Homework 1 – Deep Learning (CS/DS541, Whitehill, Spring 2021)

1. Python and Numpy Warm-up Exercises This part of the homework is intended to help you review your linear algebra and learn (or refresh your understanding of) how to implement linear algebraic and statistical operations in Python using numpy (to which we refer in the code below as np). For each of the problems below, write a method (e.g., problem_1a) that returns the answer for the corresponding problem.

In all problems, you may assume that the dimensions of the matrices and/or vectors are compatible for the requested mathematical operations. **Note**: Throughout the assignment, please use np.array, not np.matrix.

- (a) Given matrices A and B, compute and return an expression for A + B. [1 pts]
 Answer (freebie!): While it is completely valid to use np.add(A, B), this is unnecessarily verbose; you really should make use of the "syntactic sugar" provided by Python's/numpy's operator overloading and just write: A + B. Similarly, you should use the more compact (and arguably more elegant) notation for the rest of the questions as well.
- (b) Given matrices A, B, and C, compute and return AB C (i.e., right-multiply matrix A by matrix B, and then subtract C). Use dot or np.dot. [1 pts]
 Answer: return A.dot(B) C
- (c) Given matrices A, B, and C, return $A \odot B + C^{\top}$, where \odot represents the element-wise (Hadamard) product and \top represents matrix transpose. In numpy, the element-wise product is obtained simply with *. [1 pts]

 Answer: return A * B + C
- (d) Given column vectors \mathbf{x} and \mathbf{y} , compute the inner product of \mathbf{x} and \mathbf{y} (i.e., $\mathbf{x}^{\top}\mathbf{y}$). [1 pts] Answer: return $\mathbf{x}.dot(\mathbf{y})$
- (e) Given matrix A, return a matrix with the same dimensions as A but that contains all zeros. Use np.zeros. [1 pts] Answer: return np.zeros_like(A)
- (f) Given square matrix **A** and column vector **x**, use np.linalg.solve to compute **A**⁻¹**x**. Do not explicitly calculate the matrix inverse itself (e.g., np.linalg.inv, A ** -1) because this is numerically unstable (and yes, it can sometimes make a big difference!). [**2** pts] Answer: return np.linalg.solve(A, x)
- (g) Given square matrix \mathbf{A} and row vector \mathbf{x} , use np.linalg.solve to compute $\mathbf{x}\mathbf{A}^{-1}$. Hint: $\mathbf{A}\mathbf{B} = (\mathbf{B}^{\top}\mathbf{A}^{\top})^{\top}$. [3 pts] Answer: return np.linalg.solve(A.T, x).T
- (h) Given square matrix $\bf A$ and (scalar) α , compute $\bf A + \alpha \bf I$, where $\bf I$ is the identity matrix with the same dimensions as $\bf A$. Use np.eye. [1 pts] Answer: return $\bf A$ + np.eye(A.shape[0])
- (i) Given matrix A and integer i, return the sum of all the entries in the ith row whose column index is even, i.e., ∑_{j:j} is even A_{ij}. Do not use a loop, which in Python can be very slow. Instead use the np.sum function. [2 pts]
 Answer: return np.sum(A[i, 0::2])
- (j) Given matrix **A** and scalars c,d, compute the arithmetic mean over all entries of A that are between c and d (inclusive). In other words, if $S = \{(i,j) : c \leq \mathbf{A}_{ij} \leq d\}$, then compute $\frac{1}{|S|} \sum_{(i,j) \in S} \mathbf{A}_{ij}$. Use np.nonzero along with np.mean. [**2** pts] Answer: return np.mean(A[np.nonzero((A >= c) * (A <= d))])
- (k) Given an $(n \times n)$ matrix **A** and integer k, return an $(n \times k)$ matrix containing the right-eigenvectors of **A** corresponding to the k largest eigenvalues of **A**. Use np.linalg.eig. [3 pts]

Answer:

l, v = np.linalg.eig(A)
return v[:, np.argsort(np.abs(l))[-k:]]

- (1) Given a column vector (with n components) \mathbf{x} , an integer k, and positive scalars m, s, return an $(n \times k)$ matrix, each of whose columns is a sample from multidimensional Gaussian distribution $\mathcal{N}(\mathbf{x} + m\mathbf{z}, s\mathbf{I})$, where \mathbf{z} is column vector (with n components) containing all ones and \mathbf{I} is the identity matrix. Use either np.random.multivariate_normal or np.random.randn. [3 pts] Answer: return np.random.multivariate_normal($\mathbf{x} + \mathbf{m}$, $\mathbf{s} * np.eye(\mathbf{x}.shape[0])$, \mathbf{k}).T
- (m) Given a matrix **A** with *n* rows, return a matrix that results from **randomly permuting** the rows (but not the columns) in **A**. [**2 pts**]

 Answer: return A[np.random.permutation(A.shape[0]), :]
- (n) Z-scoring: Given a vector \mathbf{x} , return a vector \mathbf{y} such that each $y_i = (x_i \overline{\mathbf{x}})/\sigma$, where $\overline{\mathbf{x}}$ is the mean (use np.mean) of the elements of \mathbf{x} and σ is the standard deviation (use np.std). [2 pts] Answer: return (x np.mean(x)) / np.std(x)
- (o) Given an n-vector x and a non-negative integer k, return a n × k matrix consisting of k copies of x. Use np.atleast_2d on x and then use np.repeat. [2 pts]
 Answer: return np.repeat(np.atleast_2d(x), k, axis=0)
- (p) Given an $m \times n$ matrix $\mathbf{X} = \begin{bmatrix} \mathbf{x}^{(1)} & \dots & \mathbf{x}^{(n)} \end{bmatrix}$, compute an $n \times n$ matrix $\mathbf{D} = \begin{bmatrix} d_{11} & \dots & d_{1n} \\ & \ddots & \\ d_{n1} & \dots & d_{nn} \end{bmatrix}$

consisting of all pairwise L_2 distances $d_{ij} = \|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|_2$. In this problem you may **not** use loops. Instead, use np.atleast_3d, np.repeat, and np.swapaxes. **Hint**: construct two different 3-d arrays that each contain n copies of each of the n vectors in \mathbf{X} ; then subtract them. [5 pts] Answer:

Y = np.repeat(np.atleast_3d(X), X.shape[1], axis=2)
return ((np.swapaxes(Y, 1, 2) - Y) ** 2).sum(axis=0) ** .5

2. Linear Regression via Analytical Solution

- (a) Train an age regressor that analyzes a $(48 \times 48 = 2304)$ -pixel grayscale face image and outputs a real number \hat{y} that estimates how old the person is (in years). Your regressor should be implemented using linear regression. The training and testing data are available here:
 - https://s3.amazonaws.com/jrwprojects/age_regression_Xtr.npy
 - https://s3.amazonaws.com/jrwprojects/age_regression_ytr.npy
 - https://s3.amazonaws.com/jrwprojects/age_regression_Xte.npy
 - https://s3.amazonaws.com/jrwprojects/age_regression_yte.npy

To get started, see the train_age_regressor function in homework1_template.py.

Note: you must complete this problem using only linear algebraic operations in numpy – you may not use any off-the-shelf linear regression software, as that would defeat the purpose.

Compute the optimal weights $\mathbf{w} = (w_1, \dots, w_{2304})$ for a linear regression model by deriving the expression for the gradient of the cost function w.r.t. \mathbf{w} , setting it to 0, and then solving. Do **not** solve using gradient descent. The cost function is

$$f_{\text{MSE}}(\mathbf{w}) = \frac{1}{2n} \sum_{i=1}^{n} (\hat{y}^{(i)} - y^{(i)})^2$$

where $\hat{y} = g(\mathbf{x}; \mathbf{w}) = \mathbf{x}^{\top} \mathbf{w}$ and n is the number of examples in the training set $\mathcal{D}_{\mathrm{tr}} = \{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(n)}, y^{(n)})\}$, each $\mathbf{x}^{(i)} \in \mathbb{R}^{2304}$ and each $y^{(i)} \in \mathbb{R}$. Note that this simple

regression model does not include a bias term (which we will add later); correspondingly, please do **not** include one in your own implementation. After optimizing **w** only on the **training set**, compute and report the cost f_{MSE} on the training set \mathcal{D}_{tr} and (separately) on the testing set \mathcal{D}_{te} . Please report these numbers in the PDF file. [**12 pts**]

Answer: Assuming X is $k \times n$ and y is of length n, where n is number of training examples and k is number of features (i.e., pixels), then compute: w = np.linalg.solve(X.dot(X.T), X.dot(y)) Then, to obtain the (half) MSE, compute: loss = 1./(2*X.shape[1]) * np.sum((X.dot(w) - y) ** 2)

- 3. **Proofs** For the proofs, please create a PDF (which you can generate using LaTeX, or, if you prefer, a scanned copy of your **legible** handwriting).
 - (a) Let $\nabla_{\mathbf{x}} f(\mathbf{x})$ represent the column vector containing all the partial derivatives of f w.r.t. \mathbf{x} , i.e.,

$$\nabla_{\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

For any two column vectors $\mathbf{x}, \mathbf{a} \in \mathbb{R}^n$, prove that

$$abla_{\mathbf{x}} \left(\mathbf{x}^{ op} \mathbf{a}
ight) =
abla_{\mathbf{x}} \left(\mathbf{a}^{ op} \mathbf{x}
ight) = \mathbf{a}$$

Hint: differentiate w.r.t. each element of \mathbf{x} , and then gather the partial derivatives into a column vector. [4 pts]

Answer: For each $k \in \{1, ..., n\}$,

$$\frac{\partial}{\partial x_k} \left(\mathbf{x}^\top \mathbf{a} \right) = \frac{\partial}{\partial x_k} \left(\mathbf{a}^\top \mathbf{x} \right) = \frac{\partial}{\partial x_k} \left(\sum_{i=1}^n a_i x_i \right) = a_k$$

Therefore,

$$\nabla_{\mathbf{x}}(\mathbf{x}^{\top}\mathbf{a}) = \nabla_{\mathbf{x}}(\mathbf{a}^{\top}\mathbf{x}) = \begin{bmatrix} \frac{\partial(\sum_{i=1}^{n} a_{i}x_{i})}{\partial x_{1}} \\ \vdots \\ \frac{\partial(\sum_{i=1}^{n} a_{i}x_{i})}{\partial x_{n}} \end{bmatrix} = \begin{bmatrix} a_{1} \\ \vdots \\ a_{n} \end{bmatrix} = \mathbf{a}$$

(b) Prove that

$$abla_{\mathbf{x}} (\mathbf{x}^{\top} \mathbf{A} \mathbf{x}) = (\mathbf{A} + \mathbf{A}^{\top}) \mathbf{x}$$

for any column vector $\mathbf{x} \in \mathbb{R}^n$ and any $n \times n$ matrix **A**. [**6 pts**] *Answer*:

$$\mathbf{x}^{\top} \mathbf{A} \mathbf{x} = \begin{bmatrix} \sum_{i} x_{i} A_{i1} & \dots & \sum_{i} x_{i} A_{in} \end{bmatrix} \begin{bmatrix} x_{1} \\ \vdots \\ x_{n} \end{bmatrix} = \sum_{j} \sum_{i} x_{i} A_{ij} x_{j} = \sum_{i} \sum_{j} x_{i} A_{ij} x_{j}$$

In other words, $\mathbf{x}^{\top} \mathbf{A} \mathbf{x}$ is the sum over a 2-d "grid" of terms. For any $k \in \{1, \dots, n\}$, 2n-1 of the terms in the grid involve x_k : 2(n-1) are linear in x_k , and 1 term is quadratic in x_k . We handle

these separately when taking the derivative:

$$\frac{\partial (\mathbf{x}^{\top} \mathbf{A} \mathbf{x})}{\partial x_k} = \frac{\partial}{\partial x_k} \left(\sum_{j \neq k} x_k x_j A_{kj} + \sum_{i \neq k} x_i x_k A_{ik} + x_k x_k A_{kk} \right)$$
(1)

$$= \sum_{j \neq k} x_j A_{kj} + \sum_{i \neq k} x_k A_{ik} + 2x_k A_{kk}$$
 (2)

$$= \sum_{j \neq k} x_j A_{kj} + \sum_{i \neq k} x_k A_{ik} + x_k A_{kk} + x_k A_{kk}$$
 (3)

Now we can complete each summation by including the term $x_k A_{kk}$:

$$\frac{\partial(\mathbf{x}^{\top}\mathbf{A}\mathbf{x})}{\partial x_k} = \sum_{j} x_j A_{kj} + \sum_{i} x_i A_{ik}$$
(4)

$$= (\mathbf{A}_{k \cdot}) \mathbf{x} + ((\mathbf{A}^{\top})_{k \cdot}) \mathbf{x}$$
 (5)

where \mathbf{A}_k is the kth row of matrix \mathbf{A} . Finally, we obtain

$$\nabla_{\mathbf{x}}(\mathbf{x}^{\top}\mathbf{A}\mathbf{x}) = \begin{bmatrix} \frac{\partial(\mathbf{x}^{\top}\mathbf{A}\mathbf{x}))}{\partial x_1} \\ \vdots \\ \frac{\partial(\mathbf{x}^{\top}\mathbf{A}\mathbf{x}))}{\partial x_n} \end{bmatrix} = \begin{bmatrix} (\mathbf{A}_{1\cdot})\,\mathbf{x} + ((\mathbf{A}^{\top})_{1\cdot})\,\mathbf{x} \\ \vdots \\ (\mathbf{A}_{n\cdot})\,\mathbf{x} + ((\mathbf{A}^{\top})_{n\cdot})\,\mathbf{x} \end{bmatrix} = (\mathbf{A} + \mathbf{A}^{\top})\mathbf{x}$$

(c) Based on the theorem above, prove that

$$\nabla_{\mathbf{x}} \left(\mathbf{x}^{\top} \mathbf{A} \mathbf{x} \right) = 2 \mathbf{A} \mathbf{x}$$

for any column vector $\mathbf{x} \in \mathbb{R}^n$ and any symmetric $n \times n$ matrix \mathbf{A} . [**2 pts**] Answer: Since \mathbf{A} is symmetric, then $\mathbf{A} = \mathbf{A}^{\top}$, and thus $(\mathbf{A} + \mathbf{A}^{\top})\mathbf{x} = 2\mathbf{A}\mathbf{x}$.

(d) Based on the theorems above, prove that

$$\nabla_{\mathbf{x}} \left[(\mathbf{A}\mathbf{x} + \mathbf{b})^{\top} (\mathbf{A}\mathbf{x} + \mathbf{b}) \right] = 2\mathbf{A}^{\top} (\mathbf{A}\mathbf{x} + \mathbf{b})$$

for any column vector $\mathbf{x} \in \mathbb{R}^n$, any symmetric $n \times n$ matrix \mathbf{A} , and any constant column vector $\mathbf{b} \in \mathbb{R}^n$. [4 pts]

Answer:

$$\mathbf{A}\mathbf{x} + \mathbf{b})^{\top} (\mathbf{A}\mathbf{x} + \mathbf{b}) = \mathbf{x}^{\top} \mathbf{A}^{\top} \mathbf{A}\mathbf{x} + \mathbf{x}^{\top} \mathbf{A}^{\top} \mathbf{b} + \mathbf{b}^{\top} \mathbf{A}\mathbf{x} + \mathbf{b}^{\top} \mathbf{b}$$
 (6)

$$= \mathbf{x}^{\top} \mathbf{A}^{\top} \mathbf{A} \mathbf{x} + \mathbf{x}^{\top} \mathbf{A}^{\top} \mathbf{b} + (\mathbf{A}^{\top} \mathbf{b}) \mathbf{x} + \mathbf{b}^{\top} \mathbf{b}$$
 (7)

Applying the gradient rules derived above (and noting that $\mathbf{A}^{\top}\mathbf{A}$ is itself a symmetric matrix), we obtain

$$\nabla_{\mathbf{x}} \left((\mathbf{A}\mathbf{x} + \mathbf{b})^{\top} (\mathbf{A}\mathbf{x} + \mathbf{b}) \right) = 2\mathbf{A}^{\top} \mathbf{A}\mathbf{x} + \mathbf{A}^{\top} \mathbf{b} + \mathbf{A}^{\top} \mathbf{b}$$
(8)

$$= 2\mathbf{A}^{\top} \mathbf{A} \mathbf{x} + 2\mathbf{A}^{\top} \mathbf{b} \tag{9}$$

$$= 2\mathbf{A}^{\top}(\mathbf{A}\mathbf{x} + \mathbf{b}) \tag{10}$$

Submission: Create a Zip file containing both your Python and PDF files, and then submit on Canvas. If you are working as part of a group, then only **one** member of your group should submit.

Teamwork: You may complete this homework assignment either individually or in teams up to 3 people.