Mathematical background and experimental results

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1 Introduction

In this document, we will present the mathematical background and experimental results for a practical concerning image classification using convolutional kernel networks based on the paper with the name “End-to-End Kernel Learning with Supervised Convolutional Kernel Networks” [1].

2 Mathematical background

A convolutional kernel network is composed of $K \in \mathbb{N}$ convolutional kernel layers and an output layer. The first convolutional layer takes the input image for the network as its input, while the subsequent layers take the output of the previous layer as their input.
In the following sections, we will explore how the convolutional layers, the output layer and the training procedure of these layers work:

2.1 Convolutional layer

2.1.1 General case

The j-th convolutional layer recieves an image $I_{j-1} = [y_1, \dots, y_{|\Omega_{j-1}|}] \in \mathbb{R}^{p_{j-1} \times |\Omega_{j-1}|}$ (p_{j-1} being the number of input channels, $\Omega_{j-1} \subset [0,1]^2$ being the set of pixel coordinates) as input.
Let $e_{j-1} \times e_{j-1}$ with $e_{j-1} \in \mathbb{N}$ be the filter size of the convolutional layer and $x_y \in \mathbb{R}^{p_{j-1} e_{j-1}^2}$ be the patch of size $e_{j-1} \times e_{j-1}$ from the image I centered around the pixel $y \in \Omega_{j-1}$
The convolutional layer will then output an image $M_j = [\psi_j(x_{y_1}), \dots, \psi_j(x_{y_{|\Omega_{j-1}|}})] \in \mathbb{R}^{p_j \times |\Omega_{j-1}|}$ with $\psi_j : \mathbb{R}^{p_{j-1} e_{j-1}^2} \to \mathbb{R}^{p_j}$ being a function that assigns a vector $\psi_j(x_y) \in \mathbb{R}^{p_j}$ to each patch x_y of the input map I_{j-1}.

2.1.2 Convolutional kernel layer: The function ψ_j

We will now define the function ψ_j for a convolutional kernel layer.
A convolutional kernel layer consists of

1. A filter matrix $Z_j = [z_1, \dots, z_{p_j}] \in \mathbb{R}^{p_{j-1} e_{j-1}^2 \times p_j}$ with $z_1, \dots, z_{p_j} \in \mathbb{R}^{p_{j-1} e_{j-1}^2}$ being a selection of normed patches of size $e_{j-1} \times e_{j-1}$.
2. A positive-definite kernel

$$K_j : \mathbb{R}^{p_{j-1} e_{j-1}^2} \times \mathbb{R}^{p_{j-1} e_{j-1}^2} \to \mathbb{R},\ K_j(x, x') = \begin{cases} \|x\| \|x'\| \kappa_j(\langle \frac{x}{\|x\|}, \frac{x}{\|x'\|} \rangle) & x, x' \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

where $\kappa_j(\langle ., . \rangle)$ is the dot-product kernel on the sphere.
In this practical, we will always use the Radial basis function (RBF) kernel with

$$\kappa_j(\langle x, x' \rangle) = e^{\alpha_j(\langle x, x' \rangle - 1)} \text{ for } x, x' \in \mathbb{R}^{p_{j-1} e_{j-1}^2}, \|x\| = \|x'\| = 1$$

The parameter $\alpha_j > 0$ can be different from layer to layer.
According to the Moore-Aronszajn theorem [2], the positive-definite kernel K_j implicitly defines a reproducing kernel hilbert space (RKHS) $\mathcal{H}_j$ and a map $\varphi_j : \mathbb{R}^{p_{j-1} e_{j-1}^2} \to \mathcal{H}_j$ such that $\langle \varphi_j(x), \varphi_j(x') \rangle_{\mathcal{H}_j} = K_j(x, x')$.

Short explanation / interpretation:
We want to project patches $\in \mathbb{R}^{p_{j-1} e_{j-1}^2}$ into a higher dimensional space. The higher dimensional space is $\mathcal{H}_j$ and a patch $x \in \mathbb{R}^{p_{j-1} e_{j-1}^2}$ is mapped into it using the map $\varphi_j : \mathbb{R}^{p_{j-1} e_{j-1}^2} \to \mathcal{H}_j$. Neither $\mathcal{H}_j$ nor the map φ_j are ever explicitly stated, but are implicitly defined through the kernel K_j and the property $\langle \varphi_j(x), \varphi_j(x') \rangle_{\mathcal{H}_j} = K_j(x, x')$. In a sense, we explicitly state how the inner-product between two projected patches is supposed to look like through the kernel K_j. The space $\mathcal{H}_j$ and the map φ_j are then defined accordingly and only exist on paper.

The patches $z_1, \dots, z_{p_j}$ together with the map φ_j now define a subspace $\mathcal{F}_j = span\{\varphi_j(z_1), \dots, \varphi_j(z_{p_j})\}$.
For each new patch $x \in \mathbb{R}^{p_{j-1} e_{j-1}^2}$ we then project $\varphi_j(x)$ into $\mathcal{F}_j$ using the orthogonal projection, resulting in

$$f_x := proj_{\mathcal{H}_j}(\varphi_j(x)) = \sum_{i=1}^{p_j} \alpha_i \varphi_j(z_i) \in \mathcal{H}_j \text{ with } \alpha \in \arg\min_{\alpha \in \mathbb{R}^{p_j}} \Big\| \sum_{i=1}^{p_j} \alpha_i \varphi_j(z_i) - \varphi_j(x) \Big\|_{\mathcal{H}_j}$$

We are now looking for a parameterization $\psi_j(x) \in \mathbb{R}^{p_j}$ of f_x in $\mathcal{F}_j$ such that $K(f_x, f_{x'}) = \langle f_x, f_{x'} \rangle_{\mathcal{H}_j} = \langle \psi_j(x), \psi_j(x') \rangle$ for all patches $x, x' \in \mathbb{R}^{p_{j-1} e_{j-1}^2}$.
After a short calculation we obtain

$$\psi_j(x) = \begin{cases} \|x\| \kappa_j(Z_j^T Z_j)^{-\frac{1}{2}} \kappa_j(Z_j^T \frac{x}{\|x\|}) & x \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

where the dot-product kernel κ_j is applied pointwise to its arguments. A more detailed calculation can be found in appendix A of the original paper [1].

It is noteworthy that we never actually have to compute $\varphi_j(x)$. Because of the property $\langle \varphi_j(x), \varphi_j(x') \rangle_{\mathcal{H}_j} = K_j(x, x')$ we can directly compute the parameterization $\psi_j(x)$ using the kernel function. For this reason this approach is called the kernel trick.

2.1.3 Convolutional kernel layer: Formula for M_j

We will now use the formula for ψ_j to obtain a fromula for $M_j = [\psi_j(x_{y_1}), \dots, \psi_j(x_{y_{|\Omega_{j-1}|}})]$.
For simplicity we will first assume $x_{y_1}, \dots, x_{y_{|\Omega_{j-1}|}} \neq 0$
We define

1. $A_j := \kappa_j(Z_j^T Z_j)^{-\frac{1}{2}}$ to make the formula shorter
2. A linear operator E_j that extracts all $e_{j-1} \times e_{j-1}$ patches from the input image $I_{j-1} = [y_1, \dots, y_{|\Omega_{j-1}|}]$, meaning $E_j(I_{j-1}) = [x_{y_1}, \dots, x_{y_{|\Omega_{j-1}|}}]$

3. A diagonal matrix

$$S_j = \begin{bmatrix} \|x_{y_1}\| & & \\ & \ddots & \\ & & \|x_{y_{|\Omega_{j-1}|}}\| \end{bmatrix}, \ (S_j)_{km} = \begin{cases} \|x_{y_k}\| & k = m \\ 0 & k \neq m \end{cases}$$

with the norms of the patches $x_{y_1}, \dots, x_{y_{|\Omega_{j-1}|}}$ in the diagonal entries.
Hence $E_j(I_{j-1})S_j^{-1} = [\frac{x_{y_1}}{\|x_{y_1}\|}, \dots, \frac{x_{y_{|\Omega_{j-1}|}}}{\|x_{y_{|\Omega_{j-1}|}}\|}]$

Thus using the formula

$$\psi_j(x) = \|x\| \underbrace{\kappa_j(Z_j^T Z_j)^{-\frac{1}{2}}}_{=A_j} \kappa_j(Z_j^T \frac{x}{\|x\|})$$

from above we get

$$M_j = [\psi_j(x_{y_1}), \dots, \psi_j(x_{y_{|\Omega_{j-1}|}})] = A_j \kappa_j(Z_j^T E_j(I_{j-1}) S_j^{-1}) S_j$$

In practise we add 0.00001 to the diagonal-elements of the matrix S_j and define $A_j := (\kappa_j(Z_j^T Z_j) + 0.001\mathbb{1})^{-\frac{1}{2}}$ to ensure that S_j and A_j are regular.

2.1.4 Linear Pooling

After computing M_j we can use linear pooling to reduce the resolution and gain invariance to small shifts:
Let $\Omega_j \subset [0,1]^2$ be the new (smaller) set of pixel coordinates after pooling and let $P_j \in \mathbb{R}^{|\Omega_{j-1}| \times |\Omega_j|}$ be the pooling matrix.
Then the final output of the layer is $I_j = M_j P_j \in \mathbb{R}^{p_j \times |\Omega_j|}$.
If we do not wish to use pooling, we can simply set $\Omega_j := \Omega_{j-1}$ and $P_j := \mathbb{1}_{|\Omega_j|}$ and get $I_j = M_j P_j = M_j$

2.2 Output Layer

Let the network have $K \in \mathbb{N}$ convolutional layers and let the output layer have $N \in \mathbb{N}$ output nodes.
The output layer then consists of N matrices $W^{(1)}, \dots, W^{(N)} \in \mathbb{R}^{p_K \times |\Omega_K|}$ and the output of the network is

$$O = \begin{pmatrix} \langle I_K, W^{(1)} \rangle \\ \vdots \\ \langle I_K, W^{(N)} \rangle \end{pmatrix} \in \mathbb{R}^N$$

where $\langle \cdot, \cdot \rangle$ is the inner product.
Here we differ from the original paper a little bit. The original paper only presents the case $N = 1$ while we look at the general case $N \geq 1$. All calculations that get affected by this change will be presented in more detail (see appendix A and appendix B).

2.3 Backpropagation

Let a training set be given by a set of images $I_0^1, \dots, I_0^M$ and corresponding labels $y_1, \dots, y_M \in \mathbb{R}^N$.
Let $L : \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$ be a smooth loss function that gives an error $L(y_i, O^i) \in \mathbb{R}$ of the network

output O^i for the input image I_0^i given the true label y_i. Let λ be the regularisation parameter. We train the network by minimizing

$$\tilde{L}(\mathcal{Z},\mathcal{W}) := \frac{1}{M}\sum_{i=1}^{M} L(y_i, O^i) + \frac{\lambda}{2}\sum_{i=1}^{N}\|W^{(i)}\|_F^2 \quad (\|\cdot\|_F \text{ Frobenius norm})$$

with respect to the filters $\mathcal{Z} = \{Z_1, \dots, Z_K\}$ and the weights $\mathcal{W} = \{W^{(1)}, \dots, W^{(N)}\}$ by using the stochastic gradient descent method: We will pick a learning rate $\alpha > 0$ and repeatedly

1. Compute the gradients $\nabla_{W^{(k)}}\tilde{L}(\mathcal{Z},\mathcal{W})$ for $k = 1, \dots, N$ and $\nabla_{Z_j}\tilde{L}(\mathcal{Z},\mathcal{W})$ for $j = 1, \dots, K$
2. Calculate $\tilde{Z}_j = [\tilde{z}_1, \dots, \tilde{z}_{p_j}] := Z_j - \alpha\nabla_{Z_j}\tilde{L}(\mathcal{Z},\mathcal{W})$ and set $Z_j \leftarrow \left[\frac{\tilde{z}_1}{\|\tilde{z}_1\|}, \dots, \frac{\tilde{z}_{p_j}}{\|\tilde{z}_{p_j}\|}\right]$ for $j = 1, \dots, K$
3. Set $W^{(k)} \leftarrow W^{(k)} - \alpha\nabla_{W^{(k)}}\tilde{L}(\mathcal{Z},\mathcal{W})$ for $k = 1, \dots, N$

until a termination condition is reached (e.g. stop after 100 epochs). The learning rate α can change from epoch to epoch.
In the following sections we will deal with computing $\nabla_{W^{(k)}}\tilde{L}(\mathcal{Z},\mathcal{W})$ and $\nabla_{Z_j}\tilde{L}(\mathcal{Z},\mathcal{W})$

2.3.1 Gradient with respect to the output weights

Let $L^{(k)}(y, o) := \frac{\partial}{\partial o_k} L(y, o)$ be the partial derivative of L with respect to the k-th component of the vector o.
Then the gradient of $\tilde{L}$ with respect to $W^{(k)}$ $(k = 1, \dots, N)$ is given by

$$\nabla_{W^{(k)}}\tilde{L}(\mathcal{Z},\mathcal{W}) = \frac{1}{M}\sum_{l=1}^{M} L^{(k)}(y_l, O^l) I_K^l + \lambda W^{(k)}$$

A proof can be found in appendix A.

2.3.2 Gradient with respect to the filters

Let $I_0^1, \dots, I_0^M$ be training images with the true labels $y_1, \dots, y_M$ and the respective network outputs $O^1, \dots, O^M$.
After a short calculation using Lemma 1 and Proposition 1 of the paper [1] (see appendix B) we obtain

$$\nabla_{Z_j} L(y_k, O^k) = g_j^{(k)}\left(h_{j+1}^{(k)}\left(\dots h_K^{(k)}\left(\sum_{i=1}^{N} L^{(i)}(y_k, O^k) W^{(i)}\right)\right)\right)$$

where $g_j^{(k)}, h_j^{(k)}$ are linear functions for the input image I_0^k given by

$$g_j^{(k)}(U) = E_j\left(I_{j-1}^{(k)}\right)\left(B_j^{(k)}\right)^T - \frac{1}{2} Z_j\left(\kappa_j'\left(Z_j^T Z_j\right) \odot \left(\left(C_j^{(k)}\right)^T + C_j^{(k)}\right)\right)$$
$$h_j^{(k)}(U) = E_j^*\left(Z_j B_j^{(k)} + E_j\left(I_{j-1}^{(k)}\right)\left(\left(S_j^{(k)}\right)^{-2} \odot \left(\left(M_j^{(k)}\right)^T U P_j^T - E_j\left(I_{j-1}^{(k)}\right)^T Z_j B_j^{(k)}\right)\right)\right)$$

with

$$B_j^{(k)} = \kappa_j'\left(Z_j^T E_j\left(I_{j-1}^{(k)}\right)\left(S_j^{(k)}\right)^{-1}\right) \odot \left(A_j U P_j^T\right) \quad \text{and}$$
$$C_j^{(k)} = A_j^{\frac{1}{2}} I_j^{(k)} U^T A_j^{\frac{3}{2}}$$

Hence

$$\nabla_{Z_j}\tilde{L}(\mathcal{Z},\mathcal{W}) = \nabla_{Z_j}\left(\frac{1}{M}\sum_{k=1}^{M}L(y_k,O^k) + \frac{\lambda}{2}\sum_{i=1}^{N}\|W^{(i)}\|_F^2\right)$$
$$= \frac{1}{M}\sum_{k=1}^{M} g_j^{(k)}\left(h_{j+1}^{(k)}\left(\ldots h_K^{(k)}\left(\sum_{i=1}^{N}L^{(i)}(y_k,O^k)W^{(i)}\right)\right)\right)$$

3 Experiments

In this section, we will present the experiments conducted with a convolutional kernel network (implemented in python) on the MNIST dataset (28 x 28 images with 10 classes).
The following different networks were tested:

1. A network with 3 convolutional layers, 10 filters each and filter-size 3 x 3 (with zero-padding). After the first and second convolutional layer we used average pooling with pooling-size 3 x 3:

$$\begin{aligned}
1\times 28\times 28 &\xrightarrow[\text{10 3×3 filters}]{\text{convolution (zp)}} 10\times 28\times 28 && \xrightarrow[\text{3×3}]{\text{avg. pooling}} 10\times 9\times 9\\
&\xrightarrow[\text{10 3×3 filters}]{\text{convolution (zp)}} 10\times 9\times 9 && \xrightarrow[\text{3×3}]{\text{avg. pooling}} 10\times 3\times 3\\
&\xrightarrow[\text{10 3×3 filters}]{\text{convolution (zp)}} 10\times 3\times 3 && \xrightarrow{\text{output layer}} 10
\end{aligned}$$

2. A network with 3 convolutional layers, 10 filters each and filter-size 5 x 5 (with zero-padding). After the first and second convolutional layer we used average pooling with pooling-size 3 x 3:

$$\begin{aligned}
1\times 28\times 28 &\xrightarrow[\text{10 5×5 filters}]{\text{convolution (zp)}} 10\times 28\times 28 && \xrightarrow[\text{3×3}]{\text{avg. pooling}} 10\times 9\times 9\\
&\xrightarrow[\text{10 5×5 filters}]{\text{convolution (zp)}} 10\times 9\times 9 && \xrightarrow[\text{3×3}]{\text{avg. pooling}} 10\times 3\times 3\\
&\xrightarrow[\text{10 5×5 filters}]{\text{convolution (zp)}} 10\times 3\times 3 && \xrightarrow{\text{output layer}} 10
\end{aligned}$$

3. A network with 5 convolutional layers, 5 filters each, filters 1, 3, 5 with filter-size 3 x 3 and filters 2, 4 with filter-size 1 x 1 (with zero-padding). After the first and third convolutional layer we used average pooling with pooling-size 3 x 3:

$$\begin{aligned}
1\times 28\times 28 &\xrightarrow[\text{5 3×3 filters}]{\text{convolution (zp)}} 5\times 28\times 28 && \xrightarrow[\text{3×3}]{\text{avg. pooling}} 5\times 9\times 9 && \xrightarrow[\text{5 1×1 filters}]{\text{convolution (zp)}} 5\times 9\times 9\\
&\xrightarrow[\text{5 3×3 filters}]{\text{convolution (zp)}} 5\times 9\times 9 && \xrightarrow[\text{3×3}]{\text{avg. pooling}} 5\times 3\times 3 && \xrightarrow[\text{5 1×1 filters}]{\text{convolution (zp)}} 5\times 3\times 3\\
&\xrightarrow[\text{5 3×3 filters}]{\text{convolution (zp)}} 5\times 3\times 3 && \xrightarrow{\text{output layer}} 10
\end{aligned}$$

4. A network with 2 convolutional layers, 15 filters each and filter-size 3 x 3 (no zero-padding). After the first convolutional layer we used average pooling with pooling-size 3 x 3:

$$
\begin{aligned}
1 \times 28 \times 28 &\xrightarrow[\text{15 3×3 filters}]{\text{convolution}} 15 \times 26 \times 26 &&\xrightarrow[\text{3×3}]{\text{avg. pooling}} 15 \times 8 \times 8 \\
&\xrightarrow[\text{15 3×3 filters}]{\text{convolution}} 15 \times 6 \times 6 &&\xrightarrow{\text{output layer}} 10
\end{aligned}
$$

All networks use the RBF kernel $\kappa_j(\langle x, x' \rangle) = e^{\alpha_j(\langle x, x' \rangle - 1)}$ with $\alpha_j = 4$ for all layers j

The following parameters for the training algorithm were choosen:

- Initial learning rate $\alpha = 2$ (gets halved every time the loss increases in an epoch)
- Regularisation parameter $\lambda = 1/60000$

The regularisation parameter is most likely too small to have any significant impact on the training process. In side experiments with higher regularisation parameters (not further mentioned in this document), the performance of the trained networks were either roughly the same or significantly worse than the results achieved with the small regularisation parameter. A possible explanation is that the tested networks are too small for overfitting to be an issue, hence making regularisation obsolete.

We will now look at the results achieved by the 4 networks described above. To do that we first have to load the MNIST-Dataset and the trained networks together with the test-information collected during the training process:

[1]:
```
%matplotlib inline

import sys, os
analyses_dir = os.path.join(os.getcwd(), "analyses")
sys.path.append("src")

import numpy as np
import pandas as pd
from matplotlib import pyplot as plt
from mnist import MNIST
from analysis import Analysis

mnist = MNIST('mnist')
num_epochs = 20

training_analyses = {
    '3 layers|10 3x3|zpad; 3x3 pool':
        Analysis.load_from_file(os.path.join(analyses_dir,␣
 ↪"ana_3_3x3_layers_10_filters_3x3_pooling"),
                            mnist.train_images, mnist.train_labels, mnist.
 ↪test_images, mnist.test_labels),
```

```
    '3 layers|10 5x5|zpad; 3x3 pool':
        Analysis.load_from_file(os.path.join(analyses_dir,␣
↪"ana_3_5x5_layers_10_filters_3x3_pooling"),
                    mnist.train_images, mnist.train_labels, mnist.
↪test_images, mnist.test_labels),

    '5 layers|5 3x3 & 1x1|zpad; 3x3 pool':
        Analysis.load_from_file(os.path.join(analyses_dir,␣
↪"ana_3_3x3_2_1x1_layers_5_filters__3x3_pooling__zp"),
                    mnist.train_images, mnist.train_labels, mnist.
↪test_images, mnist.test_labels),

    '2 layers|15 3x3|no zpad; 3x3 pool':
        Analysis.load_from_file(os.path.join(analyses_dir,␣
↪"ana_2_3x3_layers_15_filters__3x3_pooling__no_zp"),
                    mnist.train_images, mnist.train_labels, mnist.
↪test_images, mnist.test_labels)

}
```

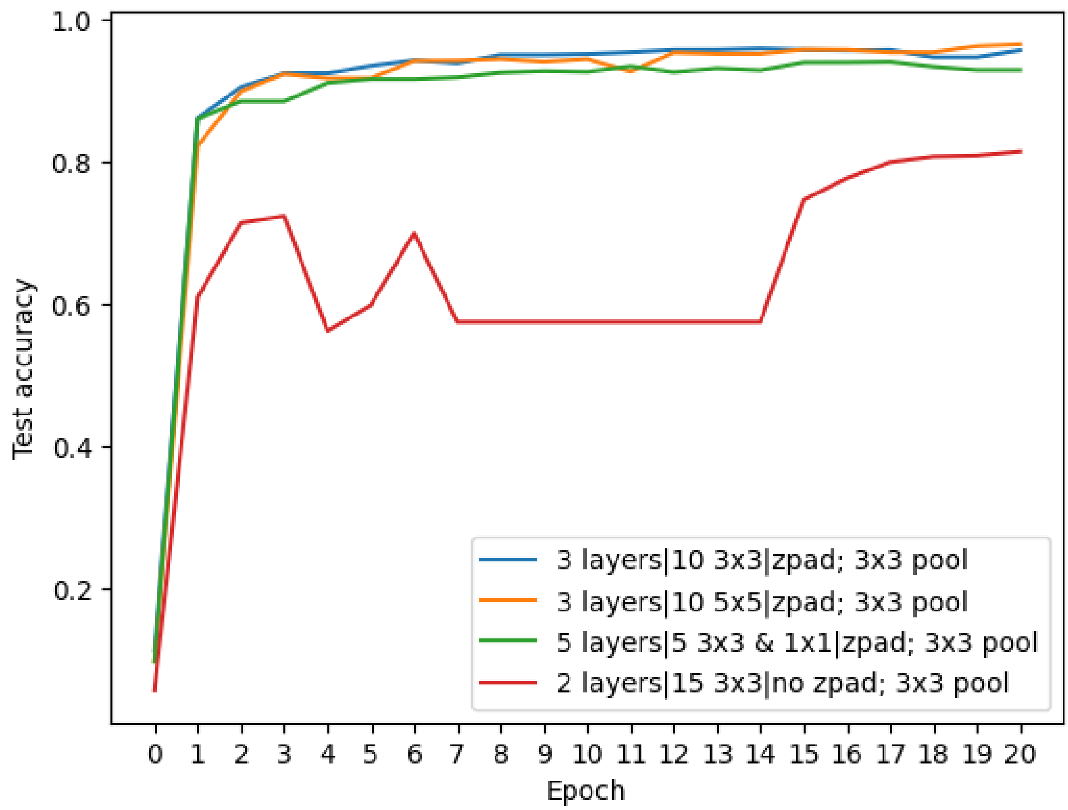
3.1 Test accuracies

The the test accuracies across the first 20 epochs were as follows:

[2]:
```
for network_name, ana in training_analyses.items():
    plt.plot([ana.test_results_epoch[i].correct_portion for i in␣
↪range(num_epochs + 1)], label=network_name)

plt.xlabel('Epoch')
plt.ylabel('Test accuracy')
plt.xticks(range(num_epochs + 1))
plt.legend(loc="lower right")

plt.show()
```



In table format:

[3]:
```
pd.set_option('display.max_columns', None)
pd.set_option('display.width', 85)

epochs = {epoch: [] for epoch in range(num_epochs + 1)}
index = []
for network_name, ana in training_analyses.items():
    index.append(network_name)
    for epoch in range(num_epochs + 1):
        epochs[epoch].append(f"{int(ana.test_results_epoch[epoch].
 ↪correct_portion * 100 + 0.5)}%")

df = pd.DataFrame(epochs)
df.index = index

print(df)
```

```
                                   0    1    2    3    4    5    6    7    8  \
3 layers|10 3x3|zpad; 3x3 pool   11%  86%  91%  92%  92%  94%  94%  94%  95%
3 layers|10 5x5|zpad; 3x3 pool   10%  82%  90%  92%  92%  92%  94%  94%  94%
```

```
5 layers|5 3x3 & 1x1|zpad; 3x3 pool  10%  86%  89%  89%  91%  92%  92%  92%  93%
2 layers|15 3x3|no zpad; 3x3 pool     6%  61%  71%  72%  56%  60%  70%  58%  58%

                                       9   10   11   12   13   14   15   16   17
\
3 layers|10 3x3|zpad; 3x3 pool       95%  95%  95%  96%  96%  96%  96%  96%  96%
3 layers|10 5x5|zpad; 3x3 pool       94%  94%  93%  95%  95%  95%  96%  96%  95%
5 layers|5 3x3 & 1x1|zpad; 3x3 pool  93%  93%  93%  93%  93%  93%  94%  94%  94%
2 layers|15 3x3|no zpad; 3x3 pool    58%  58%  58%  58%  58%  58%  75%  78%  80%

                                      18   19   20
3 layers|10 3x3|zpad; 3x3 pool       95%  95%  96%
3 layers|10 5x5|zpad; 3x3 pool       95%  96%  97%
5 layers|5 3x3 & 1x1|zpad; 3x3 pool  93%  93%  93%
2 layers|15 3x3|no zpad; 3x3 pool    81%  81%  81%
```

As we can see, the first and second network performed the best and achieved a test accuracy of 96% / 97% after 20 epochs.
Inserting convolutional layers with 1x1 filters after pooling while using less filters per layer (third network) produced worse results then the first network which it was based on (probably due to the small amount of filters per layer).
The last network with only two layers but 15 filters for each one performed the worst.

In the following sections, we will solely focus on the best performing network:

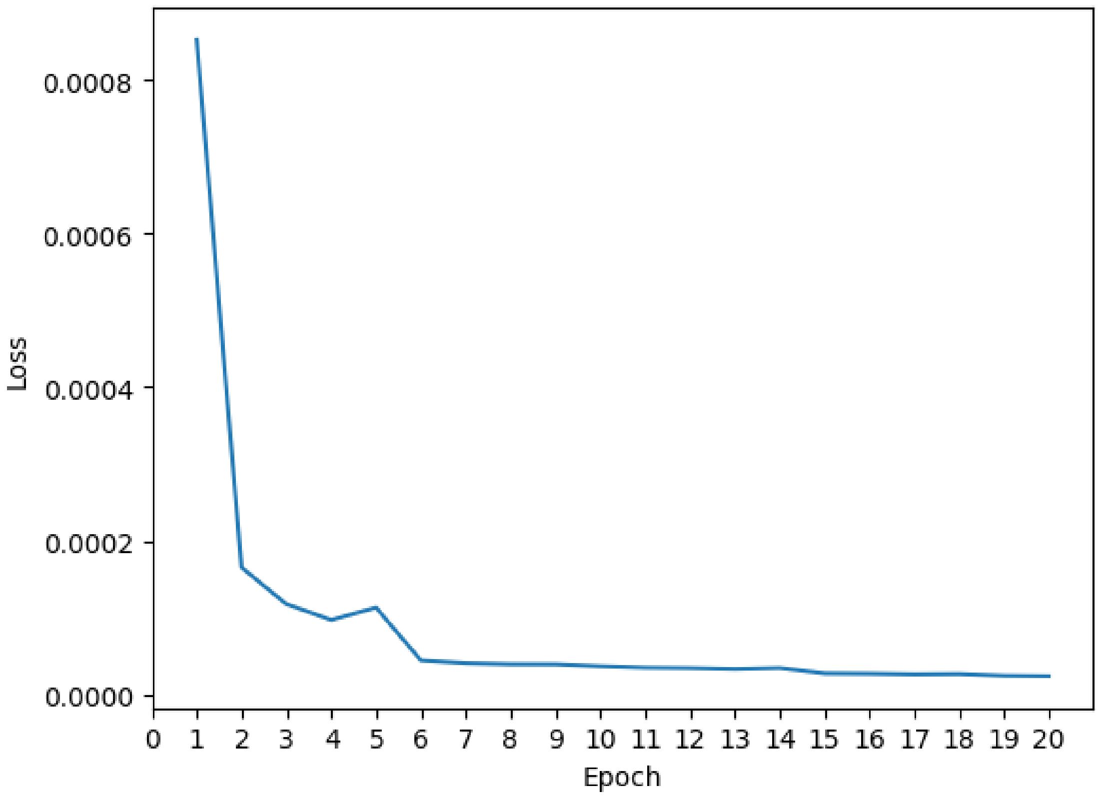
[4]:
```python
best_network_name = '3 layers|10 5x5|zpad; 3x3 pool'
best_network_training_ana = training_analyses[best_network_name]
```

3.2 Average Loss

The average loss across the 20 epochs was as follows:

[5]:
```python
plt.plot(range(1, num_epochs + 1), [best_network_training_ana.trainer.
 ↪average_loss_epoch[i] for i in range(num_epochs)])
plt.xlabel('Epoch')
plt.ylabel('Loss')
plt.xticks(range(num_epochs + 1))

plt.show()
```



In table format:

[6]:
```
pd.set_option('display.max_columns', None)
pd.set_option('display.width', 85)

epochs = {epoch: [] for epoch in range(1, num_epochs + 1)}
index = ["Avg. Loss (per thousand)"]
for epoch in range(1, num_epochs + 1):
    epochs[epoch].append(f"{best_network_training_ana.trainer.
 ↪average_loss_epoch[epoch - 1]*1000:.3f}")

df = pd.DataFrame(epochs)
df.index = index

print(df)
```

```
                              1      2      3      4      5      6      7      8  \
Avg. Loss (per thousand)  0.852  0.165  0.118  0.097  0.113  0.044  0.041  0.039

                              9     10     11     12     13     14     15     16  \
```

```
Avg. Loss (per thousand)  0.039  0.037  0.035  0.034  0.033  0.035  0.028  0.027

                             17     18     19     20
Avg. Loss (per thousand)  0.026  0.027  0.024  0.024
```

As we can see, the loss deceases drasticly within the first few epochs and than decreases a lot slower (as expected). However, we still see improvements even in the later epochs. It is possible that the network would have improved further during additional training.

3.3 Error rate of specific numbers

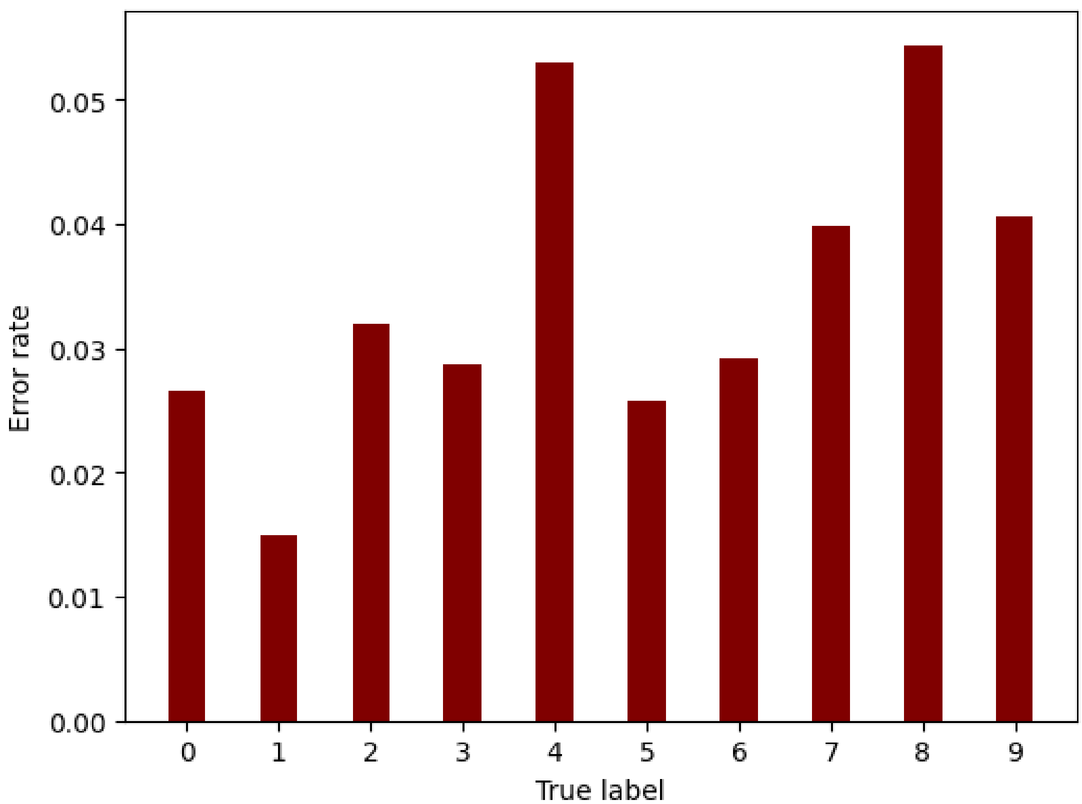
We now take a look at the ratio of misclassifications of each number as shown in the diagram below:

[7]:
```
error_rates = best_network_training_ana.test_results_epoch[-1].
 ↪label_false_portion

plt.bar(range(10), error_rates, color ='maroon',
        width = 0.4)

plt.xlabel('True label')
plt.ylabel('Error rate')
plt.xticks(range(10))

plt.show()
```



As we can see, the network has the most problems with identifying the numbers 4 and 8. We will take a closer look on the number 4:

The number 4 gets mostly misidentified as the number 9 as the diagramm below shows:

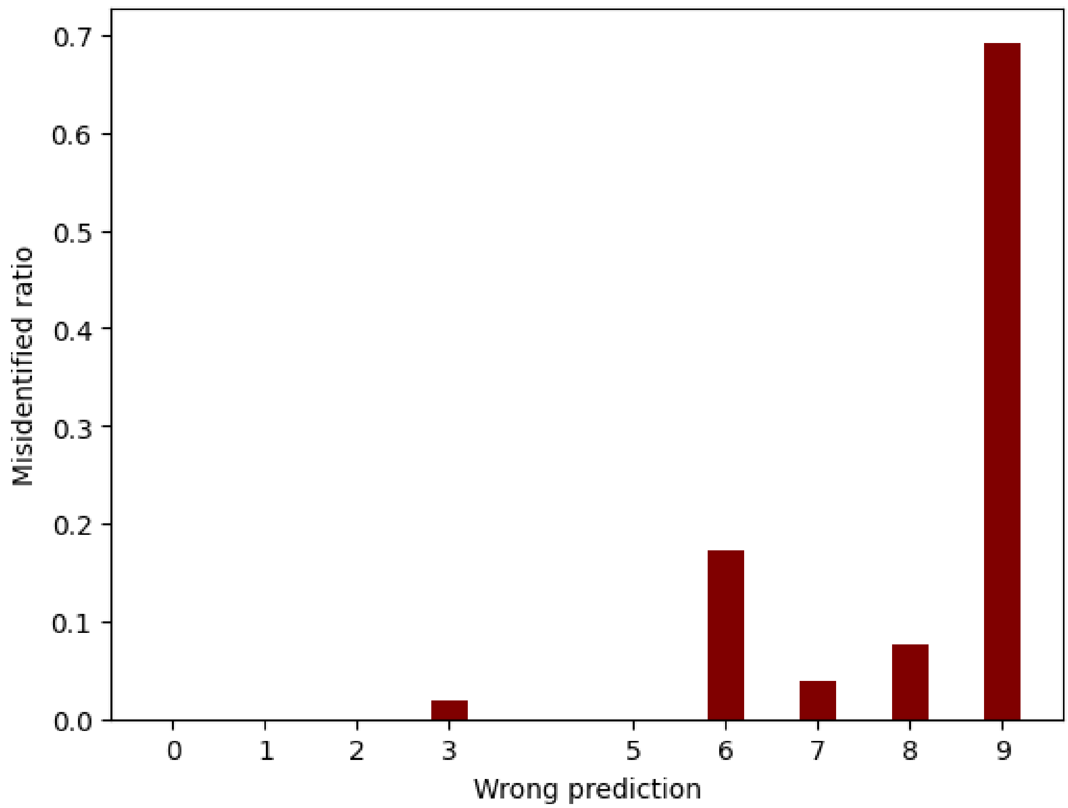
[8]:
```
label_to_test = 4

network_pred = best_network_training_ana.test_results_epoch[-1].network_pred
not_label_to_test = np.arange(10)[np.arange(10) != label_to_test]
misidentified = network_pred[label_to_test][not_label_to_test]
misidentified_ratio = misidentified / misidentified.sum()

plt.bar(not_label_to_test, misidentified_ratio, color ='maroon',
        width = 0.4)

plt.xlabel('Wrong prediction')
plt.ylabel('Misidentified ratio')
plt.xticks(not_label_to_test)

plt.show()
```



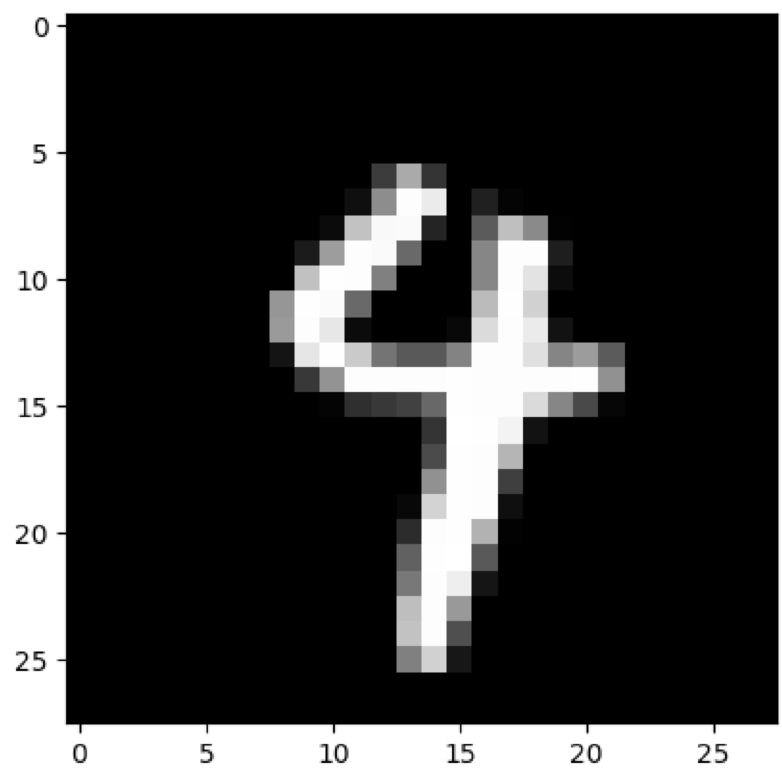
Looking through the pictures of 4s that were falsely identified as the number 9, it seems that the network tends to misinterpret the upper part of 4s as the loop of the number 9, especially if the top of the 4 is closed or almost closed. The picture shown below is a good exmple of this:

[9]:
```
label_to_test = 4
network_prediction = 9

images = []

for i in range(len(mnist.test_images)):
    if mnist.test_labels[i] == label_to_test:
        x = best_network_training_ana.trainer.best_network.forward(mnist.
 ↪test_images[i])
        if network_prediction == np.argmax(x):
            images.append(mnist.test_images[i])

plt.imshow(images[7].reshape(28, 28), cmap='gray')
plt.show()
```



4 Appendix A: Calculation of the gradient of the loss function with respect to the weights

Let $i \in \{1, \dots, p_K\},\ j \in \{1, \dots, |\Omega_K|\},\ k \in \{1, \dots, N\}$.
Then $\forall l = 1, \dots, M$:

$$\begin{aligned}\frac{\partial}{\partial W_{ij}^{(k)}} \langle I_K^l, W^{(k)} \rangle &= \frac{\partial}{\partial W_{ij}^{(k)}} \sum_{n=1}^{p_K} \sum_{m=1}^{|\Omega_K|} (I_K^l)_{nm} W_{nm}^{(k)} \\ &= (I_K^l)_{ij}\end{aligned}$$

Hence $\forall l = 1, \dots, M$:

$$\begin{aligned}\frac{\partial}{\partial W_{ij}^{(k)}} L(y_l, O^l) &= \frac{\partial}{\partial W_{ij}^{(k)}} L(y_l, O^l) \\ &= \frac{\partial}{\partial W_{ij}^{(k)}} \underbrace{\langle I_K^l, W^{(k)} \rangle}_{=O_k^l} \frac{\partial}{\partial O_k^l} L(y_l, O^l) \\ &= (I_K^l)_{ij} L^{(k)}(y_l, O^l)\end{aligned}$$

We also have

$$\begin{aligned}\frac{\partial}{\partial W_{ij}^{(k)}} \|W^{(k)}\|_F^2 &= \frac{\partial}{\partial W_{ij}^{(k)}} \sum_{n=1}^{p_K} \sum_{m=1}^{|\Omega_K|} (W_{nm}^{(k)})^2 \\ &= 2W_{ij}^{(k)}\end{aligned}$$

Bringing both together we get

$$\begin{aligned}\frac{\partial}{\partial W_{ij}^{(k)}} \tilde{L}(\mathcal{Z}, \mathcal{W}) &= \frac{\partial}{\partial W_{ij}^{(k)}} \left(\frac{1}{M} \sum_{l=1}^{M} L(y_l, O^l) + \frac{\lambda}{2} \sum_{r=1}^{N} \|W^{(r)}\|_F^2 \right) \\ &= \frac{1}{M} \sum_{l=1}^{M} (I_K^l)_{ij} L^{(k)}(y_l, O^l) + \lambda W_{ij}^{(k)}\end{aligned}$$

Therefore

$$\nabla_{W^{(k)}} \tilde{L}(\mathcal{Z}, \mathcal{W}) = \frac{1}{M} \sum_{l=1}^{M} L^{(k)}(y_l, O^l) I_K^l + \lambda W^{(k)}$$

5 Appendix B: Calculation of the gradient of the loss function with respect to the filters

For a training image I_0 with the true label y let $I_j^{\mathcal{Z}}$ be the output of the j-th convolutional layer given the filter matrices $\mathcal{Z} = \{Z_1, \dots, Z_K\}$.
Let $\varepsilon_i \in \mathbb{R}^{p_i \times |\Omega_i|}$, $(i \in \{1, \dots, K\})$, $\mathcal{E} = \{\varepsilon_1, \dots, \varepsilon_K\}$ be a pertubation of $\mathcal{Z}$ and $\mathcal{Z} + \mathcal{E} = \{Z_1 + \varepsilon_1, \dots, Z_K + \varepsilon_K\}$.

Lemma 1 and Proposition 1 of the paper [1] then state that there are linear functions g_j, h_j ($j \in \{1, \dots, K\}$) and a matrix $\Delta I_j^{\mathcal{Z},\mathcal{E}}$ such that

$$I_j^{\mathcal{Z}+\mathcal{E}} = I_j^{\mathcal{Z}} + \Delta I_j^{\mathcal{Z},\mathcal{E}} + o(\|\mathcal{E}\|) \text{ and } \langle \Delta I_j^{\mathcal{Z},\mathcal{E}}, U \rangle = \langle \varepsilon_j, g_j(U) \rangle + \langle \Delta I_{j-1}^{\mathcal{Z},\mathcal{E}}, h_j(U) \rangle$$

where $\|\mathcal{E}\| = \sum_{i=1}^{K} \|\varepsilon_i\|_F$.

Let $j \in \{1, \dots, K\},\ k \in \{1, \dots, p_j\},\ l \in \{1, \dots, |\Omega_j|\}$. We want to calculate $\frac{\partial}{\partial (Z_j)_{kl}} \tilde{L}(\mathcal{Z}, \mathcal{E})$.
To do that, we first define $\mathcal{E}(\delta) = \{\varepsilon_1(\delta), \dots, \varepsilon_K(\delta)\}$ with

$$\varepsilon_j(\delta)_{nm} = \begin{cases} \delta & n = k, m = l \\ 0 & \text{otherwise} \end{cases}$$
$$\varepsilon_i(\delta) = 0 \quad \forall i \neq j$$

for $\delta \in \mathbb{R}$.

Since $I_i^{\mathcal{Z}}$ only depends on the filters $Z_1, \dots, Z_i$ and $\varepsilon_i(\delta) = 0\ \forall i < j$, we obtain for all $i = 1, \dots, j-1$:

$$\begin{aligned} I_i^{\mathcal{Z}} &= I_i^{\mathcal{Z}+\mathcal{E}(\delta)} \\ &= I_i^{\mathcal{Z}} + \Delta I_i^{\mathcal{Z},\mathcal{E}(\delta)} + o(\|\mathcal{E}(\delta)\|) \\ &\Downarrow \\ \Delta I_i^{\mathcal{Z},\mathcal{E}(\delta)} &= o(|\delta|) \end{aligned}$$

Hence

$$\begin{aligned} \langle \Delta I_j^{\mathcal{Z},\mathcal{E}(\delta)}, U \rangle &= \langle \varepsilon_j(\delta), g_j(U) \rangle + \langle \Delta I_{j-1}^{\mathcal{Z},\mathcal{E}(\delta)}, h_j(U) \rangle \\ &= \delta g_j(U)_{kl} + \langle o(|\delta|), h_j(U) \rangle \end{aligned}$$

and for $i = j+1, \dots, K$

$$\begin{aligned} \langle \Delta I_i^{\mathcal{Z},\mathcal{E}(\delta)}, U \rangle &= \langle \underbrace{\varepsilon_i(\delta)}_{=0}, g_i(U) \rangle + \langle \Delta I_{i-1}^{\mathcal{Z},\mathcal{E}(\delta)}, h_i(U) \rangle \\ &= \langle \Delta I_{i-1}^{\mathcal{Z},\mathcal{E}(\delta)}, h_i(U) \rangle \\ &\vdots \\ &= \langle \Delta I_j^{\mathcal{Z},\mathcal{E}(\delta)}, h_{j+1}(\dots h_i(U)) \rangle \\ &= \delta g_j(h_{j+1}(\dots h_i(U)))_{kl} + \langle o(|\delta|), h_j(h_{j+1}(\dots h_i(U))) \rangle \end{aligned}$$

and therefore for $r = 1, \dots, N$

$$\begin{aligned}\frac{\partial}{\partial (Z_j)_{kl}} \langle I_k^{\mathcal{Z}}, W^{(r)} \rangle &= \lim_{\delta \to 0} \frac{\langle I_k^{\mathcal{Z}+\mathcal{E}(\delta)}, W^{(r)} \rangle - \langle I_k^{\mathcal{Z}}, W^{(r)} \rangle}{\delta} \\ &= \lim_{\delta \to 0} \frac{\langle I_k^{\mathcal{Z}} + \Delta I_k^{\mathcal{Z},\mathcal{E}(\delta)} + o(\|\mathcal{E}(\delta)\|), W^{(r)} \rangle - \langle I_k^{\mathcal{Z}}, W^{(r)} \rangle}{\delta} \\ &= \lim_{\delta \to 0} \frac{\langle \Delta I_k^{\mathcal{Z},\mathcal{E}(\delta)}, W^{(r)} \rangle}{\delta} + \underbrace{\lim_{\delta \to 0} \frac{\langle o(|\delta|), W^{(r)} \rangle}{\delta}}_{=0} \\ &= \lim_{\delta \to 0} \frac{\delta g_j(h_{j+1}(\dots h_K(W^{(r)})))_{kl}}{\delta} + \underbrace{\lim_{\delta \to 0} \frac{\langle o(|\delta|), h_j(h_{j+1}(\dots h_i(W^{(r)}))) \rangle}{\delta}}_{=0} \\ &= g_j(h_{j+1}(\dots h_K(W^{(r)})))_{kl}\end{aligned}$$

Hence

$$\begin{aligned}\frac{\partial}{\partial (Z_j)_{kl}} L(y, O^{\mathcal{Z}}) &= \sum_{r=1}^{N} \frac{\partial}{\partial (Z_j)_{kl}} \underbrace{\langle I_k^{\mathcal{Z}}, W^{(r)} \rangle}_{=O_r^{\mathcal{Z}}} \ \frac{\partial}{\partial O_r^{\mathcal{Z}}} L(y, O^{\mathcal{Z}}) \\ &= \sum_{r=1}^{N} g_j\left(h_{j+1}\left(\dots h_K\left(W^{(r)}\right)\right)\right)_{kl} L^{(r)}(y, O^{\mathcal{Z}}) \\ &= g_j\left(h_{j+1}\left(\dots h_K\left(\sum_{r=1}^{N} L^{(r)}(y, O^{\mathcal{Z}}) W^{(r)}\right)\right)\right)_{kl}\end{aligned}$$

since g_i, h_i are linear.

The gradient of L with respect to the filter matrix Z_j is therefore given by

$$\nabla_{Z_j} L(y, O^{\mathcal{Z}}) = g_j\left(h_{j+1}\left(\dots h_K\left(\sum_{r=1}^{N} L^{(r)}(y, O^{\mathcal{Z}}) W^{(r)}\right)\right)\right)$$

6 References

1. Mairal, J. (2016). End-to-End Kernel Learning with Supervised Convolutional Kernel Networks. ArXiv.Org. https://doi.org/10.48550/arXiv.1605.06265
2. N. Aronszajn (1950), “Theory of reproducing kernels,” Transactions of the American Mathematical Society, vol. 68, no. 3, pp. 337–404