

Artificial Intelligence Data Analysis (AIDA)

1st School for Heliophysicists

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LECTURE 4



Supervised Learning – Multi-Class Classification & Generalization

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FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE





Review of Lecture 3 – Unsupervised Learning

Petal length

Petal length

Setosa



(IRIS dataset initially used for classification, cf. Lecture 1)

[9] Scitkit-Learn

[10] M.Goetz, M. Riedel et al., 'HPDBSCAN – Highly Parallel DBSCAN', MLHPC Workshop at Supercomputing 2015





(using DBSCAN for outlier detection, e.g. to clean a dataset for data classification)



Estimated number of clusters: 3 Estimated number of noise points: 18

Homogeneity: 0.953

Completeness: 0.883 V-measure: 0.917

Out:



(clustering example of tweets from Twitter)

(parallelization of machine learning algorithms not trivial)

Outline of the School

Time	Day 1	Day 2	Day 3
9 - 10	Welcome and intro to the school (Giovanni Lapenta, Jorge Amaya)	Space missions data acquisition (Hugo Breuillard)	Review of ML applied to heliophysics (Peter Wintoft)
10 - 11	Introduction and differences between AI, ML, NN and Big Data (Morris Riedel)	Data manipulation in python with pandas, xarray, and additional python tools (Geert Jan Bex)	Review of ML applied to heliophysics (Peter Wintoft)
	Coffee break	Coffee break	Coffee break
11:30 - 12:30	Unsupervised learning (Morris Riedel)	Feature engineering and data reduction (Geert Jan Bex)	Reinforcement learning (Morris Riedel)
	Lunch	Lunch	Lunch
14 - 15	Unsupervised learning (Morris Riedel)	Data reduction and visualization (Geert Jan Bex)	Physics informed ML (Romain Dupuis)
15 -16	Supervised learning (Morris Riedel)	CNN, DNN (Morris Riedel)	Explainable AI (Jorge Amaya)
	Coffee break	Coffee break	Coffee break
16:30 - 18:00	Supervised learning (Morris Riedel)	CNN, DNN (Morris Riedel)	Performance and tuning of ML (Morris Riedel)

Outline

- Supervised Learning & Multi-Class Classification Problems
 - Supervised Learning Revisited & Role of Deep Learning Frameworks
 - Formalization of Machine Learning Fundamentals & Perceptron Model
 - MNIST & Multi-Class Classification Problems
 - Relevance of Data Exploration, Data Preparation & Normalization
 - Multi-Output Perceptron Learning Model
- Supervised Learning & Theory of Generalization
 - Formalization of Supervised Learning & Mathematical Building Blocks
 - Feasibility of Learning & Understanding the Theory of Generalization
 - Role Learning Algorithms, and Final Hypothesis
 - Different Models in Hypothesis Set & Unlimited 'Degrees of Freedom'
 - Using Training Dataset as Training Dataset and as Testing Dataset



Supervised Learning and Multi-Class Classification Problems



Learning Approaches – What means Learning from data – Revisited

wers of type 'IRIS Setosa'

- The basic meaning of learning is 'to use a set of observations to uncover an underlying process'
- The three different learning approaches are supervised, unsupervised, and reinforcement learning

Supervised Learning

- Majority of methods follow this approach in this course
- Example: credit card approval based on previous customer applications
- Unsupervised Learning
 - Often applied before other learning \rightarrow higher level data representation
 - Example: Coin recognition in vending machine based on weight and size
- Reinforcement Learning
 - Typical 'human way' of learning
 - Example: Toddler tries to touch a hot cup of tea (again and again)

Day 1 offers details about unsupervised & supervised learning with examples & Day 3 offers an introduction to reinforcement learning



(what type of flower is this?)

[1] Image sources: Species Iris Group of North America Database, www.signa.org



[2] A.C. Cheng et al., 'InstaNAS:



Instance-aware Neural









Learning Approaches – Supervised Learning – Revisited

- Each observation of the predictor measurement(s) has an associated response measurement:
 - Input $\mathbf{x} = x_1, ..., x_d$
 - Output $y_i, i = 1, .., n$
 - Data $(\mathbf{x}_1, y_1), ..., (\mathbf{x}_N, y_N)$
 - (the output guides the learning process as a 'supervisor')



- Goal: Fit a model that relates the response to the predictors
 - Prediction: Aims of accurately predicting the response for future observations
 - Inference: Aims to better understanding the relationship between the response and the predictors
 - Supervised learning approaches fits a model that related the response to the predictors
 - Supervised learning approaches are used in classification algorithms such as SVMs
 - Supervised learning works with data = [input, correct output]

Deep Learning Frameworks using GPUs also good for Artificial Neural Networks

TensorFlow

- One of the most popular deep learning frameworks available today
- Execution on multi-core CPUs or many-core GPUs



worker A $\overline{GPU_0}$ $\overline{CPU_0}$

worker B

 $CPU_0 \mid CPU_1$

run

master

client

[3] Tensorflow Web page



[4] Keras Web page

- Tensorflow is an open source library for deep learning models using a flow graph approach
 Tensorflow nodes model mathematical operations and graph edges between the nodes are
- so-called tensors (also known as multi-dimensional arrays)
- The Tensorflow tool supports the use of CPUs and GPUs (much more faster than CPUs)
- Tensorflow work with the high-level deep learning tool Keras in order to create models fast
- New versions of Tensorflow have Keras shipped with it as well & many further tools

Keras

- Often used in combination with low-level frameworks like Tensorflow
- Keras is a high-level deep learning library implemented in Python that works on top of existing other rather low-level deep learning frameworks like Tensorflow, CNTK, or Theano
- Created deep learning models with Keras run seamlessly on CPU and GPU via low-level deep learning frameworks
- The key idea behind the Keras tool is to enable faster experimentation with deep networks

> Day 2 offers more details on how these frameworks and tools are used with GPUs and for selected Deep Learning Techniques

Exercises – Preparing & Installing the Keras Framework



DEEP Cluster: Preparing & Installing the Keras Framework

[riedel1@deepv ~]\$ module load Python/3.6.8



[riedel1@deepv DeepLearning]\$ pip install --user keras

[4] Keras Web page



Perceptron Model – Mathematical Notation for one Neuron



Handwritten Character Recognition MNIST Dataset

- Metadata
 - Not very challenging dataset, but good for benchmarks & tutorials
- When working with the dataset
 - Dataset is not in any standard image format like jpg, bmp, or gif (i.e. file format not known to a graphics viewer)
 - Data samples are stored in a simple file format that is designed for storing vectors and multidimensional matrices (i.e. numpy arrays)
 - The pixels of the handwritten digit images are organized row-wise with pixel values ranging from 0 (white background) to 255 (black foreground)
 - Images contain grey levels as a result of an anti-aliasing technique used by the normalization algorithm that generated this dataset



NPZ file format of numpy that provides
storage of array data using gzip compression)
data()

(downloads data into ~home/.keras/datasets as

- Handwritten Character Recognition MNIST dataset is a subset of a larger dataset from US National Institute of Standards (NIST)
- MNIST handwritten digits includes corresponding labels with values 0-9 and is therefore a labeled dataset
- MNIST digits have been size-normalized to 28 * 28 pixels & are centered in a fixedsize image for direct processing
- Two separate files for training & test: 60000 training samples (~47 MB) & 10000 test samples (~7.8 MB)



MNIST Dataset – Data Access in Python & HPC Download Challenges

- Warning for very secure HPC environments
 - Note that HPC batch nodes often do not allow for download of remote files





from keras.datasets import mnist

download and shuffled as training and testing set
(X_train, y_train), (X_test, y_test) = mnist.load_data()

(downloads data into ~home/.keras/datasets as NPZ file format of numpy that provides storage of array data using gzip compression)

Exercises – Download MNIST Data



DEEP Cluster: Download MNIST Data

- Execute on Login-Node the Data Exploration Script to Download MNIST Data
 - Load the following module environment:



Python explore-MNIST-training.py
Provide use with the descent with the with training of the use with the descent with training of the use with the descent with training of the use with the descent with training of the use with training

MNIST Dataset – Training/Testing Datasets & One Character Encoding

- Different phases in machine learning
- Training phases is a hypothesis search
- Testing phase checks if we are on the right track once the hypothesis is clear
- Validation phane for model selection (set fixed parameters and set model types)
- Work on two disjoint datasets
 - One for training only (i.e. training set)
 - One for testing only (i.e. test set)
 - Exact seperation is rule of thumb per use case (e.g. 10 % training, 90% test)
 - Practice: If you get a dataset take immediately test data away ('throw it into the corner and forget about it during modelling')
 - Once we learned from training data it has an 'optimistic bias'
 - Usually start by exploring the dataset and its format & labels



(historical records, groundtruth data, examples)

MNIST Dataset – Data Exploration Script Training Data & JupyterLab Example



MNIST Dataset with Perceptron Learning Model – Need for Reshape

- Two dimensional dataset (28 x 28)
 - Does not fit well with input to Perceptron Model
 - Need to prepare the data even more
 - Reshape data → we need one long vector



Label:

Lecture 4 – Supervised Learning – Multi-Class Classification & Generalization

- Note that the reshape from two dimensional MNIST data to one long vector means that we loose the surrounding context
- Loosing the surrounding context is one factor why later in this lecture deep learning networks achieving essentially better performance by, e.g., keeping the surrounding context



18 / 50

MNIST Dataset – Reshape & Normalization – Example



								(tv	vo	di	me	ens	io	na	١o	rig	in	al i	inp	out	:)						
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0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	Θ	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	3	18	18	18	126	136	175	26	166	255	247	127	0	0	0	0
0	0	0	0	0	0	0	0	30	36	94	154	170	253	253	253	253	253	225	172	253	242	195	64	0	0	0	Θ
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Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	14	1	154	253	90	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ	Θ
0	0	0	0	0	0	0	0	0	0	0	139	253	190	2	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	Θ	0	0	0	11	190	253	70	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	35	241	225	160	108	1	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	81	240	253	253	119	25	0	0	0	0	0	0	0	0	0
0	0	0	0	Θ	0	0	Θ	0	0	0	0	0	0	45	186	253	253	150	27	0	0	0	0	0	0	0	Θ
0	0	0	0	0	0	0	Θ	0	0	0	0	0	0	0	16	93	252	253	187	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Θ	0	249	253	249	64	0	0	0	Θ	0	0	Θ
0	0	0	0	0	0	0	0	0	0	0	0	0	0	46	130	183	253	253	207	2	0	0	0	Θ	0	0	Θ
0	0	0	0	0	0	0	0	0	0	0	0	39	148	229	253	253	253	250	182	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	Θ	0	0	24	114	221	253	253	253	253	201	78	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	23	66	213	253	253	253	253	198	81	2	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	18	171	219	253	253	253	253	195	80	9	0	0	0	0	0	0	0	0	0	0	0	0
Θ	Θ	0	Θ	55	172	226	253	253	253	253	244	133	11	0	Θ	Θ	0	Θ	0	Θ	Θ	Θ	Θ	Θ	0	0	Θ
0	0	0	0	136	253	253	253	212	135	132	16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	Θ	Θ	0	0	Θ	Θ	Θ	Θ	0	Θ	Θ	Θ	0	Θ	Θ	Θ	0	Θ	Θ	Θ	0	Θ	0	Θ	Θ
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Label:

Exercises – Perform Reshape & Normalization on Different Training / Testing Data



MNIST Dataset & Multi Output Perceptron Model

10 Class Classification Problem

Use 10 Perceptrons for 10 outputs with softmax activation function (enables probabilities for 10 classes)



- Note that the output units are independent among each other in contrast to neural networks with one hidden layer
- The output of softmax gives class probabilities
- The non-linear Activation function 'softmax' represents a generalization of the sigmoid function it squashes an n-dimensional vector of arbitrary real values into a n-dimenensional vector of real values in the range of 0 and 1 – here it aggregates 10 answers provided by the Dense layer with 10 neurons

= 7850)

Layer (type)	Output	Shape	Param #
dense_1 (Dense)	(None,	10)	7850
activation_1 (Activation) Total params: 7,850 Trainable params: 7,850 Non-trainable params: 0	(None,	10)	0

MNIST Dataset & Compile Multi Output Perceptron Model

Compile the model

- Optimizer as algorithm used to update weights while training the model
- Specify loss function (i.e. objective function) that is used by the optimizer to navigate the space of weights
- (note: process of optimization is also called loss minimization, cf. Invited lecture Gabriele Cavallaro)
- Indicate metric for model evaluation (e.g., accuracy)
- Specify loss function
 - Compare prediction vs. given class label
 - E.g. categorical crossentropy

specify loss, optimizer and metric model.compile(loss='categorical_crossentropy', optimizer=OPTIMIZER, metrics=['accuracy'])



- Compile the model to be executed by the Keras backend (e.g. TensorFlow)
- Optimizer Gradient Descent (GD) uses all the training samples available for a step within a iteration
- Optimizer Stochastic Gradient Descent (SGD) converges faster: only one training samples used per iteration
- Loss function is a multi-class logarithmic loss: target is *ti,j* and prediction is *pi,j*
- Categorical crossentropy is suitable for multiclass label predictions (default with softmax)

$$L_i = -\Sigma_j t_{i,j} \log(p_{i,j})$$

[6] Big Data Tips, Gradient Descent

Full Script: MNIST Dataset – Model Parameters & Data Normalization



print(X_train.shape[0], 'train samples')
print(X test.shape[0], 'test samples')

(historical records, groundtruth data, examples)

Full Script: MNIST Dataset – Fitting a Multi Output Perceptron Model



Exercises – Execute Multi Output Perceptron Model



MNIST Dataset – A Multi Output Perceptron Model – Output & Evaluation

Epoch 7/20							
60000/60000	[=====]	- 2	s 26us/step	- loss:	0.4419 -	- acc:	0.8838
Epoch 8/20							
60000/60000	[=====]	- 2	s 26us/step	- loss:	0.4271 -	- acc:	0.8866
Epoch 9/20							
60000/60000	[=====]	- 2	s 25us/step	- loss:	0.4151 -	- acc:	0.8888
Epoch 10/20							
60000/60000	[=====]	- 2	s 26us/step	- loss:	0.4052 -	- acc:	0.8910
Epoch 11/20							
60000/60000	[=====]	- 2	s 26us/step	- loss:	0.3968 -	- acc:	0.8924
Epoch 12/20							
60000/60000	[=====]	- 2	s 25us/step	- loss:	0.3896 -	- acc:	0.8944
Epoch 13/20							
60000/60000	[=====]	- 2	s 26us/step	- loss:	0.3832 -	- acc:	0.8956
Epoch 14/20							
60000/60000	[=====]	- 2	s 25us/step	- loss:	0.3777 -	- acc:	0.8969
Epoch 15/20							
60000/60000	[]	- 2	s 25us/step	- loss:	0.3727 -	- acc:	0.8982
Epoch 16/20							
60000/60000	[=====]	- 1	s 24us/step	- loss:	0.3682 -	- acc:	0.8989
Epoch 17/20							
60000/60000	[]	- 1	s 25us/step	- loss:	0.3641 -	- acc:	0.9001
Epoch 18/20							
60000/60000	[=====]	- 1	s 25us/step	- loss:	0.3604 -	- acc:	0.9007
Epoch 19/20							
60000/60000	[=====]	- 2	s 25us/step	- loss:	0.3570 -	- acc:	0.9016
Epoch 20/20							
60000/60000	[]	- 1	s 24us/step	- loss:	0.3538 -	- acc:	0.9023

model evaluation

score = model.evaluate(X_test, Y_test, verbose=VERBOSE)
print("Test score:", score[0])
print('Test accuracy:', score[1])

10000/10000 [======] - 0s 41us/step Test score: 0.33423959468007086 Test accuracy: 0.9101



- How to improve the model design by extending the neural network topology?
- Which layers are required?
- Think about input layer need to match the data what data we had?
- Maybe hidden layers?
- How many hidden layers?
- What activation function for which layer (e.g. maybe ReLU)?
- Think Dense layer Keras?
- Think about final Activation as Softmax → output probability

[Video] Multi Output Perceptron – More Details



[8] YouTube Video, The Linear model with Multiple Inputs and Multiple Outputs Detail Explanation

Formalization of Supervised Learning & Theory of Generalization



Exercises – Execute Multi Output Perceptron Model and Test on Training Dataset



Learning Approaches – Supervised Learning – Formalization

- Each observation of the predictor measurement(s) has an associated response measurement:
 - Input $\mathbf{x} = x_1, ..., x_d$
 - Output $y_i, i = 1, .., n$
 - Data $(\mathbf{x}_1, y_1), ..., (\mathbf{x}_N, y_N)$
 - (the output guides the learning process as a 'supervisor')



- Goal: Fit a model that relates the response to the predictors
 - Prediction: Aims of accurately predicting the response for future observations
 - Inference: Aims to better understanding the relationship between the response and the predictors
 - Supervised learning approaches fits a model that related the response to the predictors
 - Supervised learning approaches are used in classification algorithms such as SVMs
 - Supervised learning works with data = [input, correct output]

Training Exa	mples
$(\mathbf{x}_{_{1}},y_{_{1}}),,($	$(\mathbf{x}_{_N},y_{_N})$

(historical records, groundtruth data, examples)

Feasibility of Learning from Data – Formalization

- Theoretical framework underlying practical learning algorithms
 - E.g. Support Vector Machines (SVMs)
 - Best understood for 'Supervised Learning'
 - Valid for bascially all machine learning algorithms
- Theoretical background used to solve 'A learning problem'
 - Inferring one 'target function' that maps between input and output
 - Learned function can be used to predict output from future input (fitting existing data is not enough)

Unknown Target Function	
$f:X\to Y$	

(ideal function)

Summary Terminologies & Importance of Theory of Generalization

Target Function

- Ideal function that 'explains' the data we want to learn
- Labelled Dataset (samples)
 - 'in-sample' data given to us:
- Learning vs. Memorizing
 - The goal is to create a system that works well 'out of sample'
 - In other words we want to classify 'future data' (ouf of sample) correct
- Dataset Part One: Training set
 - Used for training a machine learning algorithms
 - Result after using a training set: a trained system

Dataset Part Two: Test set

- Used for testing whether the trained system might work well
- Result after using a test set: accuracy of the trained model







Mathematical Building Blocks (1) – Our Linear Example



Feasibility of Learning – Hypothesis Set & Final Hypothesis

- The 'ideal function' will remain unknown in learning
 - Impossible to know and learn from data
 - If known a straightforward implementation would be better than learning
 - E.g. hidden features/attributes of data not known or not part of data
- But '(function) approximation' of the target function is possible
 - Use training examples to learn and approximate it
 - Hypothesis set \mathcal{H} consists of m different hypothesis (candidate functions)







Mathematical Building Blocks (2) – Our Linear Example



Lecture 4 - Supervised Learning - Multi-Class Classification & Generalization

The Learning Model: Hypothesis Set & Learning Algorithm

- The solution tools the learning model:
 - 1. Hypothesis set \mathcal{H} a set of candidate formulas /models
 - 2. Learning Algorithm \mathcal{A} 'train a system' with known algorithms





Mathematical Building Blocks (3) – Our Linear Example



Lecture 4 – Supervised Learning – Multi-Class Classification & Generalization

Different Models – Hypothesis Set & Unlimited 'Degrees of Freedom'

Hypothesis Set

$$\mathcal{H} = \{h\}; g \in \mathcal{H}$$

 $\mathcal{H} = \{h_1, ..., h_m\};$
(all candidate functions
derived from models
and their parameters)
Choosing from various model approaches h₁,
..., h_m is a different hypothesis
additionally a change in model parameters of
h₁, ..., h_m means a different hypothesis too
'select one function'
that best approximates
Final Hypothesis

Final Hypothesis g pprox f



(e.g. support vector machine model)



(e.g. artificial neural network model)

Lecture 4 - Supervised Learning - Multi-Class Classification & Generalization

MNIST Data – Testing on Training Dataset – Results & Discussion

- Memorizing vs. Generalization
 → How much we got?
 - We memorize the data and created a model from it
 - No unseen data used → this no generalization!

L0112/60000	[====>] - ETA: 1s
1552/60000	[====>] - ETA: 1s
12960/60000	[====>] - ETA: 1s
14400/60000	[=====>] - ETA: 1s
15840/60000	[=====>] - ETA: 1s
17280/60000	[=====>] - ETA: 1s
L8752/60000	[======>] - ETA: 1s
20192/60000	[=======>] - ETA: 1s
21632/60000	[=======>] - ETA: 1s
23072/60000	[========>] - ETA: 1s
24512/60000	[========>] - ETA: 1s
25952/60000	[========>] - ETA: 1s
27392/60000	[========>] - ETA: 1s
28832/60000	[=============>] - ETA: 1s
30272/60000	[==============>] - ETA: 1s
31712/60000	[==============>] - ETA: 0s
33152/60000	[==============>] - ETA: 0s
34592/60000	[================>] - ETA: Os
36032/60000	[======] - ETA: 0s
37472/60000	[=================>] - ETA: Os
88912/60000	[=================>] - ETA: Os
10352/60000	[==================>] - ETA: 0s
1792/60000	[==================>] - ETA: Os
3232/60000	[======] - ETA: Os
4672/60000	[======] - ETA: Os
6080/60000	[======] - ETA: 0s
7520/60000	[======] - ETA: 0s
18768/60000	[=====================================
50208/60000	[=====================================
51648/60000	[======] - ETA: 0s
3088/60000	[======] - ETA: Os
54528/60000	[=====================================
5968/60000	[=====================================
57408/60000	[=====>] - ETA: Os
58848/60000	[=====================================
60000/60000	[=====] - 2s 35us/step
lsing Tensor	Flow backend.
est score:	0.035654142725043254
est accuracy	y: 0.9916

Exercises – Train Perceptron on Testing Dataset and Test on Training Dataset



Exercises – Train on Testing Dataset & Test on Training Dataset & Increase Epochs



[Video] Neural Networks Summary



[7] YouTube Video, Neural Networks – A Simple Explanation

Lecture Bibliography



Lecture Bibliography

- [1] Species Iris Group of North America Database, Online: <u>http://www.signa.org</u>
- [2] Cheng, A.C, Lin, C.H., Juan, D.C., InstaNAS: Instance-aware Neural Architecture Search, Online: https://arxiv.org/abs/1811.10201
- [3] Tensorflow, Online: <u>https://www.tensorflow.org/</u>
- [4] Keras Python Deep Learning Library, Online: <u>https://keras.io/</u>
- [5] Jupyter Web Page, Online: <u>https://jupyter.org/</u>
- [6] Big Data Tips, 'Gradient Descent', Online: <u>http://www.big-data.tips/gradient-descent</u>
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Enjoying our yearly research group dinner 'Iceland Section' to celebrate our

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