1. Regression and MLE [20 points]

Assume we have a large dataset of \( k \) tuples, in which the \( i^{th} \) tuple has one real-valued input attribute \( x_i \) and one real-valued output attribute \( y_i \). To fit the data, we assume the following model with unknown parameter \( w \) that needs to be learned from the data.

\[
y_i = \log(w^2 x_i)
\]

(1)

**Q1.1** Derive the gradient descent update for \( w \).

Define the error as:

\[
E = \sum_i (y_i - \log(w^2 x_i))^2
\]

Then:

\[
\frac{\partial E}{\partial w} = \sum_i 2 \left( y_i - \log(w^2 x_i) \right) \frac{1}{w^2 x_i} \cdot 2wx_i
\]

\[
= \sum_i -4 \left( \frac{y_i - \log(w^2 x_i)}{w} \right)
\]

So:

\[
\omega_{new} = \omega_{old} + \lambda \sum_i \left( \frac{y_i - \log(w^2 x_i)}{w} \right)
\]

[8 pts]

Suppose we want to learn the following quadratic regression model with \( k \) input attributes:

\[
y = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_k x_k
\]

\[
pos 1 \quad pos 2 \quad pos 3 \quad \ldots \quad pos k
\]

\[
+ w_1 x_1^2 + w_2 x_1 x_2 + \ldots + w_k x_1 x_k
\]

\[
\vdots
\]

\[
\vdots
\]

\[
\ldots + \ldots + w_k x^2_k
\]

**Q1.2** What is the computational complexity in terms of \( k \) of learning the MLE weights using matrix inversion? Use big-O notation.

\[
O(k^6): \text{It's } O(\left[ \# \text{ of basis functions} \right]^3) \text{ to solve the equations}
\]

and the \# of basis functions is \( \frac{1}{2}(k+1)(k+2) \)

[3 pts]
Q1.3 Same question as above, but assume a cubic regression model (this will include terms such as \( w_{111}x_1^3, w_{112}x_1^2x_2, \) etc).

\[ O(k^3) \]

[3 pts]

Q1.4 What is the computational complexity of one iteration of batch gradient descent of the quadratic model?

\[ O(k^2) \] computing each \( \theta_k \) takes \( \frac{1}{2}(k+1)(k+2) \) ops. and you need one weight update for each weight.

[3 pts]

Q1.5 Same question as above, but using the cubic model.

\[ O(k^3) \]

[3 pts]

2. Neural networks short answer [30 points]

Consider neural networks with a single hidden layer. Each unit has a weight \( w \) and uses the following activation functions:

- Hard-threshold function: for a constant \( a \),

\[
h(x) = \begin{cases} 1 & \text{if } w^T x \geq a \\ 0 & \text{otherwise} \end{cases}
\]

- Linear:

\[ h(x) = w^T x \]

Q2.1 How many boolean functions \( f(x_1, x_2) \), where \( x_{1,2} \in \{0, 1\} \), are there?

\[ 2^4 = 16. \]

There are 4 possible inputs and for each input there are 4 possible outputs.

[3 pts]
Q2.2 For any boolean function $f(x_1, x_2)$, can we build a neural network to compute $f$? If so, prove by construction. If not, explain why not.

Any boolean function can be represented using a combination of AND, NOT, and OR gates, and each of these gates is easily representable using a neural network. For example:

Consider neural networks with a hidden layer with only one input signal $x$ and one output signal $y$. Using hard threshold and/or linear activation functions, which of the following cases can be exactly represented by a neural network? For each case, if representable, draw the network with choice of activations for both levels and briefly explain how the function is represented. If not representable, explain why not.

Q2.3 Polynomials of degree one.

Yes, a poly. of degree one is just $f(x) = ax + b$ which can be represented using one unit and a linear activation function.

Q2.4 Polynomials of degree two.

No, it's not possible to represent $x^2$.

Q2.5 Hinge loss: $L(x) = \max(1 - x, 0)$.

No, not with these activation functions. You need to be able to multiply 2 input signals.
Assume we have the following neural network with linear activation units. The output of each unit is a constant $c$ multiplied by the weighted sum of inputs.

![Neural Network Diagram]

**Q2.6** Is it possible for any function that can be represented by the above network to also be represented using a single unit network? If so, draw such a network, including the weights and activation function. If not, explain why not.

*Yes.*

![Single Unit Network Diagram]

(4 pts)

**Q2.7** Is it possible for any function that can be represented by the above network to also be represented by linear regression? If so, provide an equation for $Y$. If not, explain why not.

*Yes.*

$y = c^2(w_{1}x_1 + w_{10}x_2) + c^2(w_3x_3 + w_{10}x_4) + c^2(w_{5}x_5 + w_{12}x_3) + c^2(w_{7}x_7 + w_{12}x_4)$

(3 pts)
Q2.8 Draw a fully connected three unit neural network that has binary inputs \( X_1, X_2, 1 \) and output \( Y \), where \( Y \) implements the XOR function: \( Y = (X_1 \text{ XOR } X_2) \). Assume that each unit uses a \textit{hard threshold} activation function.

\[
h(x) = \begin{cases} 
1 & \text{if } w^T x > 2 \\
0 & \text{otherwise}
\end{cases}
\]

[4 pts]

Q2.9 Same question as above, but now assume each unit uses a \textit{summation} activation function.

\[
h(x) = \begin{cases} 
\text{Sigmoid} & \text{if } w^T x > 0 \\
0 & \text{otherwise}
\end{cases}
\]

[3 pts]
3. Neural networks training [30 points]

We train a neural network on a set of input vectors \( \{x_n\} \) where \( n = 1, \ldots, N \), together with a corresponding set of target \( K \)-dimensional vectors \( \{t_n\} \). We assume that \( t \) has a Gaussian distribution with an \( \mathbf{x} \)-dependent mean, so that:

\[
p(t|x, w) = \mathcal{N}(t|y(x, w), \beta^{-1}I)
\]

where \( \beta \) is the precision of the Gaussian noise. We would like to find the parameters \( w \) using the MLE principle:

\[
w_{\text{MLE}} = \arg\max_w \prod_{n=1}^{N} p(t_n|x_n, w)
\]

\( \text{(2)} \)

Q3.1 Show that solving (2) is equivalent to minimizing the sum-of-squares error function:

\[
E(w) = \frac{1}{2} \sum_{n=1}^{N} \|y(x_n, w) - t_n\|^2
\]

\( \text{(3)} \)

Take the negative log-likelihood:

\[
-\log L(w) = \frac{\beta}{2} \sum_{n=1}^{N} \|y(x_n, w) - t_n\|^2 - \frac{N}{2} \log \beta + \frac{N}{2} \log (2\pi)
\]

Thus, minimizing the log-likelihood equals minimizing:

\[
E(w) = \frac{1}{2} \sum_{n=1}^{N} \|y(x_n, w) - t_n\|^2
\]

[15 pts]
Consider a network with one hidden layer as shown below. Assume that each hidden unit $j$ computes a weighted sum of its inputs $x$ of the form: $a_j = \sum_i w_{ji} x_i$, where $w_j$ and $z$ are the weights and input of this hidden unit, respectively. The activation function $h$ is $h(a_j) = z_j$. Each output unit $k$ computes a weighted sum of its inputs $z$ of the form $b_k = \sum_j w'_{kj} z_j$, where $w'_k$ are the weights of this output unit. This unit outputs $y_k = b_k$. Together, the output of this network is: $y(x_n, w) = [y_1, y_2, \ldots, y_k]^T$.

To train a neural network, we need to compute the derivatives of $E(w)$. We can do so by considering a simpler quantity, $E_n = \frac{1}{2} \| y(x_n, w) - t_n \|_2^2$.

Q3.2 Show that:

$$\frac{\partial E_n}{\partial w_{ji}} = (h'(a_j) \sum_k w'_{kj}\delta_k) x_i$$

where $w'_k$ are weights of the output units and $\delta_k = y_k - t_k$.

It's easiest to break this up into 3 factors:

$$\frac{\partial E_n}{\partial w_{ji}} = \frac{\partial E_n}{\partial a_j} \frac{\partial a_j}{\partial w_{ji}} = x_i$$

$$= \frac{\partial E_n}{\partial z_j} \frac{\partial z_j}{\partial a_j} = h'(a_j)$$

$$= (y(x_n, w) - t_n) w'_j$$

$$= \sum_k \delta_k w'_{kj}$$

Together, we get: 

$$h'(a_j) \sum_k \delta_k w'_{kj} x_i$$
4. Neural networks example [20 points]

Consider the following classification training data (where ‘x’ means True and ‘o’ means False) and neural network that uses a sigmoid response function \( g(t) = \frac{1}{1 + \exp(-t)} \).

Q4.1 We want to set the weights \( w \) of the neural network so that it is capable of correctly classifying the entire dataset. Plot the decision boundaries of \( N_1 \) and \( N_2 \) (e.g. for neuron \( N_1 \), plot the line where \( w_{10} + w_{11}x_1 + w_{12}x_2 = 0 \)) on the following two graphs.