Solution 1: Gradient Computation

We use the knowledge of the following rules to calculate the gradients: $\nabla_{\mathbf{w}}(\mathbf{w}^{\top}\mathbf{v}) = \nabla_{\mathbf{w}}(\mathbf{v}^{\top}\mathbf{w}) = \mathbf{v}$ and $\nabla_{\mathbf{w}}(\mathbf{w}^{\top}\mathbf{A}\mathbf{w}) = (\mathbf{A} + \mathbf{A}^{\top})\mathbf{w}$ for some matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ and $\mathbf{w}, \mathbf{v} \in \mathbb{R}^{d}$.

- i) The gradient reduces to $\nabla_{\mathbf{w}} f = 2(\mathbf{A} + \mathbf{A}^{\top})\mathbf{v}$
- ii) $\nabla_{\mathbf{w}} f = (\mathbf{A} + \mathbf{A}^{\top}) \mathbf{w}$
- iii) $\nabla_{\mathbf{w}} f = \begin{bmatrix} \theta(w_1) & \dots & \theta(w_d) \end{bmatrix}^{\top}$, where $\theta(s) = \frac{e^s}{1 + e^s} = \frac{1}{1 + e^{-s}}$ is the logistic function.
- iv) $\nabla_{\mathbf{w}} f = \frac{\mathbf{w}}{\sqrt{1+||\mathbf{w}||^2}}$

Solution 2: Logistic Regression

For the dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$, where $\mathbf{x}_i \in \mathbb{R}^{d+1}$ is an augmented datavector $\begin{bmatrix} 1 & x_{i,1} & \dots & x_{i,d} \end{bmatrix}^\top$ with label $y_i \in \{-1, 1\}$, and given any datavector $\mathbf{x}_n \in \mathbb{R}^{d+1}$, the logistic regression model outputs the probability estimate for the true class y_n as

$$\hat{p}_{\mathbf{w}}(y_n \mid \mathbf{x}_n) = \theta\left(y_n \mathbf{w}^\top \mathbf{x}_n\right). \tag{1}$$

The loss function (in-sample error) for the model is defined to be

$$E_{\rm in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \underbrace{-\log\left(\hat{p}_{\mathbf{w}}(y_n \mid \mathbf{x}_n)\right)}_{e_n(\mathbf{w})}$$
(2)

a) From (2) we can see that since there are only two classes, we can rewite the loss function as

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \left[-I(y_n = 1) \log(\hat{p}_{\mathbf{w}}(1 \mid \mathbf{x}_n)) - I(y_n = -1) \log(\hat{p}_{\mathbf{w}}(-1 \mid \mathbf{x}_n)) \right]$$

$$= \frac{1}{N} \sum_{n=1}^{N} \left[-\frac{1+y_n}{2} \log(\hat{p}_{\mathbf{w}}(1 \mid \mathbf{x}_n)) - \frac{1-y_n}{2} \log(1-\hat{p}_{\mathbf{w}}(1 \mid \mathbf{x}_n)) \right], \tag{3}$$

where $I(y_n = 1)$ and $I(y_n = -1)$ are the indicator functions.

b) From (1) and (2) we can see that

$$e_n(\mathbf{w}) = -\log(\hat{p}_{\mathbf{w}}(y_n \mid \mathbf{x}_n)) = \log(1 + e^{-y_n \mathbf{w}^{\top} \mathbf{x}_n})$$

Therefore, we can also rewrite the loss function as

$$E_{\rm in}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \log(1 + e^{-y_n \mathbf{w}^{\top} \mathbf{x}_n})$$

$$\tag{4}$$

c) Now, from (4) we can see that the gradient of the loss function is given by

$$\nabla_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \nabla_{\mathbf{w}} \log(1 + e^{-y_n \mathbf{w}^{\top} \mathbf{x}_n}) = \frac{1}{N} \sum_{n=1}^{N} \frac{-y_n \mathbf{x}_n e^{-y_n \mathbf{w}^{\top} \mathbf{x}_n}}{1 + e^{-y_n \mathbf{w}^{\top} \mathbf{x}_n}}$$
$$= \frac{1}{N} \sum_{n=1}^{N} -y_n \mathbf{x}_n \theta(-y_n \mathbf{w}^{\top} \mathbf{x}_n).$$
(5)

Continuing with what we established in Homework 1, here notice that for a confidently missclassified point $y_n \mathbf{w}^{\top} \mathbf{x}_n \ll 0$ which gives $\theta(-y_n \mathbf{w}^{\top} \mathbf{x}_n) \approx 1$, whereas for a confidently correctly classified point, we have $y_n \mathbf{w}^{\top} \mathbf{x}_n \gg 0$ which gives $\theta(-y_n \mathbf{w}^{\top} \mathbf{x}_n) \approx 0$, meaning that there is little contribution compared to the misclassified case.

d) From (3) notice that

$$\nabla_{\mathbf{w}} E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} \left[-\frac{1+y_n}{2} \nabla_{\mathbf{w}} \log(\hat{p}_{\mathbf{w}}(1 \mid \mathbf{x}_n)) - \frac{1-y_n}{2} \nabla_{\mathbf{w}} \log(1-\hat{p}_{\mathbf{w}}(1 \mid \mathbf{x}_n)) \right]$$

$$= \frac{1}{2N} \sum_{n=1}^{N} \left[-(1+y_n)(1+e^{-\mathbf{w}^{\top}\mathbf{x}_n}) \nabla_{\mathbf{w}}(1+e^{-\mathbf{w}^{\top}\mathbf{x}_n})^{-1} - (1-y_n)(1+e^{\mathbf{w}^{\top}\mathbf{x}_n}) \nabla_{\mathbf{w}}(1+e^{\mathbf{w}^{\top}\mathbf{x}_n})^{-1} \right]$$

$$= \frac{1}{2N} \sum_{n=1}^{N} \left[-(1+y_n)\mathbf{x}_n \underbrace{\frac{e^{-\mathbf{w}^{\top}\mathbf{x}_n}}{(1+e^{-\mathbf{w}^{\top}\mathbf{x}_n})}}_{\theta(-\mathbf{w}^{\top}\mathbf{x}_n)=1-\theta(\mathbf{w}^{\top}\mathbf{x}_n)} + (1-y_n)\mathbf{x}_n \underbrace{\frac{e^{\mathbf{w}^{\top}\mathbf{x}_n}}{(1+e^{\mathbf{w}^{\top}\mathbf{x}_n})}}_{\theta(\mathbf{w}^{\top}\mathbf{x}_n)} \right]$$

$$= \frac{1}{2N} \sum_{n=1}^{N} \mathbf{x}_n \left(2\theta(\mathbf{w}^{\top}\mathbf{x}_n) - y_n - 1 \right)$$

$$= \frac{1}{N} \mathbf{X}^{\top} \underbrace{\left(\theta(\mathbf{X}\mathbf{w}) - \frac{\mathbf{y}}{2} - \frac{\mathbf{I}}{2} \right)}_{n},$$
(6)

where $\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top & \dots & \mathbf{x}_N^\top \end{bmatrix}^\top \in \mathbb{R}^{N \times (d+1)}$. Notice that the expression p is similar to $\mathbf{X}\mathbf{w} - \mathbf{y}$ in the gradient of the mean squared error loss function (for linear regression) derived in Homework 1.

Solution 3: Midterm 2017, Problem 4

We are given $\mathcal{D} = \left\{ \begin{pmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix}^\top, 1 \end{pmatrix}, \begin{pmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix}^\top, -1 \end{pmatrix} \right\} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2)\}$ and the corresponding regularized loss function for logistic regression

$$E_{\rm in}(\mathbf{w}) = \lambda ||\mathbf{w}||^2 + \frac{1}{N} \sum_{n=1}^{N} e_n(\mathbf{w}), \tag{7}$$

which is a shorthand for (4) except for the weight regularization term.

a) Since $\lambda = 0$, we can evaluate the loss function for $\mathbf{w} = \begin{bmatrix} w_1 & w_2 \end{bmatrix}^\top$ as follows

$$E_{\rm in}(\mathbf{w}) = \log(1 + e^{-(w_1 + w_2)}) + \log(1 + e^{w_1}).$$

This expression can be minimized if $w_1 \to -\infty$ and $w_1 + w_2 \to \infty$. This can be realized with $w_2 = -2w_1$ and $w_1 \to \infty$, which will yield $E_{\rm in} = 0$.

b) For $\lambda \gg 0$, we can consider $||w|| \ll 1$ while minimizing the loss function. For this case, we are given the Taylor approximation of the loss function for $e_n(\mathbf{w}) \approx \log(2) - \frac{1}{2}y_n\mathbf{w}^{\top}\mathbf{x}_n$, which we can substituted into the expression loss in part a) to then minimize it, i.e.,

$$E_{\rm in}(\mathbf{w}) = \lambda(w_1^2 + w_2^2) + \log(1 + e^{-(w_1 + w_2)}) + \log(1 + e^{w_1})$$
$$= \lambda(w_1^2 + w_2^2) + \log(2) - \frac{1}{2}(w_1 + w_2) + \log(2) + \frac{1}{2}w_1.$$

Now to minimize the loss, we set

$$\begin{split} \frac{\partial E_{\rm in}}{\partial w_1} &= 0 \implies 2\lambda w_1 - \frac{1}{2} + \frac{1}{2} = 0 \iff w_1 = 0 \\ \frac{\partial E_{\rm in}}{\partial w_2} &= 0 \implies 2\lambda w_2 - \frac{1}{2} = 0 \iff w_2 = \frac{1}{4\lambda}. \end{split}$$

Thus, $\mathbf{w}^* = \begin{bmatrix} 0 & \frac{1}{4\lambda} \end{bmatrix}^\top$ is the minimizer.