Homework 1

Deep Learning

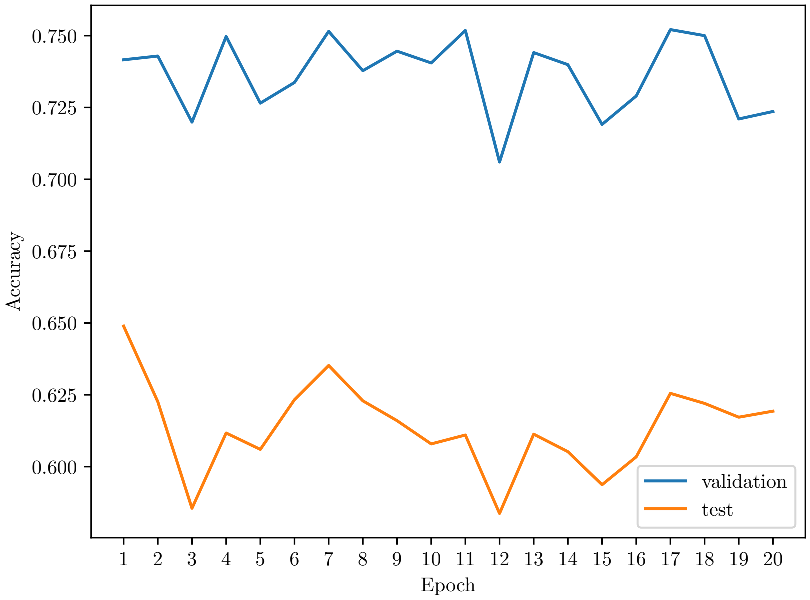
Duarte Calado de Almeida
95565

André Lopes Rodrigues
96576

Question 1

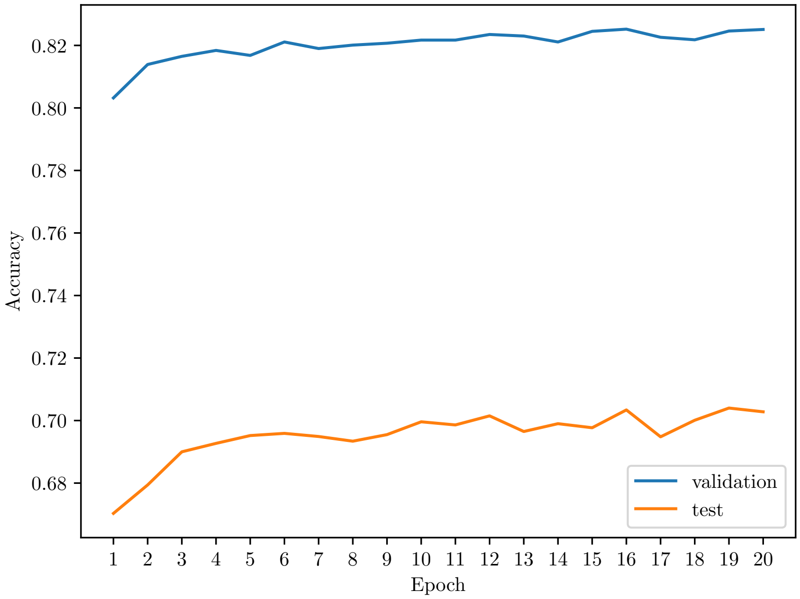
1. (a)

Final accuracy on validation set: 0.7236
Final accuracy on test set: 0.6193



(b)

Final accuracy on validation set: 0.8251
Final accuracy on test set: 0.7028

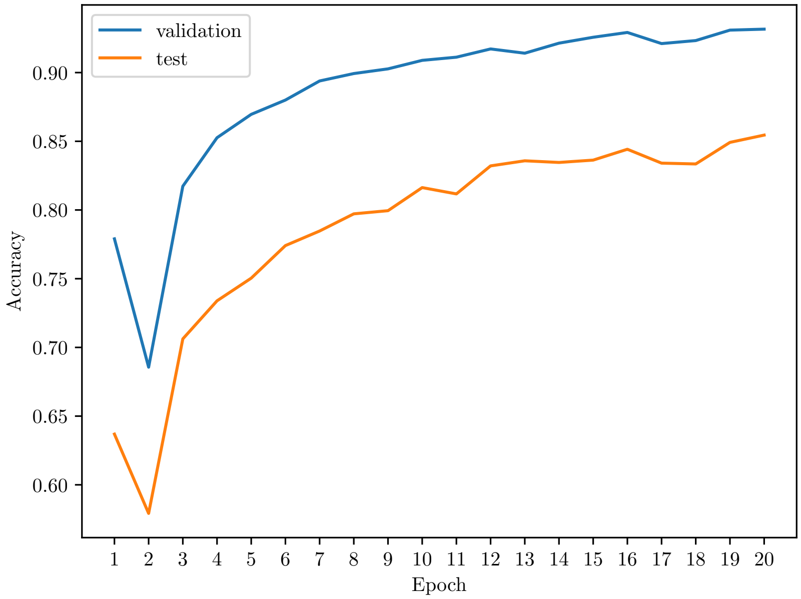


2. (a) The use of multilayer perceptrons provide a form of **representation learing** through the composition of multiclass perceptrons with non-linear activation functions; in particular, they are able to search through some subspace of feature transformations and find one for which the linear separation of data is easier. In practical terms, this layering provides **hierarchical compositionality**, i.e., each layer encodes a distributed representation that is more abstract the closer it is to the output layer, finding meaningful features at different levels of granularity.
In the context of character recognition, MLPs are usually able to successively detect features of symbols (i.e., edges and parts), combine them in coarser features and perform an accurate classification at the end. This is usually not the case if we use simple perceptrons, as plain linear combinations of grayscale values are less capable of detecting those distinctive features and be flexible to the variability that the same character may show.
Nevertheless, an MLP that uses linear activation functions ($g(z) = z$) **does not display this feature**, it corresponds to a linear classifier, effectively functioning like a simple perceptron:

$$\begin{aligned}
\boldsymbol{f}(\boldsymbol{x}) &= g(\boldsymbol{z}^{(L+1)}) = \boldsymbol{z}^{(L+1)} \\
&= \boldsymbol{W}^{(L+1)}\boldsymbol{h}^{(L)} + \boldsymbol{b}^{(L+1)} \\
&= \boldsymbol{W}^{(L+1)}(\boldsymbol{W}^{(L)}\boldsymbol{h}^{(L-1)} + \boldsymbol{b}^{(L)}) + \boldsymbol{b}^{(L+1)} \\
&\qquad \dots \\
&= \boldsymbol{W}^{(L+1)}(\boldsymbol{W}^{(L)}(\dots\ (\boldsymbol{W}^{(1)}\boldsymbol{x} + \boldsymbol{b}^{(1)})) + \boldsymbol{b}^{(L)}) + \boldsymbol{b}^{(L+1)} \\
&= \underbrace{\boldsymbol{W}^{(L+1)}\dots\boldsymbol{W}^{(1)}}_{\widetilde{\boldsymbol{W}}}\boldsymbol{x} + \underbrace{\boldsymbol{W}^{(L+1)}\dots\boldsymbol{W}^{(2)}\boldsymbol{b}^{(1)} + \dots + \boldsymbol{W}^{(L+1)}\boldsymbol{b}^{(L)} + \boldsymbol{b}^{(L+1)}}_{\widetilde{\boldsymbol{b}}}
\end{aligned}$$

(b)

Final accuracy on validation set: 0.9316
Final accuracy on test set: 0.8545

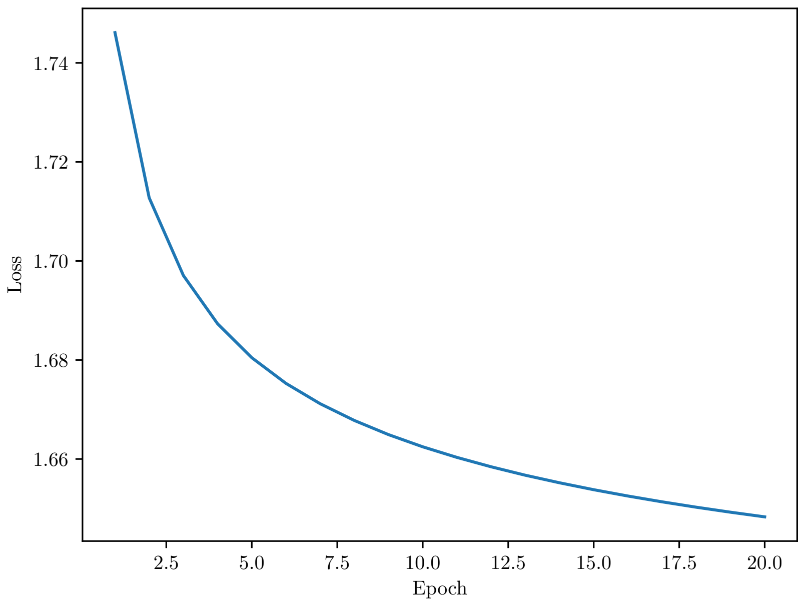


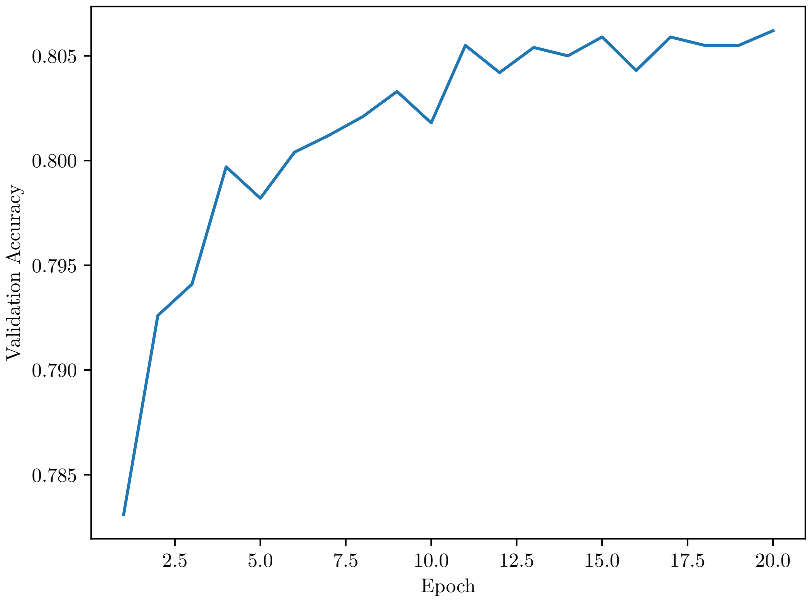
Question 2

1. The best configuration in terms of **validation accuracy** is the on with learning rate of **0.01**, as shown in the table below. The final **test error** in that configuration is 0.6641.

	learning rate		
	0.001	0.01	0.1
validation accuracy	0.795 / 0.6504	0.8062/0.6641	0.7947 / 0.6331

Plots of loss and validation error vs epoch for learning parameter 0.01:





2. The best configuration in terms of **validation accuracy** is the on with learning rate of **xxxx**, as shown in the table below. The final **test error** in that configuration is yyyy.

	learning rate			hidden size		dropout		activation	
	0.001	0.01	0.1	100	200	0.3	0.5	relu	tanh
validation accuracy	xxxxx	xxxx	xxxx	xxxx	xxxx	xxxx	xxxx	xxxx	xxxx

3. The best configuration in terms of **validation accuracy** is the on with learning rate of **xxxx**, as shown in the table below. The final **test error** in that configuration is yyyy.

	layers		
	1	2	3
validation accuracy	xxxx	xxxx	xxxx

Question 3

1. Let x_i denote the i-th component of $\boldsymbol{x}$ and let w_{ij} denote the entry in the i-th row and j-th column in matrix $\boldsymbol{W}$. We then have that:

$$
\begin{aligned}
h_i(\boldsymbol{x}) = g\left(\sum_{j=1}^{D} w_{ij}x_j\right) &= \left(\sum_{j=1}^{D} w_{ij}x_j\right)^2 = \left(\sum_{j=1}^{D} w_{ij}x_j\right)\left(\sum_{k=1}^{D} w_{ik}x_k\right) \\
&= \sum_{j=1}^{D}\sum_{k=1}^{D} w_{ij}x_j w_{ik}x_k = \sum_{j=1}^{D} w_{ij}^2 x_j^2 + \sum_{j=1}^{D}\sum_{k\neq j} w_{ij}w_{ik}x_jx_k \\
&= \sum_{j=1}^{D} w_{ij}^2 x_j^2 + \sum_{j=1}^{D}\sum_{k=1}^{j-1} w_{ij}w_{ik}x_jx_k + \sum_{j=1}^{D}\sum_{k=j+1}^{D} w_{ij}w_{ik}x_jx_k \\
&= \sum_{j=1}^{D} w_{ij}^2 x_j^2 + \sum_{k=1}^{D}\sum_{j=k+1}^{D} w_{ij}w_{ik}x_jx_k + \sum_{j=1}^{D}\sum_{k=j+1}^{D} w_{ij}w_{ik}x_jx_k \\
&= \sum_{j=1}^{D} w_{ij}^2 x_j^2 + \sum_{k=1}^{D}\sum_{j=k+1}^{D} w_{ij}w_{ik}(2x_jx_k) \\
&= \begin{bmatrix} w_{i1}^2 & w_{i1}w_{i2} & \dots & w_{i1}w_{iD} & w_{i2}^2 & w_{i2}w_{i3} & \dots & w_{i(D-1)}^2 & w_{i(D-1)}w_{iD} & w_{iD}^2 \end{bmatrix}
\begin{bmatrix} x_1^2 \\ 2x_1x_2 \\ \dots \\ 2x_1x_D \\ x_2^2 \\ 2x_2x_3 \\ \dots \\ x_{D-1}^2 \\ 2x_{D-1}x_D \\ x_D^2 \end{bmatrix}
\end{aligned}
$$

As such, $\boldsymbol{h}$ is linear in some feature transformation $\boldsymbol{\phi}$, that is, $\boldsymbol{h}$ can be written as $\boldsymbol{A}_\Theta\boldsymbol{\phi}(\boldsymbol{x})$. In particular, we have that such matrix $\boldsymbol{A}_\Theta$ can be defined as:

$$
\boldsymbol{A}_\Theta = \begin{bmatrix} — \boldsymbol{a}_1^T — \\ — \boldsymbol{a}_2^T — \\ \vdots \\ — \boldsymbol{a}_K^T — \end{bmatrix}
$$

where

$$
\boldsymbol{a}_i = \begin{bmatrix} w_{i1}^2 & w_{i1}w_{i2} & \dots & w_{i1}w_{iD} & w_{i2}^2 & w_{i2}w_{i3} & \dots & w_{i(D-1)}^2 & w_{i(D-1)}w_{iD} & w_{iD}^2 \end{bmatrix}^T
$$

and so $\boldsymbol{A}_\Theta \in \mathbb{R}^{K\times\frac{D(D+1)}{2}}$ (since $\sum_{k=1}^{D} k = \frac{D(D+1)}{2}$). Furthermore, we can define the feature transformation $\boldsymbol{\phi} : \mathbb{R}^D \mapsto \mathbb{R}^{\frac{D(D+1)}{2}}$ as:

$$
\boldsymbol{\phi}(\boldsymbol{x}) = (x_1^2, 2x_1x_2, \dots, 2x_1x_D, x_2^2, 2x_2x_3, \dots, x_{D-1}^2, 2x_{D-1}x_D, x_D^2)
$$

2. Given that the predicted output $\hat{y}$ is defined as:

$$\hat{y} = \boldsymbol{v}^T \boldsymbol{h}$$

the linearity of $\boldsymbol{h}$ in the feature transformation $\boldsymbol{\phi}(\boldsymbol{x})$ proven above leads to following equality:

$$\hat{y} = \boldsymbol{v}^T \boldsymbol{A}_\Theta \boldsymbol{\phi}(\boldsymbol{x}) = (\boldsymbol{A}_\Theta^T \boldsymbol{v})^T \boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{c}_\Theta^T \boldsymbol{\phi}(\boldsymbol{x})$$

where we take $\boldsymbol{c}_\Theta$ to be equal to $\boldsymbol{A}_\Theta^T \boldsymbol{v}$, thereby proving that $\hat{y}$ is also a linear transformation of $\boldsymbol{\phi}(\boldsymbol{x})$. However, $\hat{y}$ is **not** linear in terms of the original parameters Θ. To see this, note that the model is now a linear combination of **products** of entries of $\boldsymbol{W}$ and $\boldsymbol{v}$ rather than being linear in **each** individual entry:

$$\hat{y} = \boldsymbol{v}^T \boldsymbol{A}_\Theta \boldsymbol{\phi}(\boldsymbol{x}) = \sum_{i=1}^{D} v_i (\boldsymbol{w}_i^T \boldsymbol{x})^2 = \sum_{i=1}^{K} \sum_{j=1}^{D} \sum_{k=1}^{D} v_i w_{ij} w_{ik} x_i x_k$$

where we define $\boldsymbol{w}_i$ to be the vector in the i-th row of matrix $\boldsymbol{W}$.

3. To prove the desired result, for $\boldsymbol{c}_\Theta$ defined in the previous subquestion and for any $\boldsymbol{c} \in \mathbb{R}^{\frac{D(D+1)}{2}}$, we make the observation that the inner products $\boldsymbol{c}_\Theta^T \boldsymbol{\phi}(\boldsymbol{x})$ and $\boldsymbol{c}^T \boldsymbol{\phi}(\boldsymbol{x})$ actually correspond to quadratic forms in $\boldsymbol{x}$:

$$\begin{aligned}
\boldsymbol{c}_\Theta^T \boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{v}^T \boldsymbol{h} &= \sum_{i=1}^{K} v_i (\boldsymbol{A}_\Theta \boldsymbol{\phi}(\boldsymbol{x}))_i^2 = \sum_{i=1}^{K} v_i (\boldsymbol{w}_i^T \boldsymbol{x})^2 \\
&= \begin{bmatrix} \boldsymbol{w}_1^T \boldsymbol{x} & \boldsymbol{w}_2^T \boldsymbol{x} & \dots & \boldsymbol{w}_K^T \boldsymbol{x} \end{bmatrix} \operatorname{diag}(\boldsymbol{v}) \begin{bmatrix} \boldsymbol{w}_1^T \boldsymbol{x} \\ \boldsymbol{w}_2^T \boldsymbol{x} \\ \dots \\ \boldsymbol{w}_K^T \boldsymbol{x} \end{bmatrix} \\
&= (\boldsymbol{W}\boldsymbol{x})^T \operatorname{diag}(\boldsymbol{v}) \boldsymbol{W}\boldsymbol{x} = \boldsymbol{x}^T \boldsymbol{W}^T \operatorname{diag}(\boldsymbol{v}) \boldsymbol{W}\boldsymbol{x}
\end{aligned}$$

and

$$\begin{aligned}
\boldsymbol{c}^T \boldsymbol{\phi}(\boldsymbol{x}) &= \sum_{i=1}^{\frac{D(D+1)}{2}} c_i \phi_i(x) = \sum_{i=1}^{D} c_{(i-1)D+i-\frac{(i-1)i}{2}}\, x_i^2 + \sum_{i=1}^{D} \sum_{j=i+1}^{D} c_{(i-1)D+j-\frac{(j-1)j}{2}}\, (2x_i x_j) \\
&= \boldsymbol{x}^T \mathcal{M}(\boldsymbol{c}) \boldsymbol{x}
\end{aligned}$$

where $\mathcal{M}(\boldsymbol{c}) \in \mathbb{R}^{D \times D}$ is a symmetric matrix obtained from $\boldsymbol{c}$ such that:

- the diagonal and the part above the diagonal of the matrix $\mathcal{M}(\boldsymbol{c})$ is filled row-wise with the elements of vector $\boldsymbol{c}$, i.e.:

$$\mathcal{M}(\boldsymbol{c}) = \begin{bmatrix} c_1 & c_2 & c_3 & \cdots & c_D \\ c_2 & c_{D+1} & c_{D+2} & \cdots & c_{2D-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_D & c_{D-1} & c_{D-2} & \cdots & c_{\frac{D(D+1)}{2}} \end{bmatrix}$$

- for $1 \leq i \leq D$ and $j < i$, $(\mathcal{M}(\boldsymbol{c}))_{ij} = (\mathcal{M}(\boldsymbol{c}))_{ji}$

Furthermore, we also recur to the following lemma:

Lemma 1. *Two vectors* $\boldsymbol{a}$, $\boldsymbol{b} \in \mathbb{R}^{\frac{D(D+1)}{2}}$ *are equal if and only if* $\boldsymbol{a}^T \boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{b}^T \boldsymbol{\phi}(\boldsymbol{x})$, *for all* $\boldsymbol{x} \in \mathbb{R}^D$

Proof. If $\boldsymbol{a} = \boldsymbol{b}$, then $\boldsymbol{a}^T \boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{b}^T \boldsymbol{\phi}(\boldsymbol{x})$ is trivially verified. For the reverse implication, note that, according to the previously made observation, for any $\boldsymbol{x} \in \mathbb{R}^D$:

$$\boldsymbol{a}^T \boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{b}^T \boldsymbol{\phi}(\boldsymbol{x}) \Rightarrow \boldsymbol{x}^T \mathcal{M}(\boldsymbol{a}) \boldsymbol{x} = \boldsymbol{x}^T \mathcal{M}(\boldsymbol{b}) \boldsymbol{x}$$

Since both $\mathcal{M}(\boldsymbol{a})$ and $\mathcal{M}(\boldsymbol{a})$ are symmetric and the associated quadratic forms are twice continuously differentiable, taking the hessian on both sides of the equation yields:

$$\mathcal{M}(\boldsymbol{a}) = \mathcal{M}(\boldsymbol{b})$$

that is, $\mathcal{M}(\boldsymbol{a})$ and $\mathcal{M}(\boldsymbol{b})$ are equal entry-wise. In particular, we have that $a_i = b_i$, for $i = 1, \ldots, \frac{D(D+1)}{2}$. □

We are now equipped with the tools needed for the proof. Since $\mathcal{M}(\boldsymbol{c})$ is symmetric, the **Spectral Decomposition Theorem** tells us that there is an orthonormal matrix $\boldsymbol{Q}$ and a diagonal matrix $\boldsymbol{\Lambda}$ such that $\mathcal{M}(\boldsymbol{c}) = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^T$. Let $\boldsymbol{q_i}$ denote the eigenvector of $\mathcal{M}(\boldsymbol{c})$ that is present in i-th column of $\boldsymbol{Q}$ and let λ_i be the corresponding eigenvalue (note that $\{\boldsymbol{q}_i\}_{i=1}^D$ forms an orthonormal basis of $\mathbb{R}^D$). Then, we can write $\boldsymbol{c}^T\boldsymbol{\phi}(\boldsymbol{x})$ as:

$$\boldsymbol{c}^T\boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{x}^T\mathcal{M}(\boldsymbol{c})\boldsymbol{x} = (\boldsymbol{Q}^T\boldsymbol{x})^T\boldsymbol{\Lambda}(\boldsymbol{Q}^T\boldsymbol{x}) = \sum_{i=1}^{D}\lambda_i(\boldsymbol{q}_i^T\boldsymbol{x})^2$$

Now, if we assume that $K \geq D$, we can find a matrix $\boldsymbol{W}$ and a vector $\boldsymbol{v}$ that make $\boldsymbol{c}_\Theta^T\boldsymbol{\phi}(\boldsymbol{x})$ equal to $\boldsymbol{c}^T\boldsymbol{\phi}(\boldsymbol{x})$ in the following way:

- we make $\boldsymbol{v}$ to be equal to $(\lambda_1, \lambda_2, \ldots, \lambda_D, \underbrace{0, \ldots, 0}_{K-D \text{ times}})$;
- we make $\boldsymbol{W}$ to be equal to the vertical concatenation of $\boldsymbol{Q}^T$ with a $(K-D) \times D$ matrix of zeros, i.e.:

$$\boldsymbol{W} = \begin{bmatrix} \boldsymbol{Q}^T \\ \boldsymbol{0}_{(K-D)\times D} \end{bmatrix}$$

We then have that:

$$\boldsymbol{c}_\Theta^T\boldsymbol{\phi}(\boldsymbol{x}) = \sum_{i=1}^{K}\boldsymbol{v}_i(\boldsymbol{w}_i^T\boldsymbol{x})^2 = \sum_{i=1}^{D}\lambda_i(\boldsymbol{q}_i^T\boldsymbol{x})^2 = (\boldsymbol{Q}^T\boldsymbol{x})^T\boldsymbol{\Lambda}(\boldsymbol{Q}^T\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^T\boldsymbol{x} = \boldsymbol{c}^T\boldsymbol{\phi}(\boldsymbol{x})$$

and, by Lemma 1, we prove that the previous choice of $\boldsymbol{W}$ and $\boldsymbol{v}$ originate a vector $\boldsymbol{c}_\Theta$ such that $\boldsymbol{c}_\Theta = \boldsymbol{c}$. Furthermore, we have proven that the sets of classifiers $\mathcal{C}_1 = \{\boldsymbol{c}_\Theta^T\phi(x) : \Theta = (\boldsymbol{W}, \boldsymbol{v}) \in \mathbb{R}^{K\times D\times K}\}$ and $\mathcal{C}_2 = \{\boldsymbol{c}^T\phi(x) : \boldsymbol{c} \in \mathbb{R}^{\frac{D(D+1)}{2}}\}$ are exactly the same, and so the original neural network reduces to a **linear model** in terms of $\boldsymbol{c}_\Theta$. □

Consider now the case when $K < D$. Then, the nullspace of $\boldsymbol{W}$ has at least dimension $D - K \geq 1$, and thus there is some **non-null** vector $\boldsymbol{x}^*$ such that $\boldsymbol{W}\boldsymbol{x}^* = 0$. Now, choose $\boldsymbol{c}$ to be a vector such that $\mathcal{M}(\boldsymbol{c}) = \boldsymbol{I}_{D\times D}$ (i.e., the $D \times D$ identity matrix). We then have:

$$\boldsymbol{c}_\Theta^T\boldsymbol{\phi}(\boldsymbol{x}^*) = \boldsymbol{x}^{*T}\boldsymbol{W}^T\text{diag}(\boldsymbol{v})\boldsymbol{W}\boldsymbol{x}^* = 0$$

and

$$\boldsymbol{c}^T\boldsymbol{\phi}(\boldsymbol{x}^*) = \boldsymbol{x}^{*T}\mathcal{M}(\boldsymbol{c})\boldsymbol{x}^* = \boldsymbol{x}^{*T}\boldsymbol{I}_{D\times D}\boldsymbol{x}^* = \|\boldsymbol{x}^*\|_2^2 > 0$$

Thus, for $K < D$, we have constructed an instance of $\boldsymbol{c}$ for which there exists some $\boldsymbol{x} \in \mathbb{R}^D$ such that $\boldsymbol{c}_\Theta^T\boldsymbol{\phi}(\boldsymbol{x}) \neq \boldsymbol{c}^T\boldsymbol{\phi}(\boldsymbol{x})$. Applying Lemma 1, we conclude that there is no choice of parameters $\boldsymbol{W}$ and $\boldsymbol{v}$ that make $\boldsymbol{c}_\Theta$ equal to $\boldsymbol{c}$ and so the model cannot be parametrized by $\boldsymbol{c}_\Theta$ in this case.

4. Given that $\hat{y} = \boldsymbol{c}_\Theta^T\boldsymbol{\phi}(\boldsymbol{x})$, we can write the squared loss as:

$$L(\boldsymbol{c}_\Theta^T;\mathcal{D}) = \frac{1}{2}\sum_{n=1}^{N}(\hat{y}_n(\boldsymbol{x}_n;\boldsymbol{c}_\Theta^T) - y_n)^2 = \frac{1}{2}\sum_{n=1}^{N}(\boldsymbol{c}_\Theta^T\boldsymbol{\phi}(\boldsymbol{x}) - y_n)^2 = \frac{1}{2}\|\boldsymbol{X}\boldsymbol{c}_\Theta - \boldsymbol{y}\|_2^2$$

where $\boldsymbol{y} = (y_1, y_2, \ldots, y_n)$. As such, the minimization of the squared lost corresponds to a linear least squares problem, which in this case has a unique solution $\boldsymbol{c}_\Theta^*$ that is found simply by setting the gradient to zero:

$$\begin{aligned}\nabla_{\boldsymbol{c}_\Theta} L(\boldsymbol{c}_\Theta^T; \mathcal{D}) = \mathbf{0} \Leftrightarrow \nabla_{\boldsymbol{c}_\Theta}(\boldsymbol{X}\boldsymbol{c}_\Theta)\nabla_{\boldsymbol{z}}(\|\boldsymbol{z}\|_2^2)|_{\boldsymbol{z}=\boldsymbol{X}\boldsymbol{c}_\Theta-\boldsymbol{y}} = \mathbf{0} \Leftrightarrow 2\boldsymbol{X}^T(\boldsymbol{X}\boldsymbol{c}_\Theta - \boldsymbol{y}) = \mathbf{0} \\ \Rightarrow \boldsymbol{c}_\Theta^* = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}\end{aligned}$$

To prove the existence of $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$, note that the dimensions of the nullspaces of and $\boldsymbol{X}$ and $\boldsymbol{X}^T\boldsymbol{X}$ are equal, since, for every $\boldsymbol{x} \in \mathbb{R}^{\frac{D(D+1)}{2}}$:

$$\boldsymbol{X}\boldsymbol{x} = \mathbf{0} \Rightarrow \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{x} = \mathbf{0}$$

and

$$\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{x} = \mathbf{0} \Rightarrow x^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{x} = \mathbf{0} \Rightarrow \|\boldsymbol{X}\boldsymbol{x}\|_2^2 = \mathbf{0} \Rightarrow \boldsymbol{X}\boldsymbol{x} = \mathbf{0}$$

Since $N > \frac{D(D+1)}{2}$ and $\boldsymbol{X}$ has full column rank ($\frac{D(D+1)}{2}$), its nullspace has dimension 0. Hence, $\boldsymbol{X}^T\boldsymbol{X}$ is a $\frac{D(D+1)}{2} \times \frac{D(D+1)}{2}$ square matrix with rank $\frac{D(D+1)}{2} - 0 = \frac{D(D+1)}{2}$, and so it is invertible.

Usually, loss functions of feedforward neural networks are non-convex in their parameters due to multiple compositions of non-linear activation functions, making the global minimization of said functions especially hard. In spite of that, since the presented architecture only has a single hidden layer with at least as many units as the input layer and uses only quadratic activations, we managed to reduce it to a **linear regression** by defining the underlying **feature transformation $\boldsymbol{\phi}$** and **weight vector $\boldsymbol{c}_\Theta$**. Hence, the minimization of the loss function becomes much easier, since the global minimizer can be computed in closed form.