# **Multilayer Perceptron Project Report MATH 6373 - Deep Learning and Neural Networks**

Ravik Chand Lucas Smith Huy Nguyen

### Part 0

For this project, our team used The Superconductivity Data Data Set, shared by Hamidieh Kam of the University of Pennsylvania and hosted on the University of California Machine Learning Repository. This dataset contains information about 21,263 instances, n, of superconducting materials, their composition, and their respective chemical characteristics.

## UCI Machine Learning Repository: Superconductivty Data Data Set

In addition to the number of unique elements found in each material, eight variables regarding each material are recorded such as Atomic Mass, First Ionization Energy (FIE), Atomic Radius, Density, Fusion Heat, Thermal Conductivity, and Valence. The definitions of each variable are as below:

Variable	Units	Description
Atomic Mass	Atomic mass units (AMU)	Total proton and neutron rest masses
First Ionization Energy	Kilo-Joules per mole (kJ/mol)	Energy required to remove a valence electron
Atomic Radius	Picometer (pm)	Calculated atomic radius
Density	Kilograms per meters cubed $(kg/m^3)$	Density at standard temperature and pressure
Electron Affinity	Kilo-Joules per mole (kJ/mol)	Energy required to add an electron to a neutral atom
Fusion Heat	Kilo-Joules per mole (kJ/mol)	Energy to change from solid to liquid without temperature change
Thermal Conductivity	Watts per meter-Kelvin (W/(mK))	Thermal conductivity coefficient $\kappa$
Valence	No units	Typical number of chemical bonds formed by the element

From these variables, 80 feature columns, p, are derived containing the mean, range, entropy, and standard deviation data of the variables. As an example, regarding the variable "thermal conductivity," the mean feature column represents the arithmetic average of thermal conductivity

coefficients of elements found within a material. The weighted mean represents the average adjusted to the proportion of each element found within the material. The geometric mean is an alternative calculation of the average, and likewise, the weighted variant feature column represents the geometric mean calculation with consideration to the proportion of each element found in a material. The range and weighted range represent the difference between the greatest and weakest coefficients. Entropy represents disorder, while standard deviation represents the variation between coefficients of elements within a material. The formulas used to calculate these features, specifically in the case of a superconductor composed of 7Re+1Zr are as below:

Feature & description	Formula	Sample value
Mean	$=\mu=(t_1+t_2)\\/2$	35.5
Weighted mean	$= u = (p_1t_1) \ + (p_2t_2)$	44.43
Geometric mean	$= (t_1 t_2)^{1/2} $	33.23
Weighted geometric mean	$= (t_1)^{p_1} (t_2)^{p_2}$	43.21
Entropy	$= -w_1 \ln(w_1) \ -w_2 \ln(w_2)$	0.63
Weighted entropy	$=-A\ln(A) \ -B\ln(B)$	0.26
Range	$=t_{1}-t_{2} \ (t_{1}>t_{2})$	25
Weighted range	$= p_1 t_1 - p_2 t_2 \\$	37.86
Standard deviation	$egin{aligned} &= \left[ (1 \ /2)((t_1 - \mu)^2 \ &+ (t_2 - \mu)^2)  ight]^{1/2} \end{aligned}$	12.5
Weighted standard deviation	$=\left[p_{1}(t_{1}- u)^{2} ight. \ \left.+p_{2}(t_{2}- u)^{2}) ight]^{1/2}$	8.75

colname	Description
number_of_elements	Number of unique elements
mean_atomic_mass	Mean atomic mass
wtd_mean_atomic_mass	Weighted mean atomic mass
gmean_atomic_mass	Geometric mean atomic mass
wtd_gmean_atomic_mass	Weighted geometric mean atomic mass
entropy_atomic_mass	Entropy of atomic mass
wtd_entropy_atomic_mass	Weighted entropy of atomic mass
range_atomic_mass	Range of atomic mass
wtd_range_atomic_mass	Weighted range of atomic mass
std_atomic_mass	Standard deviation of atomic mass
wtd_std_atomic_mass	Weighted standard deviation of atomic mass
mean_fie	Mean first ionization energy
wtd_mean_fie	Weighted mean first ionization energy
gmean_fie	Geometric mean first ionization energy
wtd_gmean_fie	Weighted geometric mean first ionization energy
entropy_fie	Entropy of first ionization energy
wtd_entropy_fie	Weighted entropy of first ionization energy
range_fie	Range of first ionization energy
wtd_range_fie	Weighted range of first ionization energy
std_fie	Standard deviation of first ionization energy
wtd_std_fie	Weighted standard deviation of first ionization energy
mean_atomic_radius	Mean atomic radius
wtd_mean_atomic_radius	Weighted mean atomic radius
gmean_atomic_radius	Geometric mean atomic radius
wtd_gmean_atomic_radius	Weighted geometric mean atomic radius
entropy_atomic_radius	Entropy of atomic radius
wtd_entropy_atomic_radius	Weighted entropy of atomic radius
range_atomic_radius	Range of atomic radius
wtd_range_atomic_radius	Weighted range of atomic radius
std_atomic_radius	Standard deviation of atomic radius
wtd_std_atomic_radius	Weighted standard deviation of atomic radius
mean_Density	Mean density

wtd_mean_Density		
wtd_gmean_Density	wtd_mean_Density	Weighted mean density
entropy_Density	gmean_Density	Geometric mean density
wtd_entropy_Density range_Density Range of density wtd_range_Density Standard deviation of density wtd_std_Density Weighted standard deviation of density mean_ElectronAffinity Weighted mean electron affinity wtd_mean_ElectronAffinity Weighted geometric mean electron affinity wtd_mean_ElectronAffinity Entropy of electron affinity wtd_entropy_ElectronAffinity Weighted entropy of electron affinity wtd_mange_ElectronAffinity Weighted entropy of electron affinity wtd_entropy_ElectronAffinity Weighted entropy of electron affinity wtd_range_ElectronAffinity Weighted entropy of electron affinity wtd_range_ElectronAffinity Weighted range of electron affinity std_ElectronAffinity Weighted standard deviation of electron affinity wtd_std_ElectronAffinity Weighted standard deviation of electron affinity wtd_std_ElectronAffinity Weighted standard deviation of electron affinity wtd_mean_FusionHeat Weighted mean fusion heat wtd_mean_FusionHeat Weighted mean fusion heat wtd_gmean_FusionHeat Weighted geometric mean fusion heat wtd_gmean_FusionHeat Weighted entropy of fusion heat wtd_entropy_FusionHeat Weighted entropy of fusion heat std_entropy_FusionHeat Weighted range of fusion heat std_FusionHeat Standard deviation of fusion heat wtd_range_FusionHeat Weighted range of fusion heat wtd_std_FusionHeat Weighted standard deviation of fusion heat wtd_std_FusionHeat Weighted standard deviation of fusion heat wtd_mean_ThermalConductivity Weighted mean thermal conductivity wtd_mean_ThermalConductivity Weighted mean thermal conductivity wtd_gmean_ThermalConductivity wtd_gmean_ThermalConductivity wtd_gmean_ThermalConductivity	wtd_gmean_Density	Weighted geometric mean density
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wtd_range_Density  std_Density  Standard deviation of density  wtd_std_Density  Weighted standard deviation of density  mean_ElectronAffinity  wtd_mean_ElectronAffinity  wtd_mean_ElectronAffinity  wtd_gmean_ElectronAffinity  wtd_gmean_ElectronAffinity  wtd_gmean_ElectronAffinity  wtd_gmean_ElectronAffinity  wtd_gmean_ElectronAffinity  wtd_gmean_ElectronAffinity  wtd_gmean_ElectronAffinity  wtd_gmean_ElectronAffinity  wtd_entropy_ElectronAffinity  wtd_entropy_ElectronAffinity  wtd_entropy_ElectronAffinity  wtd_ange_of electron affinity  wtd_range_ElectronAffinity  wtd_range_ElectronAffinity  wtd_std_ElectronAffinity  weighted range of electron affinity  std_ElectronAffinity  weighted range of electron affinity  wtd_std_ElectronAffinity  weighted standard deviation of electron affinity  mean_FusionHeat  wtd_mean_FusionHeat  weighted mean fusion heat  wtd_mean_FusionHeat  wtd_gmean_FusionHeat  weighted geometric mean fusion heat  wtd_gmean_FusionHeat  wtd_gmean_FusionHeat  wtd_entropy_FusionHeat  wtd_entropy_FusionHeat  wtd_entropy_FusionHeat  wtd_range_FusionHeat  weighted entropy of fusion heat  wtd_range_FusionHeat  weighted range of fusion heat  std_FusionHeat  weighted range of fusion heat  wtd_range_FusionHeat  weighted range of fusion heat  wtd_range_FusionHeat  weighted standard deviation of fusion heat  std_FusionHeat  weighted standard deviation of fusion heat  wtd_std_FusionHeat  weighted range of fusion heat  wtd_std_FusionHeat  weighted	wtd_entropy_Density	Weighted entropy of density
std_Density Standard deviation of density  wtd_std_Density Weighted standard deviation of density  mean_ElectronAffinity Weighted mean electron affinity  gmean_ElectronAffinity Weighted mean electron affinity  wtd_gmean_ElectronAffinity Weighted geometric mean electron affinity  wtd_gmean_ElectronAffinity Weighted geometric mean electron affinity  wtd_entropy_ElectronAffinity Weighted entropy of electron affinity  wtd_entropy_ElectronAffinity Weighted entropy of electron affinity  wtd_range_ElectronAffinity Weighted range of electron affinity  std_ElectronAffinity Weighted range of electron affinity  wtd_std_ElectronAffinity Weighted standard deviation of electron affinity  wtd_std_ElectronAffinity Weighted standard deviation of electron affinity  mean_FusionHeat Weighted mean fusion heat  wtd_mean_FusionHeat Weighted mean fusion heat  wtd_gmean_FusionHeat Weighted geometric mean fusion heat  wtd_gmean_FusionHeat Weighted geometric mean fusion heat  wtd_entropy_FusionHeat Weighted entropy of fusion heat  wtd_entropy_FusionHeat Weighted entropy of fusion heat  wtd_range_FusionHeat Weighted range of fusion heat  std_FusionHeat Standard deviation of fusion heat  wtd_std_FusionHeat Weighted standard deviation of fusion heat  wtd_mean_ThermalConductivity Mean thermal conductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity	range_Density	Range of density
wtd_std_Density Weighted standard deviation of density mean_ElectronAffinity Weighted mean electron affinity wtd_mean_ElectronAffinity Geometric mean electron affinity wtd_gmean_ElectronAffinity Weighted geometric mean electron affinity wtd_gmean_ElectronAffinity Entropy of electron affinity wtd_entropy_ElectronAffinity Weighted entropy of electron affinity wtd_entropy_ElectronAffinity Weighted entropy of electron affinity range_ElectronAffinity Weighted range of electron affinity wtd_range_ElectronAffinity Weighted range of electron affinity std_ElectronAffinity Weighted standard deviation of electron affinity wtd_std_ElectronAffinity Weighted standard deviation of electron affinity mean_FusionHeat Weighted mean fusion heat wtd_mean_FusionHeat Weighted mean fusion heat wtd_gmean_FusionHeat Weighted geometric mean fusion heat wtd_gmean_FusionHeat Weighted entropy of fusion heat wtd_entropy_FusionHeat Weighted entropy of fusion heat wtd_ange_FusionHeat Weighted range of fusion heat std_range_FusionHeat Weighted range of fusion heat std_FusionHeat Standard deviation of fusion heat wtd_std_FusionHeat Weighted standard deviation of fusion heat mean_ThermalConductivity Mean thermal conductivity gmean_ThermalConductivity gmean_ThermalConductivity wtd_gmean_ThermalConductivity wtd_gmean_ThermalConductivity	wtd_range_Density	Weighted range of density
mean_ElectronAffinity wtd_mean_ElectronAffinity wtd_mean_ElectronAffinity gmean_ElectronAffinity wtd_gmean_ElectronAffinity wtd_gmean_ElectronAffinity wtd_gmean_ElectronAffinity entropy_ElectronAffinity wtd_entropy_ElectronAffinity wtd_range_ElectronAffinity wtd_range_ElectronAffinity wtd_range_ElectronAffinity wtd_std_ElectronAffinity wtd_std_ElectronAffinity wteighted range of electron affinity wtd_std_ElectronAffinity wteighted standard deviation of electron affinity wtd_std_ElectronAffinity weighted standard deviation of electron affinity mean_FusionHeat wtd_mean_FusionHeat wteighted mean fusion heat wtd_gmean_FusionHeat wtd_gmean_FusionHeat wtd_gmean_FusionHeat wtd_entropy_FusionHeat wtd_entropy_FusionHeat wtd_entropy_FusionHeat wtd_range_FusionHeat wtd_range_FusionHeat wtd_range_FusionHeat wtd_range_FusionHeat wtd_std_FusionHeat wtd_std_FusionHeat wtd_std_FusionHeat wteighted standard deviation of fusion heat	std_Density	Standard deviation of density
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gmean_ElectronAffinity	mean_ElectronAffinity	Mean electron affinity
wtd_gmean_ElectronAffinity	wtd_mean_ElectronAffinity	Weighted mean electron affinity
entropy_ElectronAffinity	gmean_ElectronAffinity	Geometric mean electron affinity
wtd_entropy_ElectronAffinity Range of electron affinity  wtd_range_ElectronAffinity Weighted range of electron affinity  wtd_range_ElectronAffinity Weighted range of electron affinity  std_ElectronAffinity Standard deviation of electron affinity  wtd_std_ElectronAffinity Weighted standard deviation of electron affinity  mean_FusionHeat Mean fusion heat  wtd_mean_FusionHeat Weighted mean fusion heat  gmean_FusionHeat Weighted geometric mean fusion heat  wtd_gmean_FusionHeat Entropy of fusion heat  wtd_entropy_FusionHeat Weighted entropy of fusion heat  wtd_entropy_FusionHeat Range of fusion heat  wtd_range_FusionHeat Weighted range of fusion heat  std_FusionHeat Standard deviation of fusion heat  wtd_std_FusionHeat Weighted standard deviation of fusion heat  mean_ThermalConductivity Mean thermal conductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity	wtd_gmean_ElectronAffinity	Weighted geometric mean electron affinity
range_ElectronAffinity	entropy_ElectronAffinity	Entropy of electron affinity
wtd_range_ElectronAffinity	wtd_entropy_ElectronAffinity	Weighted entropy of electron affinity
std_ElectronAffinity  wtd_std_ElectronAffinity  wtd_std_ElectronAffinity  weighted standard deviation of electron affinity  mean_FusionHeat  wtd_mean_FusionHeat  wtd_gmean_FusionHeat  wtd_gmean_FusionHeat  wtd_gmean_FusionHeat  wtd_gmean_FusionHeat  wtd_gmean_FusionHeat  wtd_entropy_FusionHeat  wtd_entropy_FusionHeat  wtd_range_FusionHeat  wtd_range_FusionHeat  wtd_range_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_mean_ThermalConductivity  wtd_mean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity	range_ElectronAffinity	Range of electron affinity
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mean_FusionHeat	std_ElectronAffinity	Standard deviation of electron affinity
wtd_mean_FusionHeat  gmean_FusionHeat  wtd_gmean_FusionHeat  wtd_gmean_FusionHeat  entropy_FusionHeat  wtd_entropy_FusionHeat  wtd_entropy_FusionHeat  wtd_range_FusionHeat  wtd_range_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  mean_ThermalConductivity  wtd_gmean_ThermalConductivity	wtd_std_ElectronAffinity	Weighted standard deviation of electron affinity
gmean_FusionHeat  wtd_gmean_FusionHeat  wtd_gmean_FusionHeat  entropy_FusionHeat  wtd_entropy_FusionHeat  wtd_entropy_FusionHeat  Range of fusion heat  wtd_range_FusionHeat  wtd_range_FusionHeat  wtd_range_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_mean_ThermalConductivity  wtd_mean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivity	mean_FusionHeat	Mean fusion heat
wtd_gmean_FusionHeat wtd_entropy_FusionHeat wtd_entropy_FusionHeat wtd_entropy_FusionHeat wtd_entropy_FusionHeat wtd_range_FusionHeat wtd_range_FusionHeat wtd_range_FusionHeat wtd_std_FusionHeat wtd_std_FusionHeat wtd_std_FusionHeat wtd_mean_ThermalConductivity wtd_mean_ThermalConductivity wtd_gmean_ThermalConductivity	wtd_mean_FusionHeat	Weighted mean fusion heat
entropy_FusionHeat Entropy of fusion heat  wtd_entropy_FusionHeat Weighted entropy of fusion heat  range_FusionHeat Range of fusion heat  wtd_range_FusionHeat Weighted range of fusion heat  std_FusionHeat Standard deviation of fusion heat  wtd_std_FusionHeat Weighted standard deviation of fusion heat  wtd_std_FusionHeat Weighted standard deviation of fusion heat  mean_ThermalConductivity Mean thermal conductivity  wtd_mean_ThermalConductivity Weighted mean thermal conductivity  gmean_ThermalConductivity Geometric mean thermal conductivity  wtd_gmean_ThermalConductivit	gmean_FusionHeat	Geometric mean fusion heat
wtd_entropy_FusionHeat  range_FusionHeat  wtd_range_FusionHeat  wtd_range_FusionHeat  wtd_range_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  weighted standard deviation of fusion heat  mean_ThermalConductivity  wtd_mean_ThermalConductivity  wtd_mean_ThermalConductivity  Geometric mean thermal conductivity  wtd_gmean_ThermalConductivit  wtd_gmean_ThermalConductivit	wtd_gmean_FusionHeat	Weighted geometric mean fusion heat
range_FusionHeat  wtd_range_FusionHeat  wtd_range_FusionHeat  std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  weighted standard deviation of fusion heat  mean_ThermalConductivity  wtd_mean_ThermalConductivity  wtd_mean_ThermalConductivity  wtd_gmean_ThermalConductivity  wtd_gmean_ThermalConductivit  wtd_gmean_ThermalConductivit  ### Conductivity  ### Con	entropy_FusionHeat	Entropy of fusion heat
wtd_range_FusionHeat  std_FusionHeat  wtd_std_FusionHeat  wtd_std_Fusion heat  wtd_std_	wtd_entropy_FusionHeat	Weighted entropy of fusion heat
std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  wtd_std_FusionHeat  weighted standard deviation of fusion heat  mean_ThermalConductivity  wtd_mean_ThermalConductivity  wtd_mean_ThermalConductivity  Geometric mean thermal conductivity  wtd_gmean_ThermalConductivit  wtd_gmean_ThermalConductivit	range_FusionHeat	Range of fusion heat
wtd_std_FusionHeat  mean_ThermalConductivity  wtd_mean_ThermalConductivity  Weighted standard deviation of fusion heat  Mean thermal conductivity  wtd_mean_ThermalConductivity  Weighted mean thermal conductivity  gmean_ThermalConductivity  wtd_gmean_ThermalConductivit	wtd_range_FusionHeat	Weighted range of fusion heat
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wtd_gmean_ThermalConductivit	wtd_mean_ThermalConductivity	Weighted mean thermal conductivity
l	gmean_ThermalConductivity	Geometric mean thermal conductivity
		Weighted geometric mean thermal conductivity

entropy_ThermalConductivity	Entropy of thermal conductivity
wtd_entropy_ThermalConductivi ty	Weighted entropy of thermal conductivity
range_ThermalConductivity	Range of thermal conductivity
wtd_range_ThermalConductivity	Weighted range of thermal conductivity
std_ThermalConductivity	Standard deviation of thermal conductivity
wtd_std_ThermalConductivity	Weighted standard deviation of thermal conductivity
mean_Valence	Mean valence
wtd_mean_Valence	Weighted mean valence
gmean_Valence	Geometric mean valence
wtd_gmean_Valence	Weighted geometric mean valence
entropy_Valence	Entropy of valence
wtd_entropy_Valence	Weighted entropy of valence
range_Valence	Range of valence
wtd_range_Valence	Weighted range of valence
std_Valence	Standard deviation of valence
wtd_std_Valence	Weighted standard deviation of valence
critical_temp	Critical temperature in Kelvin

The remaining column denotes the critical temperature required to achieve a superconductive state, which will be used to define our classes as below.

Critical Temp.	Class	Cases
3.32 <	Class 1	3541
3.32 — 8.40	Class 2	3524
8.40 — 20.00	Class 3	3493
20.00 — 40.57	Class 4	3459
40.57 — 79.00	Class 5	3411
> 79.00	Class 6	3621

The objective of this classification activity is to identify relationships between the elemental variables of materials and the critical temperatures required to achieve a superconductive state. This may help to guide research towards creating superconductive materials which are viable at ambient temperatures.

#### Part 1

The data set was split into 6 dataframes e1, e2, e3, e4, e5, and e6 such that each data frame contained a single class, j, as outlined in the above class definition table. Because our classes were of a similar size. SMOTE or other such oversampling techniques were not required to balance the data set. The "critical\_temp" column was removed from dataframes ej. A new column, "label," was then added containing class identification as CLi to each data frame ei, for i 1 through k = 6. The train test split function was applied to create training sets, train ei. consisting of 80% of observations, and test sets, test ei, containing 20% of observations from each data frame ej. The individual train ej data frames were then concatenated into the data frame train data, and likewise the individual test ej data frames formed the data frame test data. The get dummies function from the Pandas package was applied to the label column for the train data and test data to create the data frames one hot train and one hot test which contained the one-hot encoded categorical variable of class identification. The label columns in both the train data and test data were removed, and columns from the corresponding one-hot encoded frames were added in their respective places. The data frames x train and x test were derived from the test and train data frames by removing the one-hot encoded class information. This class information was isolated to create the *y train* and *y test* data frames.

## Part 2

A sequential model from the TensorFlow package was used to create a multilayer perceptron consisting of three layers. The first layer, L1, accepted an input vector Xn. This was followed by a hidden layer H. The third layer, L3, served as an output layer. The vector of k outputs then passed through the softmax function which translated the values into a probability vector Pn in which Pn(j) was expressed as a value between 0 and 1 that described the likelihood of case n belonging to a particular class j. Case n was determined to belong to the class which expressed the strongest probability. Pn(j) was calculated as the exponential of j divided by the sum of all exponentials of j for a particular case n:

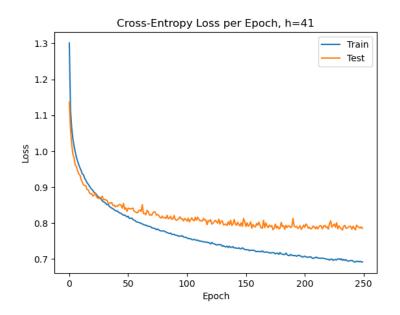
$$Pn(j) = e^{j} / \sum_{i=1}^{k} e^{j}$$

Cross entropy (CRE), is a measure of the difference between two probability distributions, in our case the true CLj, y(n), or  $y\_train(n)$  and  $y\_test(n)$  versus the CLj predicted by Pn. This serves as the loss function in our models and is defined by the below formula:

$$CRE[y(n), Pn] = -y(n) * log(Pn)$$

The cross entropy loss is minimized during the training process to adjust the weights and biases of the model in order to improve its performance. The average cross entropy for the training set,  $train\_avCRE$ , and test set,  $test\_avCRE$ , were defined. The ADAM optimizer was specified as well as the RELU response function. The initial weights were randomized, the number of epochs, m, was set to 150. The batch size of 152 was determined by the count of n cases in

 $train\_data$  divided by 100. The initial value of h, the count of neurons in the hidden layer, was set as half the count of features, p, or 41. Because the training loss showed signs of continuing decline beyond 150 epochs, the number of epochs was extended to 250. The performance of the model as determined by cross entropy loss is displayed in the following graph:

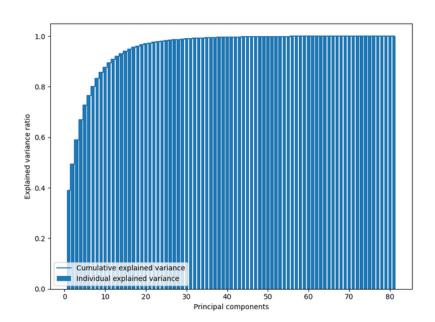


This incurred an additional minute of compute time per 50 epochs or about 0.46 seconds per epoch. Though the training loss continued to decrease beyond 250 epochs, the test loss leveled off leading us to conclude that 250 epochs was the optimal amount,  $m^*$ . The below confusion matrix was generated using the  $test\_data$  by MLP\* which had a number of epochs equal to  $m^*$ .

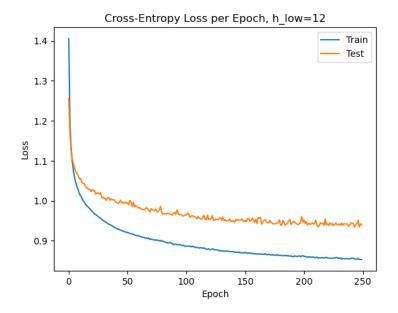
	CL1	CL2	CL3	CL4	CL5	CL6
CL1	80.40	16.23	3.06	0.15	0.00	0.15
CL2	20.99	69.48	8.59	0.79	0.16	0.00
CL3	6.71	18.33	65.96	8.18	0.65	0.16
CL4	1.17	6.23	22.21	60.65	8.44	1.30
CL5	0.28	0.14	5.83	18.86	58.67	16.23
CL6	0.00	0.12	1.09	3.98	22.92	71.89

CL1, materials with critical temperatures less than 3.32°K, exhibited the greatest prediction accuracy while CL5, materials with critical temperatures greater than 40.57°K but less than 79.00°K, had the weakest.

**Part 3**Principal component analysis was performed on the training data, *x\_train*, to identify the number of features which could explain 90% of variance. From this, 12 principal components were determined.



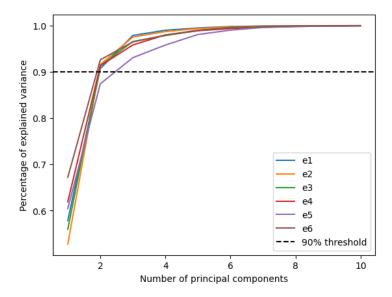
However, prediction accuracy given this reduced count of features was roughly 6-8% less than the complete feature count, and as such, we maintained usage of all 80 features moving forward. Another MLP was created, MLP<sub>LOW</sub>, which was given identical attributes to MLP\* with the exception of the number of neurons in layer H. While the hidden layer of MLP\* was equipped with 41 neurons, MLP<sub>LOW</sub>'s hidden layer was reduced to 12,  $h_{LOW}$ . The results of MLP<sub>LOW</sub> are as below with the confusion matrix pertaining to the *test\_data*:



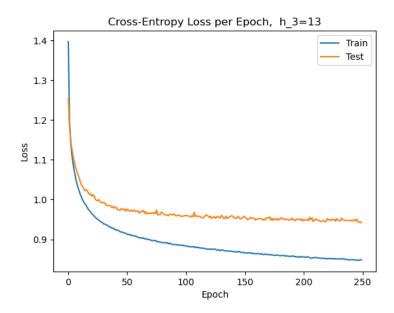
	CL1	CL2	CL3	CL4	CL5	CL6
CL1	72.18	24.16	3.07	0.15	0.15	0.29
CL2	27.01	58.14	13.11	1.26	0.47	0.00
CL3	5.52	20.07	66.30	7.73	0.00	0.37
CL4	1.46	6.89	23.18	60.40	7.42	0.66
CL5	0.36	0.95	6.27	17.63	50.89	23.91
CL6	0.13	0.40	0.93	4.77	25.60	68.17

Part 4

PCA was implemented again, however, separately for each homogenous class data frame ej. The count of principal components that captured 90% of variation for each data frame ej was determined to be 2, with the exception of e5 which had 3 principal components. The sum of principal components, equal to 13, was used to define  $h_{PCA}$ . Using  $h_{PCA}$  as the count of neurons in its hidden layer, MLP<sub>PCA</sub> was created.

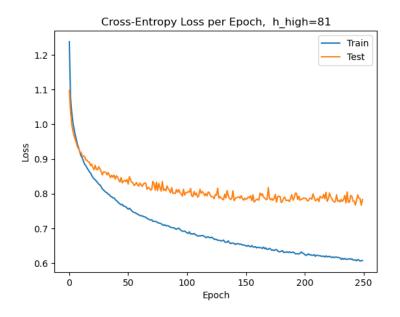


The performance of MLP<sub>3</sub> and corresponding confusion matrix corresponding to the *test\_data* is as follows:



	CL1	CL2	CL3	CL4	CL5	CL6
CL1	72.98	22.20	4.04	0.62	0.16	0.00
CL2	27.56	58.15	13.28	0.72	0.29	0.00
CL3	6.27	18.12	63.94	10.63	0.35	0.70
CL4	1.01	7.07	21.93	61.62	7.36	1.01
CL5	0.38	0.51	6.61	19.82	52.48	20.20
CL6	0.24	0.24	1.22	4.74	26.03	67.52

Because  $h_3$  was less than the initial value of h used in MLP\*, we opted to use the value p to define  $h_{HIGH}$ . The model MLP<sub>HIGH</sub> was then created with a count of neurons  $h_{HIGH}$ , which performed as below along with the confusion matrix for  $test\_data$ :



	CL1	CL2	CL3	CL4	CL5	CL6
CL1	80.23	17.94	1.69	0.14	0.00	0.00
CL2	18.03	71.77	9.01	0.85	0.34	0.00
CL3	3.78	16.79	67.93	10.29	0.76	0.45
CL4	1.23	6.01	19.72	66.41	6.32	0.31
CL5	0.27	0.67	6.48	20.11	57.76	14.71
CL6	0.00	0.12	1.04	4.39	23.90	70.55

The following table presents the performance of each MLP:

MLP	h	т	TRAIN CRE	TEST CRE	TEST Acc. (%)	Compute Time (sec.)
MLP_INIT	41	175	4.1170	0.0002	67.67	37.15
MLP_LOW	12	225	4.1170	0.0002	62.21	34.95
MLP_PCA	13	160	4.5746	0.0002	62.54	35.90
MLP_HIGH	81	160	4.5746	0.0002	69.05	32.92

Based on the table above, we picked MLP\_HIGH as our MLP\* due to its test accuracy and compute time.

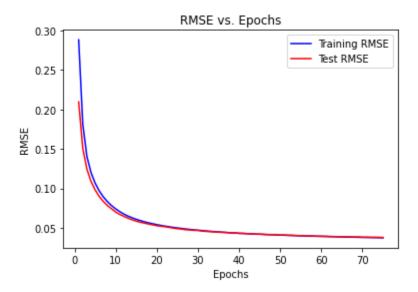
#### Part 5

Sparsity learning is a type of machine learning technique that involves reducing the number of features or weights in a model to improve its efficiency and accuracy. In sparsity learning, a model is trained to identify the most important features or weights in the input data and discard the rest. This approach is particularly useful in situations where the input data has a large number of features or weights that may not be relevant or useful for the task at hand.

Sparsity learning can be achieved through various methods, such as L1 regularization, which adds a penalty term to the loss function that encourages the weights of less important features to be set to zero. Another method is to use feature selection techniques, such as correlation-based feature selection, which identifies features that are highly correlated with the output variable and removes the rest.

Sparsity learning has several advantages, including faster training times, improved generalization performance, and increased interpretability of the model. It is commonly used in applications such as natural language processing, image and signal processing, and recommendation systems.

The **get\_weight()** method was used to obtain the thresholds, *W*, and thresholds, *B*, for MLP<sub>HIGH</sub>. A new model, hidden\_model4, was created with only an input layer and the hidden layer referred from MLP<sub>HIGH</sub> which could be used to define the data frames of activity vectors Zn\_train and Zn\_test for the x\_train and x\_test respectively. These new variables were used to train an autoencoder which could decode the activity vectors. Additionally, a Root Mean Squared Error method was defined to serve as the loss metric for automatic learning, and a Sparse Loss method as the loss function for sparsity learning. The sparsity target was defined as 10% and sparsity weight set to 0.001. The autoencoder was trained on the Zn\_train data frame and validated using the Zn\_test frame. The RMSE for the training and testing was plotted per epoch in the below graph:



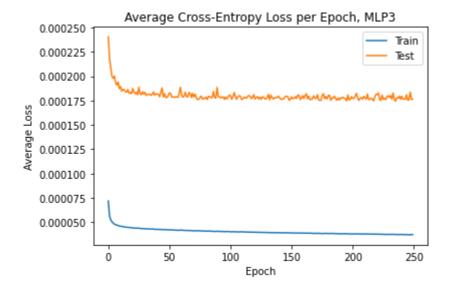
Based on this graph, 70 was selected as our optimal number of epochs,  $m_{AEC}$ . The mean, M, of the norms of the magnitude of Zn over all n cases is 5.8 and it was used to compute the ratio of testing RMSE over M as  $R_{AEC}$ , or 0.0067.

The testRMSE( $m_{AEC}$ ) represents the root mean squared error (RMSE) for a model's predictions on a test set, using the mean absolute error criterion ( $m_{AEC}$ ) as the evaluation metric. The lower the testRMSE( $m_{AEC}$ ), the better the model's performance in predicting the test set.

On the other hand, M represents the mean of the norms ||Zn|| over all cases #n. The norms ||Zn|| measure the magnitude of a vector, and taking the mean over all cases #n provides an overall measure of the "size" of the vectors. The ratio  $R_{AEC}$  can be interpreted as the ratio of the model's performance on the test set, as measured by testRMSE( $m_{AEC}$ ), relative to the overall "size" of the vectors, as measured by M. A lower value of  $R_{AEC}$  suggests that the model's performance is relatively good compared to the "size" of the vectors.

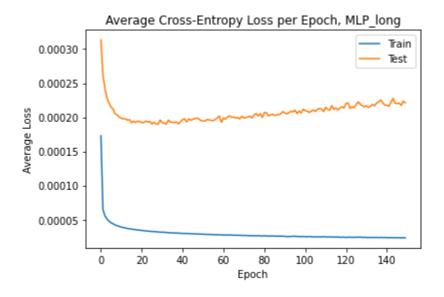
In this case, we have  $R_{AEC}$  = 0.0067, indicating that the model's performance on the test set, as measured by testRMSE(m<sub>AEC</sub>), is quite good relative to the overall "size" of the vectors, as measured by M.

We applied  $MLP_{12}$  to an original input vector Xn of dimension p, the activity of hidden layer H becomes vector Zn of dimension h=  $h_{high}$ , and the activity of layer K becomes a vector U\_n of dimension dimK=  $h_{high}$ . We now use each U\_n as a new input vector describing the case "n". These new input vectors are going to be used to train a new classifier,  $MLP_3$ , which has the test accuracy of 70.83% as the figure and confusion matrix regarding *test\_data* below:



	CL1	CL2	CL3	CL4	CL5	CL6
CL1	77.86	20.12	1.74	0.14	0	0.14
CL2	16.64	73.71	8.99	0.33	0.33	0
CL3	3.48	15.38	71.41	8.71	0.29	0.73
CL4	0.3	4.96	19.85	68.72	5.26	0.9
CL5	0.38	1.65	5.47	20.61	55.85	16.03
CL6	0	0	0.64	1.93	20.57	76.86

Now we build another model which is  $MLP_{LONG}$ . It is the concatenation of  $MLP_{12}$  and  $MLP_{3}^{*}$  with classifier with 3 hidden layers H,K,G: L1 -> H-> K ->G -> OUT -> softmax.Our  $MLP_{LONG}$  model has the test accuracy of 72.63% and has performance like below:



The final result of our model are show as the table blow:

MLP	m	TEST Acc. (%)	Compute Time(sec)
MLP_INIT	175	66.37	37.15
MLP_LOW	225	61.69	34.95
MLP_PCA	160	61.93	35.90
MLP_HIGH	160	68.57	32.92
MLP3	18	70.48	24.30
MLP_LONG	18	70.45	29.88

The compute times shown are the average computation time per epoch, multiplied by m, the ideal stopping epoch. As we can see,  $MLP_{LONG}$  and MLP3 have almost the same accuracy, therefore they are our best performance models of every model we built. However, due to the additional layers of  $MLP_{LONG}$ , which increase computing time, MLP3 is selected as our best model overall.

Q0:

#### **Code Part**

```
import pandas as pd
import numpy as np
import tensorflow as tf
from sklearn.metrics import log loss
from sklearn.model selection import train test split
from sklearn.metrics import accuracy_score
from sklearn.neural network import MLPClassifier
from sklearn.preprocessing import OneHotEncoder, StandardScaler
data = pd.read_csv("train.csv")
data = data.dropna()
quantiles = np.quantile(data["critical temp"], np.arange(0, 1.1, 0.1))
e1 = data[data["critical_temp"] < 3.32]
e2 = data[(data["critical_temp"] > 3.32) & (data["critical_temp"] < 8.4)]
e3 = data[(data["critical_temp"] > 8.4) & (data["critical_temp"] < 20)]
e4 = data[(data["critical temp"] > 20) & (data["critical temp"] < 40.56667)]
e5 = data[(data["critical_temp"] > 40.56667) & (data["critical_temp"] < 79)]
e6 = data[data["critical temp"] > 79]
column names = pd.DataFrame(data.columns)
data.head()
# Add class labels, drop temperature
e1["label"] = "CL1"
e1 = e1.drop("critical_temp", axis=1)
e2["label"] = "CL2"
e2 = e2.drop("critical_temp", axis=1)
e3["label"] = "CL3"
e3 = e3.drop("critical_temp", axis=1)
e4["label"] = "CL4"
e4 = e4.drop("critical_temp", axis=1)
e5["label"] = "CL5"
e5 = e5.drop("critical_temp", axis=1)
```

```
e6["label"] = "CL6"
e6 = e6.drop("critical_temp", axis=1)
e1.head()
Q1:
#Q1: We dont need to use SMOTE and one-hot encoding
# Randomly select 80% of cases from each class to create the training set
train e1, test e1 = train test split(e1, test size=0.2, random state=42)
train e2, test e2 = train test split(e2, test size=0.2, random state=42)
train e3, test e3 = train test split(e3, test size=0.2, random state=42)
train e4, test e4 = train test split(e4, test size=0.2, random state=42)
train_e5, test_e5 = train_test_split(e5, test_size=0.2, random_state=42)
train e6, test e6 = train test split(e6, test size=0.2, random state=42)
# Concatenate the training and test sets for each class to create the final TRAIN and TEST sets
train data = pd.concat([train e1, train e2, train e3, train e4, train e5, train e6])
test data = pd.concat([test e1, test e2, test e3, test e4, test e5, test e6])
# One-hot encoding
# train data
one hot train = pd.get dummies(train data["label"])
train data = train data.drop("label", axis=1)
train_data = pd.concat([train_data, one hot train], axis=1)
# test data
one hot test = pd.get dummies(test data["label"])
test_data = test_data.drop("label", axis=1)
test data = pd.concat([test data, one hot test], axis=1)
train_data.head()
#Q2:
# Split the dataset into features and target variable
en_col = ["CL1", "CL2", "CL3", "CL4", "CL5", "CL6"]
x train = train data.drop(en col, axis=1)
y train = train data[en col]
x test = test data.drop(en col, axis=1)
y_test = test_data[en_col]
# Standardize the features
scaler = StandardScaler()
```

```
x train = pd.DataFrame(scaler.fit transform(x train))
x test = pd.DataFrame(scaler.transform(x test))
x train.head()
from tensorflow.keras.initializers import RandomUniform
import time
# Validation Split
x train1, x valid, y train1, y valid = train test split(x train, y train, test size=0.1)
# Define the model
model = tf.keras.Sequential([
  tf.keras.layers.Dense(41, activation='relu', input_shape=(x_train.shape[1],),
kernel initializer=RandomUniform),
  tf.keras.layers.Dense(y train.shape[1], activation='softmax')
1)
# Compile the model
model.compile(optimizer='adam', loss='categorical crossentropy', metrics=['accuracy'])
# Train the model
start time = time.time()
history = model.fit(x train1, y train1, batch size=152, epochs=175, verbose=0,
validation_data=(x_valid,y_valid))
end time = time.time()
time per epoch = (end time - start time) / len(history.history['loss'])
# Calculate average cross-entropy loss for train and test sets
train preds = model.predict(x_train)
train_avCRE = log_loss(y_train, train_preds) / len(x_train)
test_preds = model.predict(x_test)
test_avCRE = log_loss(y_test, test_preds) / len(x_test)
# Extract the training and validation losses for each epoch
train losses per epoch = history.history['loss']
test losses per epoch = history.history['val loss']
# Calculate the average cross-entropy loss per epoch for train and test sets
train avCRE per epoch = [loss / len(x train) for loss in train losses per epoch]
```

```
test avCRE per epoch = [loss / len(x test) for loss in test losses per epoch]
print("Average Cross Entropy Loss for Train Set:", train avCRE)
print("Average Cross Entropy Loss for Test Set:", test_avCRE)
print("Average Cross Entropy Loss per Epoch for Train Set:", train avCRE per epoch)
print("Average Cross Entropy Loss per Epoch for Test Set:", test avCRE per epoch)
print("Computing time per epoch: ", time per epoch)
# 150 epochs was originally used, but the accuracy of the training set was still
# continuing to decrease, so I bumped it up to 200
# Computation time for 150 epochs: ~3.5 min
# Computation time for 200 epochs: ~4.5 min
# Computation time for 250 epochs: ~5.5 min
# We will use 150 epochs going forward. Test accuracy levels off at around this point.
# 200 and 250 epochs were computed to make sure no accuracy gains were left on the table.
import matplotlib.pyplot as plt
# Plot the loss per epoch
plt.plot(train losses per epoch, label='Train')
plt.plot(test_losses_per_epoch, label='Test')
plt.title('Cross-Entropy Loss per Epoch, h=41')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.show()
# Evaluate the model on the test set
test_loss, test_accuracy = model.evaluate(x_test, y_test, verbose=0)
print("Test Accuracy: {:.2f}%".format(test_accuracy * 100))
round(x train1.shape[0]/100, 0)
# Create and print the confusion matrix.
from sklearn.metrics import confusion matrix
test pred labels = np.argmax(test preds, axis=1)
y test array = y test.to numpy()
y test labels = np.argmax(y test array, axis=1)
# Compute the confusion matrix
```

```
conf matrix = confusion matrix(test pred labels,y test labels)
# Normalize the confusion matrix
normalized conf matrix = conf matrix.astype('float') / conf matrix.sum(axis=1)[:, np.newaxis]
# Convert to percentage
percentage_conf_matrix = normalized conf matrix * 100
print("Confusion Matrix (Percentage):")
print("Confusion Matrix (Percentage):")
for row in percentage conf matrix:
  formatted row = ["{:.2f}".format(x) for x in row]
  print(" ".join(formatted_row))
Q3:
from sklearn.decomposition import PCA
# Create a PCA object with 90% variance explained
pca = PCA(n components=0.9)
# Fit the PCA model on the training data
pca.fit(x train)
# Transform the training data into the new feature space
x_train_pca = pca.transform(x_train)
x_test_pca = pca.transform(x_test)
x_train_pca = pd.DataFrame(x_train_pca)
x test pca = pd.DataFrame(x test pca)
# Print the shape of the transformed data
print("Shape of transformed data:", x train pca.shape)
# Create a PCA object
pca = PCA()
# Fit the PCA model on the training data
pca.fit(x train)
# Compute the cumulative sum of explained variance
var exp = np.cumsum(pca.explained variance ratio )
# Create a bar plot of explained variance vs. number of components
```

```
plt.figure(figsize=(8, 6))
plt.bar(range(1, len(var exp) + 1), var exp, align='center', label='Individual explained variance')
plt.step(range(1, len(var_exp) + 1), var_exp, where='mid', label='Cumulative explained
variance')
plt.ylabel('Explained variance ratio')
plt.xlabel('Principal components')
plt.legend(loc='best')
plt.tight_layout()
plt.show()
# Validation Split
x train2, x valid, y train2, y valid = train test split(x train, y train, test size=0.1)
# Define the model
model2 = tf.keras.Sequential([
  tf.keras.layers.Dense(12, activation='relu', input shape=(x train.shape[1],),
kernel initializer=RandomUniform),
  tf.keras.layers.Dense(y train.shape[1], activation='softmax')
])
# Compile the model
model2.compile(optimizer='adam', loss='categorical crossentropy', metrics=['accuracy'])
# Train the model
start time = time.time()
history2 = model2.fit(x train2, y train2, batch size=152, epochs=225, verbose=0,
validation_data=(x_valid,y_valid))
end_time = time.time()
time per epoch2 = (end time - start time) / len(history2.history['loss'])
# Calculate average cross-entropy loss for train and test sets
train preds2 = model2.predict(x train)
train_avCRE2 = log_loss(y_train, train_preds2) / len(x_train)
test_preds2 = model2.predict(x_test)
test avCRE2 = \log \log(y \text{ test, test preds2}) / \ln(x \text{ test})
# Extract the training and validation losses for each epoch
train losses per epoch2 = history2.history['loss']
test losses per epoch2 = history2.history['val loss']
```

```
# Calculate the average cross-entropy loss per epoch for train and test sets
train avCRE per epoch2 = [loss / len(x train) for loss in train losses per epoch2]
test avCRE per epoch2 = [loss / len(x test) for loss in test losses per epoch2]
print("Average Cross Entropy Loss for Train Set:", train_avCRE2)
print("Average Cross Entropy Loss for Test Set:", test avCRE2)
print("Average Cross Entropy Loss per Epoch for Train Set:", train avCRE per epoch2)
print("Average Cross Entropy Loss per Epoch for Test Set:", test avCRE per epoch2)
print("Computing time per epoch: ", time per epoch2)
# Plot the loss per epoch
plt.plot(train losses per epoch2, label='Train')
plt.plot(test losses per epoch2, label='Test')
plt.title('Cross-Entropy Loss per Epoch, h low=12')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.show()
# Evaluate the model on the test set
test loss2, test accuracy2 = model2.evaluate(x test, v test, verbose=0)
print("Test Accuracy: {:.2f}%".format(test accuracy2 * 100))
# Need to work out why this model has over 100% accuracy. Will come back to it.
# There is a higher loss than the first model, but not by much.
test_pred_labels2 = np.argmax(test_preds2, axis=1)
# Compute the confusion matrix
conf matrix2 = confusion matrix(test pred labels2,y test labels)
# Normalize the confusion matrix
normalized conf matrix2 = conf_matrix2.astype('float') / conf_matrix2.sum(axis=1)[:,
np.newaxis]
# Convert to percentage
percentage conf matrix2 = normalized conf matrix2 * 100
```

```
print("Confusion Matrix (Percentage):")
print("Confusion Matrix (Percentage):")
for row in percentage conf matrix2:
  formatted row = ["{:.2f}".format(x) for x in row]
  print(" ".join(formatted_row))
Q4:
from sklearn.decomposition import PCA
# Define the variance threshold
var threshold = 0.9
# Loop through each dataframe and perform PCA on numeric columns
for i, df in enumerate([e1, e2, e3, e4, e5, e6]):
  numeric df = df.select dtypes(include=['float64', 'int64'])
  pca = PCA(n components=var threshold)
  pca.fit(numeric df)
  n components = pca.n components
  print(f"Number of features that capture 90% of the variance for e{i+1}: {n_components}")
# Our variance is highly concentrated to only a few features for every class.
# h1 + h2 ... = 13, which is the same dimension used for h low.
# Going to use h=p where p is the total number of features for h_high
# Define the variance threshold
var_{threshold} = 0.9
# Define the number of principal components to try
max components = 10
# Loop through each dataframe and perform PCA on numeric columns
for i, df in enumerate([e1, e2, e3, e4, e5, e6]):
  numeric_df = df.select_dtypes(include=['float64', 'int64'])
  pca = PCA(n components=max components)
  pca.fit(numeric df)
  var_ratio = pca.explained_variance_ratio_
  cum var ratio = np.cumsum(var ratio)
  n components = np.argmax(cum var ratio >= var threshold) + 1
  plt.plot(np.arange(1, max components+1), cum var ratio, label=f'e{i+1}')
plt.xlabel('Number of principal components')
plt.ylabel('Percentage of explained variance')
plt.axhline(y=var threshold, color='black', linestyle='--', label=f'{var threshold:.0%} threshold')
```

```
plt.legend()
plt.show()
# Validation Split
x_train3, x_valid, y_train3, y_valid = train_test_split(x_train, y_train, test_size=0.1)
# Define the model
model3 = tf.keras.Sequential([
  tf.keras.layers.Dense(13, activation='relu', input shape=(x train.shape[1],),
kernel initializer=RandomUniform),
  tf.keras.layers.Dense(y train.shape[1], activation='softmax')
1)
# Compile the model
model3.compile(optimizer='adam', loss='categorical crossentropy', metrics=['accuracy'])
# Train the model
start time = time.time()
history3 = model3.fit(x_train3, y_train3, batch_size=152, epochs=160, verbose=0,
validation_data=(x_valid,y_valid))
end time = time.time()
time_per_epoch3 = (end_time - start_time) / len(history3.history['loss'])
# Calculate average cross-entropy loss for train and test sets
train preds3 = model3.predict(x train)
train avCRE3 = log loss(y train, train preds3) / len(x train)
test_preds3 = model3.predict(x_test)
test avCRE3 = \log \log(y \text{ test, test preds3}) / \ln(x \text{ test})
# Extract the training and validation losses for each epoch
train losses per epoch3 = history3.history['loss']
test_losses_per_epoch3 = history3.history['val_loss']
# Calculate the average cross-entropy loss per epoch for train and test sets
train avCRE per epoch3 = [loss / len(x train) for loss in train losses per epoch3]
test avCRE per epoch3 = [loss / len(x test) for loss in test losses per epoch3]
print("Average Cross Entropy Loss for Train Set:", train avCRE3)
print("Average Cross Entropy Loss for Test Set:", test avCRE3)
```

```
print("Average Cross Entropy Loss per Epoch for Train Set:", train avCRE per epoch3)
print("Average Cross Entropy Loss per Epoch for Test Set:", test avCRE per epoch3)
print("Computing time per epoch: ", time_per_epoch3)
# Plot the loss per epoch
plt.plot(train losses per epoch3, label='Train')
plt.plot(test losses per epoch3, label='Test')
plt.title('Cross-Entropy Loss per Epoch, h 3=13')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.show()
# Evaluate the model on the test set
test_loss3, test_accuracy3 = model3.evaluate(x_test, y_test, verbose=0)
print("Test Accuracy: {:.2f}%".format(test_accuracy3 * 100))
test pred labels3 = np.argmax(test preds3, axis=1)
# Compute the confusion matrix
conf matrix3 = confusion matrix(test pred labels3,y test labels)
# Normalize the confusion matrix
normalized conf matrix3 = conf matrix3.astype('float') / conf matrix3.sum(axis=1)[:,
np.newaxis]
# Convert to percentage
percentage_conf_matrix3 = normalized_conf_matrix3 * 100
print("Confusion Matrix (Percentage):")
print("Confusion Matrix (Percentage):")
for row in percentage conf matrix3:
  formatted_row = ["{:.2f}".format(x) for x in row]
  print(" ".join(formatted row))
# Validation Split
x train4, x valid, y train4, y valid = train test split(x train, y train, test size=0.1)
# Define the model
model4 = tf.keras.Sequential([
```

```
tf.keras.layers.Dense(81, activation='relu', input shape=(x train.shape[1],),
kernel initializer=RandomUniform),
  tf.keras.layers.Dense(y_train.shape[1], activation='softmax')
1)
# Compile the model
model4.compile(optimizer='adam', loss='categorical crossentropy', metrics=['accuracy'])
# Train the model
start time = time.time()
history4 = model4.fit(x_train4, y_train4, batch_size=152, epochs=160, verbose=0,
validation_data=(x_valid,y_valid))
end time = time.time()
time per epoch4 = (end time - start time) / len(history4.history['loss'])
# Calculate average cross-entropy loss for train and test sets
train preds4 = model4.predict(x train)
train_avCRE4 = log_loss(y_train, train_preds4) / len(x_train)
test_preds4 = model4.predict(x_test)
test avCRE4 = log loss(v test, test preds4) / len(x test)
# Extract the training and validation losses for each epoch
train losses per epoch4 = history4.history['loss']
test losses per epoch4 = history4.history['val loss']
# Calculate the average cross-entropy loss per epoch for train and test sets
train avCRE_per_epoch4 = [loss / len(x_train) for loss in train_losses_per_epoch4]
test avCRE per epoch4 = [loss / len(x test) for loss in test losses per epoch4]
print("Average Cross Entropy Loss for Train Set:", train avCRE4)
print("Average Cross Entropy Loss for Test Set:", test avCRE4)
print("Average Cross Entropy Loss per Epoch for Train Set:", train_avCRE_per_epoch4)
print("Average Cross Entropy Loss per Epoch for Test Set:", test_avCRE_per_epoch4)
print("Computing time per epoch: ", time per epoch4)
# Plot the loss per epoch
plt.plot(train losses per epoch4, label='Train')
```

```
plt.plot(test losses per epoch4, label='Test')
plt.title('Cross-Entropy Loss per Epoch, h high=81')
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.legend()
plt.show()
# Evaluate the model on the test set
test loss4, test accuracy4 = model4.evaluate(x test, y test, verbose=0)
print("Test Accuracy: {:.2f}%".format(test_accuracy4 * 100))
test_pred_labels4 = np.argmax(test_preds4, axis=1)
# Compute the confusion matrix
conf matrix4 = confusion matrix(test pred labels4,y test labels)
# Normalize the confusion matrix
normalized conf matrix4 = conf matrix4.astype('float') / conf matrix4.sum(axis=1)[:,
np.newaxis]
# Convert to percentage
percentage conf matrix4 = normalized conf matrix4 * 100
print("Confusion Matrix (Percentage):")
print("Confusion Matrix (Percentage):")
for row in percentage conf matrix4:
  formatted_row = ["{:.2f}".format(x) for x in row]
  print(" ".join(formatted row))
Q5:
# Define the model, this time with seperate objects for each layer
input_layer = tf.keras.lnput(shape=(x_train.shape[1],))
hidden layer = tf.keras.layers.Dense(81, activation='sigmoid',
kernel initializer=RandomUniform)(input layer)
output_layer = tf.keras.layers.Dense(y_train.shape[1], activation='softmax')(hidden_layer)
mlp high = tf.keras.Model(inputs=input layer, outputs=output layer)
# Compile the model
mlp high.compile(optimizer='adam', loss='categorical crossentropy', metrics=['accuracy'])
# Train the model
```

```
history = mlp high.fit(x train, y train, batch size=42, epochs=150, verbose=0,
validation_data=(x_test,y_test))
# Create new model to study the hidden layer
hidden_layer_model = tf.keras.Model(inputs=mlp_high.input, outputs=mlp_high.layers[1].output)
# Compute Zn for each case in x train
Zn train = hidden layer model.predict(x train)
Zn test = hidden layer model.predict(x test)
latent dim = 81
input dim = 81
sparsity_target = 0.1
sparsity_weight = 1e-3
class Autoencoder(tf.keras.Model):
  def init (self, latent dim, input dim):
     super(Autoencoder, self). init ()
     self.latent dim = latent dim
     self.encoder = tf.keras.Sequential([
       tf.keras.layers.lnput(shape=(input dim,)),
       tf.keras.layers.Dense(latent_dim, activation='sigmoid'),
    ])
     self.decoder = tf.keras.Sequential([
       tf.keras.layers.Dense(input dim, activation='sigmoid'),
    ])
  def call(self, x):
     encoded = self.encoder(x)
     decoded = self.decoder(encoded)
     return decoded
autoencoder = Autoencoder(latent_dim, input_dim)
# Define RMSE as a custom metric
def rmse(y_true, y_pred):
  return tf.sqrt(tf.reduce_mean(tf.square(y_pred - y_true)))
# Define the KL divergence sparsity penalty
def kl divergence(p, p hat):
  return p * tf.math.log(p / p_hat) + (1 - p) * tf.math.log((1 - p) / (1 - p_hat))
```

```
# Define the sparse loss function
def sparse_loss(y_true, y_pred):
  mse loss = tf.reduce_mean(tf.square(y_pred - y_true))
  hidden_layer = autoencoder.encoder(y_true)
  p hat = tf.reduce mean(hidden layer, axis=0)
  sparsity loss = tf.reduce sum(kl divergence(sparsity target, p hat))
  total_loss = mse_loss + sparsity_weight * sparsity_loss
  return total loss
autoencoder.compile(optimizer='adam', loss=sparse loss, metrics=[rmse])
history_aec = autoencoder.fit(Zn_train, Zn_train,
                   epochs=75,
                   shuffle=True,
                   validation data=(Zn test, Zn test),
                   verbose=1)
train rmse = history aec.history['rmse']
val rmse = history aec.history['val rmse']
epochs = range(1, len(train_rmse) + 1)
plt.plot(epochs, train rmse, 'b', label='Training RMSE')
plt.plot(epochs, val rmse, 'r', label='Test RMSE')
plt.xlabel('Epochs')
plt.ylabel('RMSE')
plt.legend()
plt.title('RMSE vs. Epochs')
plt.show()
# Copy and paste model3 from other file
# Define the model
model3 = tf.keras.Sequential([
  tf.keras.layers.Dense(81, activation='relu', input_shape=(x_train.shape[1],),
kernel initializer=RandomUniform),
  tf.keras.layers.Dense(y train.shape[1], activation='softmax')
])
# Compile the model
model3.compile(optimizer='adam', loss='categorical crossentropy', metrics=['accuracy'])
```

```
# Train the model
history3 = model3.fit(x train, y train, batch size=42, epochs=150, verbose=0,
validation_data=(x_test,y_test))
# Extract weights and biases from the first dense layer of model3 and the encoder
model3 dense1 weights, model3 dense1 biases = model3.layers[0].get weights()
encoder weights, encoder biases = autoencoder.encoder.layers[0].get weights()
# Verify that the weights and biases have the same dimensions
print("Model3 Weights Size: ", model3 dense1 weights.shape)
print("Model3 Biases Size: ", model3 dense1 biases.shape)
print("Encoder Weights Size: ", encoder_weights.shape)
print("Encoder Biases Size: ", encoder_biases.shape)
Zn combined = np.concatenate((Zn train, Zn test), axis=0)
# Define the modified MLP 12 model
MLP 12 = tf.keras.Sequential([
  model3.layers[0],
  autoencoder.encoder,
  tf.keras.layers.Dense(81, activation='linear') # Change the output dimension to 82
])
# Compile the modified model
MLP 12.compile(optimizer='adam', loss='mse')
# Train the modified model
history MLP 12 = MLP 12.fit(x train, Zn train,
                 batch size=42,
                 epochs=150,
                 verbose=0.
                 validation_data=(x_test, Zn_test))
# Combine x train and x test
x_combined = np.concatenate((x_train, x_test), axis=0)
y combined = np.concatenate((y train, y test), axis=0)
# Predict the output using the modified MLP 12 model
U n = MLP 12.predict(x combined)
# Split the U n dataset into training and test sets (80/20)
```

```
U n train, U n test, y train new, y test new = train test split(U n, y combined,
test size=0.2, random state=42)
U_n.shape
# Define the MLP3 model
MLP3 = tf.keras.Sequential([
  tf.keras.layers.lnput(shape=(U_n_train.shape[1],)),
  tf.keras.layers.Dense(40, activation='relu'),
  tf.keras.layers.Dense(y train.shape[1], activation='softmax')
1)
# Compile the MLP3 model
MLP3.compile(optimizer='adam', loss='categorical_crossentropy', metrics=['accuracy'])
# Train the MLP3 model
history MLP3 = MLP3.fit(U n train, y train new,
              batch size=42,
              epochs=250,
              verbose=0,
              validation data=(U n test, y test new))
train preds = MLP3.predict(U n train)
train avCRE = log loss(y train new, train preds) / len(U n train)
test_preds = MLP3.predict(U_n_test)
test avCRE = log loss(y test new, test preds) / len(U n test)
# Extract the training and validation losses for each epoch
train losses per epoch = history MLP3.history['loss']
test_losses_per_epoch = history_MLP3.history['val_loss']
# Calculate the average cross-entropy loss per epoch for train and test sets
train_avCRE_per_epoch = [loss / len(U_n_train) for loss in train_losses_per_epoch]
test avCRE per epoch = [loss / len(U n test) for loss in test losses per epoch]
print("Average Cross Entropy Loss for Train Set:", train avCRE)
print("Average Cross Entropy Loss for Test Set:", test avCRE)
print("Average Cross Entropy Loss per Epoch for Train Set:", train avCRE per epoch)
print("Average Cross Entropy Loss per Epoch for Test Set:", test avCRE per epoch)
plt.plot(train avCRE per epoch, label='Train')
plt.plot(test avCRE per epoch, label='Test')
```

```
plt.title('Average Cross-Entropy Loss per Epoch, MLP3')
plt.xlabel('Epoch')
plt.ylabel('Average Loss')
plt.legend()
plt.show()
# Evaluate the MLP3 model on the U n test set
test loss MLP3, test accuracy MLP3 = MLP3.evaluate(U n test, y test new, verbose=0)
print("Test Accuracy: {:.2f}%".format(test accuracy MLP3 * 100))
# Create and print the confusion matrix.
test_pred_labels = np.argmax(test_preds, axis=1)
y test array = y test new
y_test_labels = np.argmax(y_test_array, axis=1)
# Compute the confusion matrix
conf matrix = confusion matrix(test pred labels, y test labels)
# Normalize the confusion matrix
normalized conf matrix = conf matrix.astype('float') / conf matrix.sum(axis=1)[:, np.newaxis]
# Convert to percentage
percentage conf matrix = normalized conf matrix * 100
print("Confusion Matrix (Percentage):")
print("Confusion Matrix (Percentage):")
for row in percentage_conf_matrix:
  formatted row = ["{:.2f}".format(x) for x in row]
  print(" ".join(formatted_row))
MLP_long = tf.keras.Sequential([
  MLP 12.layers[0], # First hidden layer from MLP 12
  MLP_12.layers[1], # Second hidden layer (output layer of MLP_12)
  MLP3.layers[0], #
  MLP3.layers[1], # Third hidden layer from MLP3
])
# Compile the MLP long model
MLP long.compile(optimizer='adam', loss='categorical_crossentropy', metrics=['accuracy'])
# Train the MLP long model
```

```
history MLP long = MLP long.fit(x train, y train,
                   batch size=42,
                   epochs=50,
                   verbose=0.
                   validation_data=(x_test, y_test))
train preds long = MLP long.predict(x train)
train avCRE long = log loss(y train, train preds long) / len(x train)
test preds long = MLP long.predict(x test)
test avCRE long = log loss(y test, test preds long) / len(x test)
# Extract the training and validation losses for each epoch
train losses per epoch long = history MLP long.history['loss']
test losses per epoch long = history MLP long.history['val loss']
# Calculate the average cross-entropy loss per epoch for train and test sets
train avCRE per epoch long = [loss / len(x train) for loss in train losses per epoch long]
test_avCRE_per_epoch_long = [loss / len(x_test) for loss in test_losses_per_epoch_long]
print("Average Cross Entropy Loss for Train Set:", train avCRE long)
print("Average Cross Entropy Loss for Test Set:", test avCRE long)
print("Average Cross Entropy Loss per Epoch for Train Set:", train avCRE per epoch long)
print("Average Cross Entropy Loss per Epoch for Test Set:", test_avCRE_per_epoch_long)
plt.plot(train avCRE per epoch long, label='Train')
plt.plot(test avCRE per epoch long, label='Test')
plt.title('Average Cross-Entropy Loss per Epoch, MLP long')
plt.xlabel('Epoch')
plt.ylabel('Average Loss')
plt.legend()
plt.show()
# Evaluate the MLP3 model on the U n test set
test_loss_long, test_accuracy_long = MLP_long.evaluate(x_test, y_test, verbose=0)
print("Test Accuracy: {:.2f}%".format(test accuracy long * 100))
```