

MASTER THESIS

Optimization of Neural Network

Author: Martin Bulín MSc. Supervisor: Ing. Luboš Šmídl Ph.D.

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in the

Department of Cybernetics

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Declaration of Authorship

I, Martin Bulín MSc., declare that this thesis titled, "Optimization of Neural Network" and the work presented in it are my own. The main methods follow on my work presented in (Bulín, 2016), however the workload is different.

I confirm that:

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- Where I have consulted the published work of others, this is always clearly attributed.
- Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- $\bullet\,$ I have acknowledged all main sources of help.

Signed:		
Date:		

 $"Look\ deep\ into\ nature,\ and\ then\ you\ will\ understand\ everything\ better."$

A. Einstein

UNIVERSITY OF WEST BOHEMIA

Abstract

Faculty of Applied Sciences
Department of Cybernetics

Engineer (Ing.)

Optimization of Neural Network

by Martin Bulín MSc.

abstract text...

Acknowledgements

 ${\it acknowledgements\ text...}$

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List of Abbreviations

AI Artificial Intelligence ANN Artificial Neural Network

MNIST Modified National Institute of Standards and Technology

MSE Mean Squared Error
PA Pruning Algorithm
RPE Rule Plus Exception

UFI Unbalanced Feature Information

XOR eXclusive **OR**

Introduction

Introduction text...

1.1 State of the Art

State of the art text... (Rosenblatt, 1958) (Reed, 1993)

1.2 Thesis Objectives

Thesis objectives text...

1.3 Thesis Outline

Thesis outline text...

Methods

Methods intro text...

2.1 Network Pruning

Network pruning text...

Network Shrinking...

2.2 Feature Selection

Minimal network structure text...

2.3 Network Visualization

Graphical user interface text...

2.4 Speech Data Gathering

Speech data classification text... (Šmídl, 2017)

Examples

The pruning algorithm is presented on several examples, where each of them has its purpose of being shown. The XOR problem (section 3.1) should verify the ability of finding an optimal network structure. Section 3.2 comes with another 2D problem, where one feature carries more information than the other one. The Rule-plus-Exception problem in section 3.3 deals with a minority of samples that has to be treated by a different net part than rule-based samples. The train problem (section 3.4) is a working example of the feature selection procedure. The MNIST database (section 3.5) is widely used in machine learning and can be regarded as commonly known, hence it is an ideal example to present new methods on. Finally, in section 3.6 the pruning algorithm is analysed on a large dataset of phonemes.

3.1 XOR Function

The standard Exclusive OR (XOR) function is defined by truth Table 3.1. Based on this function one can build a classification problem of two features and two classes.

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0

Table 3.1: XOR function.

This problem serves perfectly for a demonstration of network optimization methods, as two optimal architectural solutions producing the XOR function are already known (Fig. 3.1) 1 .

 $^{^{1}}$ The known (e.g. from (Bradley, 2006)) minimal network architectures producing the XOR function [2, 2, 1] and [2, 3, 1] are adjusted to [2, 2, 2] and [2, 3, 2] in Fig. 3.1 in order to comply with the conventions introduced in chapter 2. The number of output neurons always equals the number of classes. The number of hidden-output synapses might not be optimized in this study.

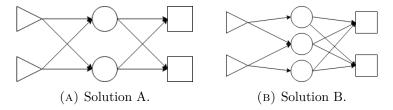


FIGURE 3.1: Optimal network architectures producing the XOR function.

With this knowledge we can prove that the pruning algorithm is (or is not) able to find the optimal solution. If the method is correct, it should end up with one of the shown architectures (Fig. 3.1a or Fig. 3.1b).

The truth Table 3.1 ruled the generation of a 2D dataset illustrated in Fig. 3.2. The two classes can be linearly separated by two lines (corresponding to two neurons, see Fig. 3.1a) and each class consists of 1000 samples. Each sample was randomly assigned to one of the two possible points belonging to its class (e.g. (0,0) or (1,1) for class 0) and then randomly placed in the surounding area within a specified range $(r = \frac{\sqrt{2}}{4})$.

The samples of each class were then splitted into three sets in the following manner: 80% to a training set, 10% to a validation set and 10% to a testing set.



FIGURE 3.2: The XOR dataset.

The goal of this example is to show that the pruning algorithm finds one of the known minimal network structures (Fig. 3.1). An oversized network [2, 50, 2] is used as the starting point. The following Table 3.2 shows all the experiment settings.

initial network		learning parameters		pruning parameters	
structure	[2, 50, 2]	learning rate 0.3		required accuracy	1.0
n synapses	200	number of epochs	50	retrain	True
transfer fcn	sigmoid	minibatch size	1	retraining epochs	50

Table 3.2: Experiment settings for the XOR example.

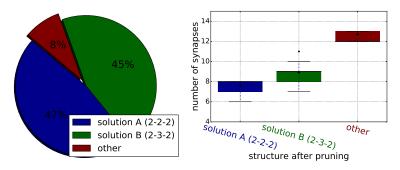
Results: XOR Function

Fig. 3.3 describes the pruning process. We can see the number of synapses, the network structure and the classification accuracy for single pruning steps (see [PA]). When the required accuracy (1.0) was not reached, the corresponding steps are transparent in the figure, indicating they were forgotten.



Figure 3.3: Illustration of the pruning procedure applied on XOR dataset (selected observation).

In Fig. 3.4 the hypothesis of this experiment is confirmed. We ran 100 observations of the experiment. In Fig. 3.4a we can see that in 47 out of 100 cases the pruning algorithm changed the network to [2, 2, 2] architecture (Fig. 3.1a), in 45% of the cases it resulted with [2, 3, 2] (Fig. 3.1b) and only in 8% it failed to find the optimal architecture. Fig. 3.4b gives statistics for the final number of synapses in these three cases.



(A) Network structure after (B) Number of synapses after pruning (100 observations). pruning (100 observations).

FIGURE 3.4: Pruning results for XOR dataset.

3.2 Unbalanced Feature Information

This example is adopted from (Karnin, 1990). The problem is again two-dimensional having two non-overlapping classes as depicted in Fig. 3.5. The samples are uniformly distributed in $[-1,1] \times [-1,1]$ and the classes are equally probable, separated by two lines in 2D space $(x_1 = a \text{ and } x_2 = b, \text{ where } a = 0.1 \text{ and } b = \frac{2}{a+1} - 1 \approx 0.82)$. Clearly, the problem can be solved by two neurons, similarly as the previous one.

What is interesting about this two-classes layout is that feature x_1 is much more important for the global classification accuracy than feature x_2 . Having x_1 information, based on Fig. 3.5 one could potentially classify more than 90% of the samples. Opposite of that, we cannot say much with information from feature x_2 only. And this is something that also the pruning algorithm should find out.

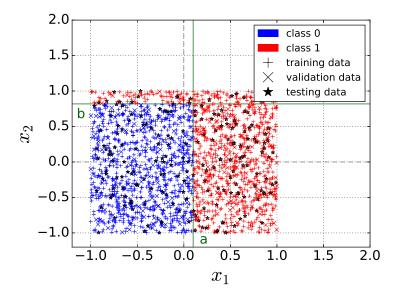


FIGURE 3.5: The UFI dataset.

Hence, we focus on synapses connecting the input and the hidden layer (shortly input-hidden synapses). We know the required network structure is [2, 2, 2], as two lines are needed to separate the data in 2D space. Actually, we even know the lines must be parallel to coordinate axes, which means that each of the hidden units needs one of the features only. Therefore, the first hypothesis here is that pruning of input-hidden synapses should result in one of the cases in Fig. 3.6.

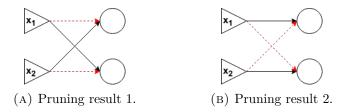


FIGURE 3.6: Expected pruning of input-hidden synapses (UFI problem).

-						
	$initial\ network$		learning parameters		pruning parameters	
	structure	[2, 2, 2]	learning rate 0.7 required accuracy		required accuracy	0.98
	n synapses	8	number of epochs	50	retrain	True
ſ	transfer fcn	sigmoid	minibatch size	1	retraining epochs	50

To prove this behaviour, we ran an experiment with settings in Table 3.3.

Table 3.3: Experiment settings for the UFI example.

The second hypothesis is that the synapse connected to the first feature (x_1) is more important and therefore, the other synapse (the one connected to feature x_2) should always be removed first.

Results: Unbalanced Feature Information

In Fig. 3.7 the first hypothesis is confirmed. We ran the experiment 100 times. In 48 cases, the pruning of input-hidden synapses finished with the result shown in Fig. 3.6a and it finished with the result shown in Fig. 3.6b in 44% of the cases.

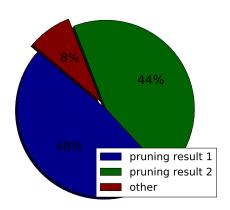


Figure 3.7: Results of pruning (see Fig. 3.6) input-hidden synapses (100 observations, UFI example).

In other words, with a probability of 92% the algorithm is able to find the axis-parallel lines and reveals that each of the lines needs the information from corresponding feature only. In the remaining 8% of the cases the pruning resulted with more than two input-hidden synapses.

The second hypothesis is confirmed in Fig. 3.8. The synapses's significance factor was always (100 observations) greater for the synapse coming from feature x_1 than for the synapse connected to x_2 . By definition (see [PA]), the pruning method eliminates the synapses with low significance factors first, therefore the information coming from feature x_1 would live longer in the network than the x_2 information.

Let's try to explain this result. Consider w_{r1} to be the weight of the synapse connecting the x_1 feature and r^{th} hidden neuron (with bias b_r) and w_{s2} to be the weight of the synapse coming from feature x_2 to s^{th} hidden neuron (with bias b_s), then by neuron definition (Rosenblatt, 1958) we created two

lines, perpendicular one to each other, as follows.

$$w_{r1} \cdot x_1 + 0 \cdot x_2 + b_r = 0 \tag{3.1}$$

$$x_1 = -\frac{b_r}{w_{r1}} \tag{3.2}$$

$$x_1 = -\frac{b_r}{w_{r1}}$$

$$0 \cdot x_1 + w_{s2} \cdot x_2 + b_s = 0$$
(3.2)
$$(3.3)$$

$$x_2 = -\frac{b_s}{w_{s2}} \tag{3.4}$$

In Fig. 3.5 we see that a < b. To generalize the problem (assuming normalised feature vectors, see chapter 2) we state |a| < |b|, meaning we want:

$$|-\frac{b_r}{w_{r1}}| < |-\frac{b_s}{w_{s2}}| \tag{3.5}$$

Hence we expect:

$$|w_{r1}| > |w_{s2}| \tag{3.6}$$

Out of this we expect a weight magnitude to be greater for more important synapses.

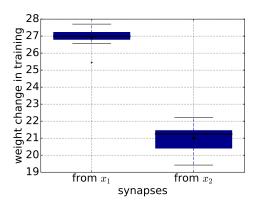


FIGURE 3.8: Weight change in training for the remaining input-hidden synapses (100 observations).

The weight magnitude seems to be a perfect measure to find feature significance factor. However, as we do not use a weight decay (see the learning approach in chapter 2), in general the more epochs we learn the greater weight magnitudes we get. Therefore small initial weight values do not affect the result significantly and so we can state:

$$|w_{ii}(t)| \approx |w_{ii}(t) - w_{ii}(0)|$$
 (3.7)

where $w_{ji}(0) \in N(0,1)$ is the initial value of weight w_{ji} and t is time. Summing it up we can say that the kitt measure [ref] based on weight change is equally good as the magnitude measure assuming enough training epochs (e.g. 50).

3.3 Rule-plus-Exception

This four-dimensional problem is originally adopted from (Mozer and Smolensky, 1989) and is also used in (Karnin, 1990). The task is to learn another Boolean function: $AB + \overline{A} \, \overline{B} \, \overline{C} \, \overline{D}$. A single function output should be on (i.e. equals 1) when both A and B are on, which is the rule, and it should also be on when the $exception \, \overline{A} \, \overline{B} \, \overline{C} \, \overline{D}$ occurs.

Clearly, the *rule* occurs more often than the *exception*, therefore the samples corresponding with the *rule* should be more important for the global classification accuracy. The hypothesis is that the pruning method should suggest the part of network, which deals with the *exception*, to be eliminated first before network elements dealing with the *rule*.

To test this hypothesis, a dataset of 10000 samples was generated. Each sample consists of four features: [a,b,c,d]. Each of these features (for every sample) was randomly set to be on (1) or off (0). Then, whenever the rule occured $(a=1 \land b=1)$, the sample was assigned to class 1 (as a rule sample). If the exception occured $(a=0 \land b=0 \land c=0 \land d=0)$, the sample was also labeled as 1 (as an exception sample). Otherwise, the sample was assigned to class 0. Thereby the generated dataset consisted of:

- 2511 *rule* samples (class 1);
- 649 exception samples (class 1);
- 6840 samples in class 0.

The function is expected to be learned by two hidden neurons, one dealing with the *rule* and the other one with the *exception*. We focus on inputhidden synapses again. Two possible expected pruning results are shown in Fig. 3.9.

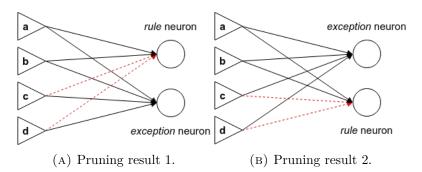


FIGURE 3.9: Expected pruning of input-hidden synapses (RPE problem).

We ran the learning-pruning procedure with the settings listed in Table 3.4.

$initial\ network$		learning parameters		pruning parameters	
structure	[2, 2, 2]	learning rate	1.0	required accuracy	1.0
n synapses	8	number of epochs	50	retrain	True
transfer fcn	sigmoid	minibatch size	1	retraining epochs	50

Table 3.4: Experiment settings for the RPE example.

Results: Rule-plus-Exception

Fig. 3.10 supports the hypothesis that one hidden neuron forms the *rule* and the other one the *exception*. With a probability of 97% the pruning finished with one of the structures in Fig. 3.9.

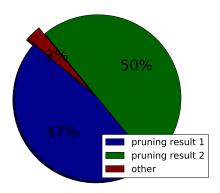


FIGURE 3.10: Results of pruning (see Fig. 3.9) input-hidden synapses (100 observations, RPE example).

The same thing is confirmed by Fig. 3.11. It shows weight change in training (kitt significance factor) for all 8 input-hidden synapses. We can see that synapses connecting the *rule* neuron with feature $c(s_{rc})$ and feature $d(s_{rd})$ were suggested as least important (resulted in structures in Fig. 3.9).



FIGURE 3.11: Weight change in training for input-hidden synapses (100 observations, RPE example).

Additionally, synapses responsible for rule (s_{ra} and s_{rb}) have a greater mean significance than the synapses connected with the exception neuron (s_{e*}).

3.4 Michalski's Trains

The train problem was originally introduced in (Larson and Michalski, 1977). The task was to determine concise decision rules distinguishing between two sets of trains (Eastbound and Westbound). In (Mozer and Smolensky, 1989), they presented a simplified version illustrated in Fig. 3.12.

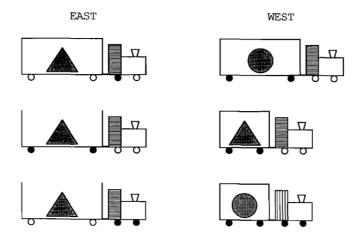


Figure 3.12: Michalski's train problem.

Each train is described by 7 binary features listed in Table 3.5.

	feature	encoded as 0	encoded as 1
0	car length	long	short
1	car type	open	closed
2	cabin pattern	vertical lines	horizontal lines
3	load shape	triangle	circle
4	color of trailer wheels	white	black
5	color of first car wheel	white	black
6	color of second car wheel	white	black

Table 3.5: Features describing a train.

Having Table 3.5 we can encode the trains shown in Fig. 3.12 into feature vectors as follows in Table 3.6.

class EAST		class WEST	
east 1	$[0, 1, 1, 0, 0, 0, 1]^T$	west 1	$[0,1,1,1,1,0,0]^T$
east 2	$[0,0,1,0,1,0,0]^T$	west 2	$[1, 1, 1, 0, 1, 0, 0]^T$
east 3	$[0,0,1,0,0,1,1]^T$	west 3	$[1,1,0,1,1,1,1]^T$

Table 3.6: Feature vectors for different train types.

The task is to determine the minimal number of input features capable of the east-west classification based on the six possible types in Table 3.6 (or in Fig. 3.12). The hypothesis is that the pruning algorithm should select the needed features by eliminating unimportant input-hidden synapses. Looking at Fig. 3.12 one of the solutions could be keeping features (0,3), because the shape of the load together with the length of the car is enough to distinguish west trains from east trains. Another solution, for example, is keeping the car length, car type and color of the second car wheel - features (0,1,6).

To test our pruning algorithm on this feature selection task, a dataset of 6000 samples (3000 west and 3000 east trains) was generated. The three possible train types for each class (Fig. 3.12) are equally distributed among the samples, meaning we have 1000 samples of each train type.

As shown in (Mozer and Smolensky, 1989), one hidden neuron is enough to learn this problem, hence we started with the network structure [7, 1, 2]. The experiment parameters are listed in Table 3.7.

initial network		learning parameters		pruning parameters	
structure	[7, 1, 2]	[1, 2] learning rate 0.3 require		required accuracy	1.0
n synapses	9	number of epochs	100	retrain	True
transfer fcn	sigmoid	minibatch size	1	retraining epochs	10

Table 3.7: Experiment settings for the train example.

We ran 100 observations of the experiment and considered the features that were not cut out, as a result of a single experiment.

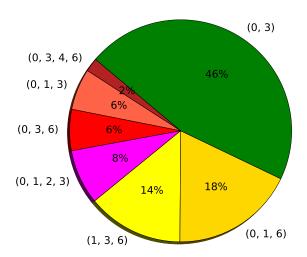


Figure 3.13: Results of feature selection by the pruning algorithm (train example). The labels corresponds with feature indices in Table 3.5.

The result pie in Fig. 3.13 shows that the pruning algorithm found the best possible solution ((0,3) - the car length and the load shape) in 46% of the cases. We can regard the (0,1,6) and (1,3,6) as another (not best but also good) solutions. The rest we consider as fail cases, as all of them include features (0,3) and the other features are redundant. To sum it up, we got a perfect solution: 46%; a good solution: 32%; a bad solution: 22%.

3.5 Handwritten digits (MNIST)

The MNIST (Modified National Institute of Standards and Technology) database (Wikipedia, 2004) is a large database of handwritten digits that is widely used for training and testing methods in the field of machine learning.

The dataset was downloaded from (LeCun and Cortes, 1998). Some of the digits were written by employees of American Census Bureau (*United States Census Bureau* 2017) and some by students of an American high school. In total 70000 samples were collected. Examples are shown in Fig. 3.14.

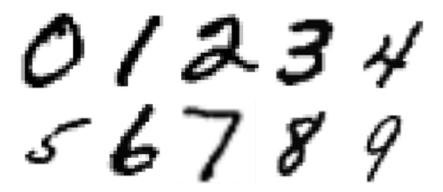


FIGURE 3.14: Examples of MNIST dataset.

Each sample is a grayscale image (normalised to [0,1]) of size 28x28 pixels. This gives row-by-row a vector of 784 features. The data was splitted into a training set of 50000 samples, a validation set of 10000 samples and a testing set of 10000 samples.

From (LeCun and Cortes, 1998) we know the problem can be learnt by a feedforward network with one hidden layer up to high accuracy (98 - 99%). The first task is to achieve similar results with the implemented neural net framework. We tested the following learning settings (Table 3.8).

network par	ameters	learning parameters		
structure	[784, 20, 10]	learning rate	0.3	
n synapses	15880	number of epochs	100	
transfer function	sigmoid	batch size	10	

Table 3.8: Settings for training a dense feedforward net on the MNIST dataset.

The training results are summarized in Table 3.9. A confusion matrix for the testing data is given in Fig. 3.15.

	accuracy	MSE
training data	97.2%	0.526
testing data	94.3%	1.025

Table 3.9: Training results on MNIST dataset.



FIGURE 3.15: Confusion matrix (MNIST, testing data).

In the following, the pruning method is analysed on networks trained on the MNIST database. Parameters of the learning-pruning procedure are listed in Table 3.10.

initial network		learning parameters		pruning parameters	
structure	[784, 20, 10]	learning rate	0.3	required accuracy	0.97
n synapses	15800	number of epochs	30	retrain	True
transfer fcn	sigmoid	minibatch size	10	retraining epochs	10

Table 3.10: Experiment settings for the MNIST example.

The hypothesis is that the initial number of synapses in the network (15800) is redundant, as well as the number of features (784). In Fig. 3.16 we can see a selected observation of the pruning process. The number of synapses was reduced to 1259 and the number of used features to 465, while the classification accuracy was kept on 97%. The pruning procedure finished in 424 pruning steps (explained in [PA]).



Figure 3.16: Illustration of the pruning procedure applied on MNIST dataset (selected observation). Required accuracy: 97%.

In Fig. 3.17, we can see a comparison of the evaluation time. We compare a fully-connected (initial) network to a pruned one. Bars are given for the three data groups (training: 50000 samples, validation: 10000 samples, testing: 10000 samples). The processing time was reduced by nearly half after the pruning, which led to a reduction of weight matrix dimension (see [SHRINK]).

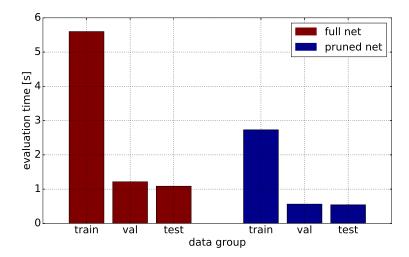


FIGURE 3.17: Evaluation (accuracy and error computation) time for all data groups (pruned vs. full net).

Fig. 3.18 gives the statistics by running 10 observations of the pruning procedure for several values of required classification accuracy. We observed the number of synapses (red axis) and used features after pruning (blue axis).



FIGURE 3.18: Minimal number of features and synapses to get required classification accuracy (MNIST data).

The results show that less than a tenth of the synapses and about a half of the features are needed to keep the maximal classification accuracy (97%). It is also worth saying that the MNIST dataset can be learnt to 50% using only 20 features and a network with 38 synapses. In the following, these two results are further analysed.

Minimal MNIST network

At first, we focus on a pruned network capable of MNIST classification with accuracy of 50% (Fig. 3.19). This example is simple enough to show the feature selection method described in [ref FS].



Figure 3.19: Result of network pruning and path tracking, MNIST data, accuracy: 50%.

Each class (digit in this case) has its color. If a hidden unit has one output connection only, it inherits the color of the class it is connected to. The features (pixels of the 28x28 image) are then colored in the same way. If a hidden unit influences more than one class, it is blacked. All features connected to a black hidden unit are then blacked as well, as they also affects more than one class.



FIGURE 3.20: Result of network pruning and path tracking (shown 17^{th} hidden neuron only), MNIST data, accuracy: 97%.

A pruned network capable of 97% accurate classification is visualized in Fig. 3.20. To make the figure clearer, only synapses coming to the 17^{th} hidden unit are drawn between the input and hidden layer.

We can see that each of the features affects more than one class in this case. Therefore we better use the visualization in Fig. 3.21.

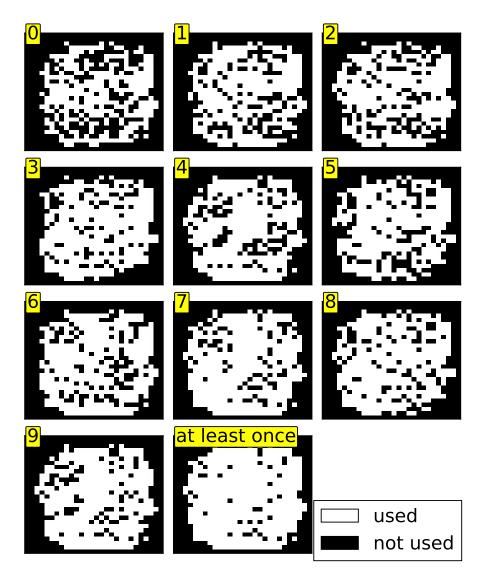


Figure 3.21: Used features for individual classes, MNIST data, accuracy: 97%.

Knowing all the remaining synapses are important for classification, we can track that paths from individual classes to features. This way we distinguish features connected to a selected class from those that do not affect that class. Fig. 3.21 shows important features for each class (digit) separately. Note that the *at-least-once* subplot corresponds to the features shown in Fig. 3.20. It shows all features used by at least one class.

Some more ideas about path tracking in pruned networks are further discussed in section 4.3.

3.6 Phonemes (Speech Data)

PHONES data...

Discussion

Discussion text...

4.1 Methods Recapitulation

Methods recapitulation text...

4.2 Comparison of Pruning Methods

Comparison of results text...

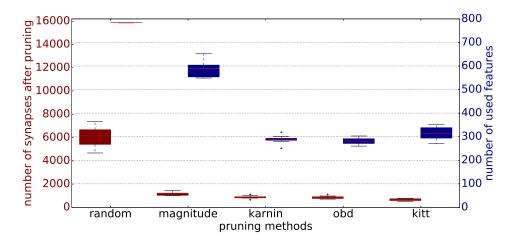


Figure 4.1: MNIST, req_acc = 0.95, retraining: 5 epochs



FIGURE 4.2: MNIST, req_acc = 0.95, no retraining

4.3 Future Work

Outlook...

Conclusion

Conclusion text...

Outlook text... shrinking layers?

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Appendix A1

Structure of the Workspace

Appendix A2

Implementation

Appendix A3

Code Documentation