Represent the derivative of the following scalar functions with respect to $\mathbf{X} \in \mathbb{R}^{D \times D}$.

- (a) $f(\mathbf{X}) = tr(\mathbf{X}^2)$. Here, tr(A) is the trace of a square matrix A.
- (b) $g(\mathbf{X}) = tr(\mathbf{X}^3)$.
- (c) $h(\mathbf{X}) = tr(\mathbf{X}^k)$ for $k \in \mathbb{N}$.

In order to alleviate overfitting in logistic regression, regularization technique can be used with the L_2 -norm of the weight parameter, $||\mathbf{w}||^2 = \sum_{i=1}^D w_i^2$. When we are given $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^D$ and $y_1, \dots, y_N \in \{0, 1\}$ for training set, we want to derive the update rule for $\mathbf{w} \in \mathbb{R}^D$ in order to minimize the following loss function $L(\mathbf{w})$ having L_2 -norm,

$$L(\mathbf{w}) = \sum_{i=1}^{N} \left(-y_i \ln f(\mathbf{x}_i; \mathbf{w}) - (1 - y_i) \ln(1 - f(\mathbf{x}_i; \mathbf{w})) \right) + ||\mathbf{w}||^2.$$
 (1)

$$f(\mathbf{x}; \mathbf{w}) = \frac{1}{1 + \exp(-\mathbf{w}^{\top} \mathbf{x})}$$
 (2)

- (1) Derive the update rule for \mathbf{w} when we use gradient descent.
- (2) Discuss the effect of L_2 -norm regularization.

Consider the following function,

$$f(\mathbf{x}; \mathbf{w}) = \frac{1 - \exp(-\mathbf{w}^T \mathbf{x})}{1 + \exp(-\mathbf{w}^T \mathbf{x})},$$
(3)

having the shape in Fig. 1.

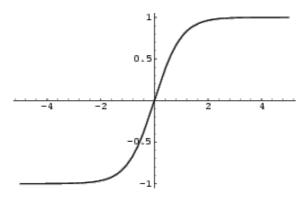


Figure 1: $f(\mathbf{x}; \mathbf{w})$

Find the gradient descent update rule for ${\bf w}$ to minimize the loss

$$L = \frac{1}{2} \sum_{i=1}^{N} (f(\mathbf{x}_i; \mathbf{w}) - y_i)^2.$$
 (4)

Here, we use N number of $\mathbf{x}_i \in \mathbb{R}^D$ and $y_i \in \{-1, 1\}$ for $i \in \{1, \dots, N\}$ which are given in advance.

For a given data set $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^N$, derive the closed-form solution for \mathbf{w} that maximizes the following probability \mathbf{P} .

$$\mathbf{P} = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2} (y_i - f(\mathbf{x}_i; \mathbf{w}))^2\right),$$
 (5)

with $f(\mathbf{x}; \mathbf{w}) = \mathbf{w}^{\top} \mathbf{x}$ for $\mathbf{x}, \mathbf{w} \in \mathbb{R}^{D}$.

The Frobenius dot product $\langle \mathbf{A}, \mathbf{B} \rangle$ is defined as

$$\langle \mathbf{A}, \mathbf{B} \rangle = tr(\mathbf{A}^{\top} \mathbf{B}), \tag{6}$$

for $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{N \times N}$ using the scalar function $tr(\cdot)$ for the trace of a matrix,

$$tr(\mathbf{M}) = \sum_{i}^{N} M_{ii}, \quad \text{for } \mathbf{M} \in \mathbb{R}^{N \times N}.$$
 (7)

Find the derivative of $\langle \mathbf{A}, \mathbf{B} \rangle$ with respect to \mathbf{A} using the definition of the matrix derivative:

$$\left[\frac{d}{d\mathbf{A}}\langle\mathbf{A},\mathbf{B}\rangle\right]_{ij} = \frac{\partial}{\partial A_{ij}}\langle\mathbf{A},\mathbf{B}\rangle. \tag{8}$$

We are given a scalar function $f(\mathbf{X}) = \mathbf{w}^{\top} \mathbf{X} \mathbf{w}$ for $\mathbf{w} \in \mathbb{R}^{D}, \mathbf{X} \in \mathbb{R}^{D \times D}$. Find the derivative of $f(\mathbf{X})$ with respect to the vector \mathbf{w} . Use the definition of the vector derivative $\left[\frac{df}{d\mathbf{w}}\right]_{k} = \frac{\partial f}{\partial w_{k}}$, where w_{k} is the k-th element of \mathbf{w} .

For a dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$ with $\mathbf{x}_i \in \mathbb{R}^D$ and $y_i \in \{0, 1\}$, Suppose that we have a two-layer neural network with residual connections shown in Figure 2. Each component is given as follows:

$$L(W) = \frac{1}{2} \sum_{i=1}^{N} (g(\mathbf{x}_i) - y_i)^2$$
 (9)

$$g(\mathbf{x}) = \sigma \left(\sum_{d=1}^{D} w_{2,d} \cdot h_d(\mathbf{x}) \right)$$
 (10)

$$h_i(\mathbf{x}) = x_i + \sigma \left(\sum_{m=1}^M w_{1,i,m} \cdot z_m(\mathbf{x}) \right)$$
 (11)

$$z_i(\mathbf{x}) = \sigma \left(\sum_{d=1}^D w_{0,i,d} \cdot x_d \right) \tag{12}$$

$$\sigma(x) = \frac{1}{1 + \exp(-x)}. (13)$$

Here, the residual connection from each x_i to the h_i node in the second layer is represented in Eq. (11). The weight $w_{i,j,k}$ connects the j-th node of i-th layer to the k-th node of (i+1)-th layer.

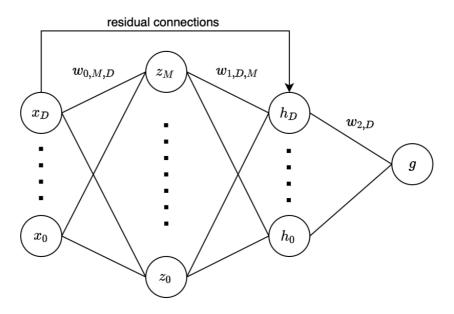


Figure 2: A two-layer network

- (a) Calculate derivative of L with respect to h_j .
- (b) Calculate derivative of L with respect to $w_{1,d,m}$.