1$ and since $\frac{1}{\sqrt{1+t}} = 1 - \frac{1}{2}t + O(t^2)$ we have

$$\frac{1}{|\mathbf{w} + \eta(\mathbf{w} \cdot \mathbf{x})\mathbf{x}|} = \frac{1}{\sqrt{|\mathbf{w}|^2 + 2\eta(\mathbf{w} \cdot \mathbf{x})^2 + \eta^2(\mathbf{w} \cdot \mathbf{x})^2 |\mathbf{x}|^2}} = 1 - \eta(\mathbf{w} \cdot \mathbf{x})^2 + O(\eta^2).$$

Hence

$$\frac{1}{|\mathbf{w} + \eta(\mathbf{w} \cdot \mathbf{x})\mathbf{x}|} (\mathbf{w} + \eta(\mathbf{w} \cdot \mathbf{x})\mathbf{x}) = (\mathbf{w} + \eta(\mathbf{w} \cdot \mathbf{x})\mathbf{x})(1 - \eta(\mathbf{w} \cdot \mathbf{x})^2 + O(\eta^2))$$
$$= \mathbf{w} + \eta(\mathbf{w} \cdot \mathbf{x})(\mathbf{x} - (\mathbf{w} \cdot \mathbf{x})\mathbf{w}) + O(\eta^2).$$

3. Assume that $x \in \mathbb{R}^{d \times 1}$. Find the gradient of the function

$$f(W) = \frac{1}{2}|X - W^{\mathrm{T}}WX|^2, \quad W \in \mathbb{R}^{m \times d},$$

at a point where $WW^{T} = I$.

Solution: We can rewrite f(W) as

$$f(W) = \frac{1}{2} \left(X^{\mathsf{T}} X - 2 X^{\mathsf{T}} W^{\mathsf{T}} W X + X^{\mathsf{T}} W^{\mathsf{T}} W W^{\mathsf{T}} W X \right).$$

If we have a function of the form g(W) = AWB where A and B are matrices with the dimensions $1 \times m$ and $d \times 1$, then

$$\frac{\partial g(W)}{\partial W(j,k)} = A(1,j)B(k,1),$$

so we can write

$$g'(W) = A^{\mathrm{T}}B^{\mathrm{T}}.$$

Similarly if $g(W) = AW^{T}B$, then $g(W) = B^{T}WA^{T}$ so that g'(W) = BA. Applying these differentiation rules to f we get

$$\begin{split} f'(W) &= \tfrac{1}{2} \left(-2WXX^{\mathrm{T}} - 2WXX^{\mathrm{T}} + WW^{\mathrm{T}}WXX^{\mathrm{T}} + WXX^{\mathrm{T}}W^{\mathrm{T}}W \right. \\ &+ WXX^{\mathrm{T}}W^{\mathrm{T}}W + WW^{\mathrm{T}}WXX^{\mathrm{T}} \right) = -WXX^{\mathrm{T}} + WXX^{\mathrm{T}}W^{\mathrm{T}}W, \end{split}$$

when we use $WW^{\mathrm{T}} = I$.