Data Science and Machine Learning in Python

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Topics covered in the online lectures

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Part 1: Data Science

	Date	Topics covered
1	Apr 13th	Course introduction Data Science motivation How to use Jupyter Notebook Python types and lists Loops, if/else, functions
2	Apr 20th	Python tuples, lists, dictionaries Functions Numpy basics, operations Image processing
3	Apr 27th	Pandas Series, DataFrame Pandas basic operations Import/export files
4	May 4th	Principles of data visualization Data cleaning and preparation Join, combine and reshape data
5	May 11th	Volkswohl Bund dataset Data visualization in Python How to write Data Science reports Data aggregation and grouping

Part 2: Machine Learning

	Date	Topics covered
6	Jun 1st	Introduction to supervised learning Classification and regression scikit-learn k-Nearest Neighbors Linear regression (ridge and lasso)
7	Jun 8th	Linear classification models Decision trees Random forests and gradient boosting
8	Jun 15th	Kernel support vector machines Neural networks
9	Jun 22nd	Introduction to unsupervised learning Preprocessing and scaling Dimensionality reduction Principal component analysis
10	Jun 29th	k-means clustering Hierarchical clustering DBSCAN
11	Jul 6th	Representing data Engineering features Model evaluation and improvement Text data analysis

Deadlines for Submission and Distribution of Grading

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Student task	Deliverables	Deadline	Work	Share of grade
W01 Assignment	Code and results	Apr 26th	Team A	5.0%
W02 Case Study	Code / presentation slides	May 22nd	Team B	18.0%
W02 Case Study	Peer review*	May 31st	Individual	2.0%
W03 Assignment	Code and results	May 29th	Team B	5.0%
W04 Assignment	Code and results	Jun 12th	Team C	10.0%
W05 Assignment	Code and results	Jun 26th	Team D	7.0%
W06 Assignment	Code and results	Jul 8th	Team D	13.0%
W07 Case Study	Code / presentation slides	Jul 17th	Team D	22.0%
W07 Case Study	Peer review*	Jul 31st	Individual	3.0%
DataCamp 1	Finish course	May 9th	Individual	2.5%
DataCamp 2	Finish course	May 30th	Individual	2.5%
DataCamp 3	Finish course	Jun 20th	Individual	2.5%
DataCamp 4	Finish course	Jul 11th	Individual	2.5%

* Peer review is mandatory. Quality of peer review itself is graded. Not providing peer review at all would result in high point deduction

Agenda for online lecture 8

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Session	Topic	Mode	Materials used	Minutes	End
14:30-16:00	Organizational questions	Q&A		10	14:40
	Bank Marketing data	Team work in break-out rooms	Lecture 08a notebook	45	15:25
	Kernel SVM	Lecture / Q&A	Lecture slides	15	15:40
	Neural networks	Lecture / Q&A	Lecture slides	15	15:55
16:10-17:40	Telco Customer Churn	Lecture / Q&A	Lecture 08b notebook	30	16:40
	Online retail exercise 1+2	Team work in break-out rooms	Lecture 08c notebook	40	17:20
	Online retail exercise 1	Lecture / Q&A	Lecture 08c notebook	15	17:35
17:50-19:20	Online retail exercise 2+3	Team work in break-out rooms	Lecture 08c notebook	30	18:20
	Online retail exercise 2	Lecture / Q&A	Lecture 08c notebook	10	18:30
	Online retail exercise 3	Team work in break-out rooms	Lecture 08c notebook	30	19:00
	Online retail exercise 3	Lecture / Q&A	Lecture 08c notebook	10	19:10
	Organizational questions	Q&A		10	19:20

Types of problems

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Supervised Approaches

- Labeled data
- Target values known

Classification

- Predict category

Regression

- Predict numeric value

Unsupervised Approaches

- Unlabeled data
- No target value provided

Cluster Analysis

- Organize similar cases into segments

Dimensionality reduction

- Reduce number of features

Question for discussion

- Find examples for each of the 4 categories

Linear Support Vector Machines

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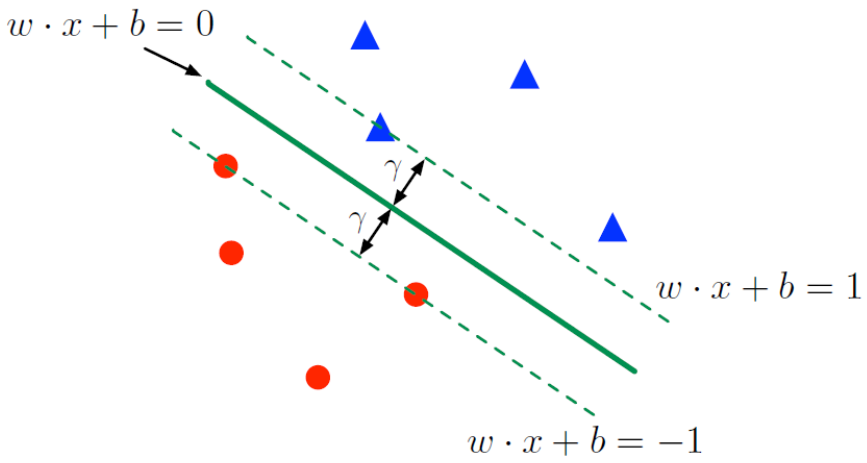
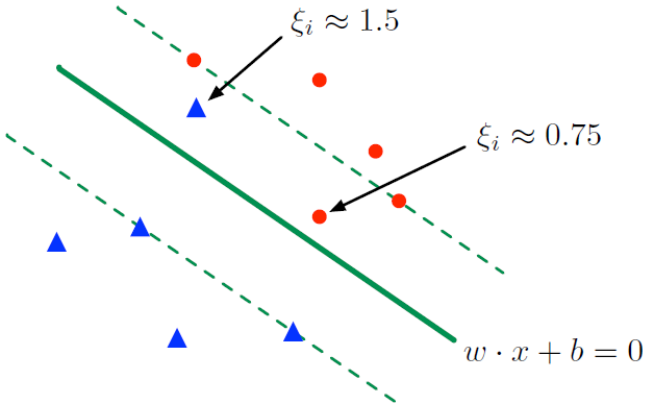
Maximize margin $\gamma = \frac{1}{\|w\|}$



Minimize slack ξ



Source: UCSanDiegoX DSE220x – Machine Learning Fundamentals

Linear Support Vector Machines

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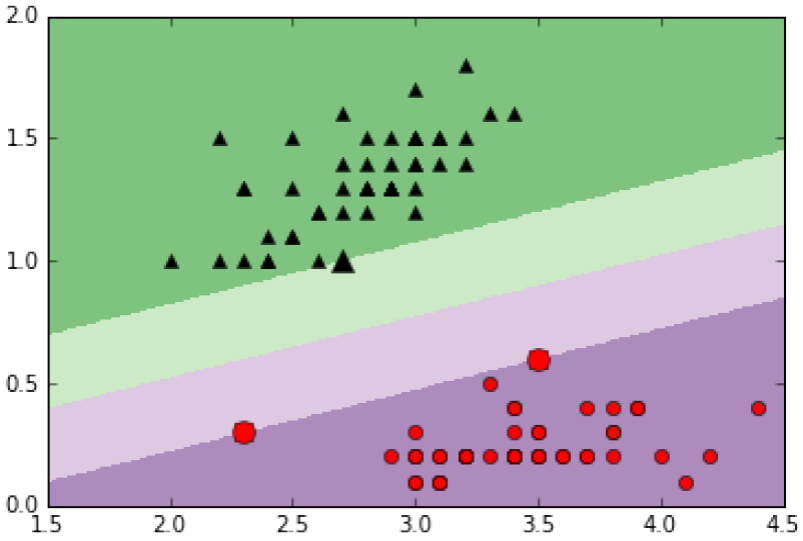
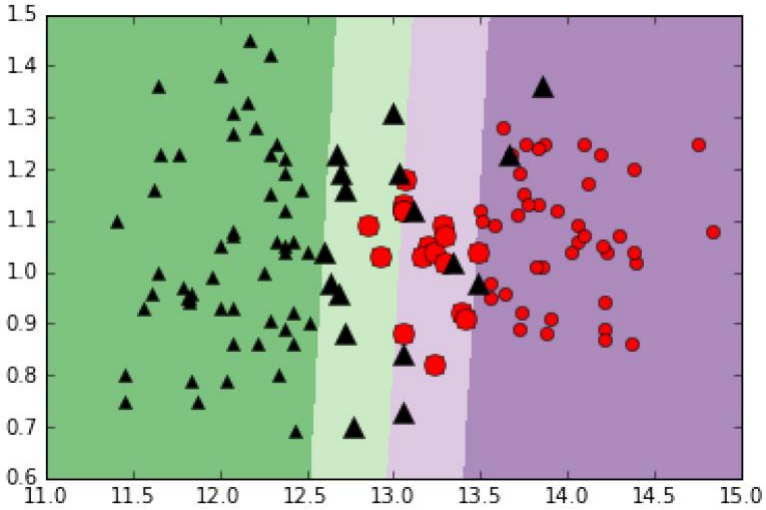
Support vectors





Source: UCSanDiegoX DSE220x – Machine Learning Fundamentals

Linear Binary Classification – Formulas

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Given training input data $\boldsymbol{x^{(1)}, \ldots, x^{(n)}} \in \mathbb{R}^{\boldsymbol{d}}$ with labels $\boldsymbol{y^{(1)}, \ldots, y^{(n)}} \in \{-\mathbf{1}, \mathbf{1}\}$.

Try to find $\boldsymbol{w} \in \mathbb{R}^{\boldsymbol{d}}$ and $\boldsymbol{b} \in \mathbb{R}$, so that

$$\mathbf{sign}\left(\boldsymbol{w} \cdot \boldsymbol{x^{(i)}} + \boldsymbol{b}\right) = \boldsymbol{y^{(i)}}$$

as often as possible.

Logistic regression

Minimize

$$\boldsymbol{L(w, b)} = -\ln\left(\prod_{\boldsymbol{i=1}}^{\boldsymbol{n}} \boldsymbol{Pr_{w,b}}\left(\boldsymbol{y^{(i)}} \mid \boldsymbol{x^{(i)}}\right)\right) + \boldsymbol{\lambda}\|\boldsymbol{w}\|_{\mathbf{2}}^{\mathbf{2}} = -\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \ln\left(\frac{\mathbf{1}}{\mathbf{1} + \boldsymbol{e}^{-\boldsymbol{y^{(i)}}\left(\boldsymbol{w} \cdot \boldsymbol{x^{(i)}} + \boldsymbol{b}\right)}}\right) + \boldsymbol{\lambda}\|\boldsymbol{w}\|_{\mathbf{2}}^{\mathbf{2}}$$

Linear support vector machines

Hard margin

$$\min_{\boldsymbol{w} \in \mathbb{R}^{\boldsymbol{d}}, \boldsymbol{b} \in \mathbb{R}} \|\boldsymbol{w}\|_{\mathbf{2}}^{\mathbf{2}} \quad \text{such that} \quad \boldsymbol{y^{(i)}}\left(\boldsymbol{w} \cdot \boldsymbol{x^{(i)}} + \boldsymbol{b}\right) \geq 1$$

Soft margin

$$\min_{\boldsymbol{w} \in \mathbb{R}^{\boldsymbol{d}}, \boldsymbol{b} \in \mathbb{R}, \boldsymbol{\xi} \in \mathbb{R}^{\boldsymbol{n}}} \|\boldsymbol{w}\|_{\mathbf{2}}^{\mathbf{2}} + \boldsymbol{K}\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \boldsymbol{\xi_i} \quad \text{such that} \quad \boldsymbol{y^{(i)}}\left(\boldsymbol{w} \cdot \boldsymbol{x^{(i)}} + \boldsymbol{b}\right) \geq \mathbf{1} - \boldsymbol{\xi_i}, \quad \boldsymbol{\xi} \geq \mathbf{0}$$

Source: UCSanDiegoX DSE220x – Machine Learning Fundamentals

Linear Models – Summary

Parameters

- Regularization parameter alpha and C
- Model type lasso vs. ridge for regression / logistic vs. SVM for classification

Strengths

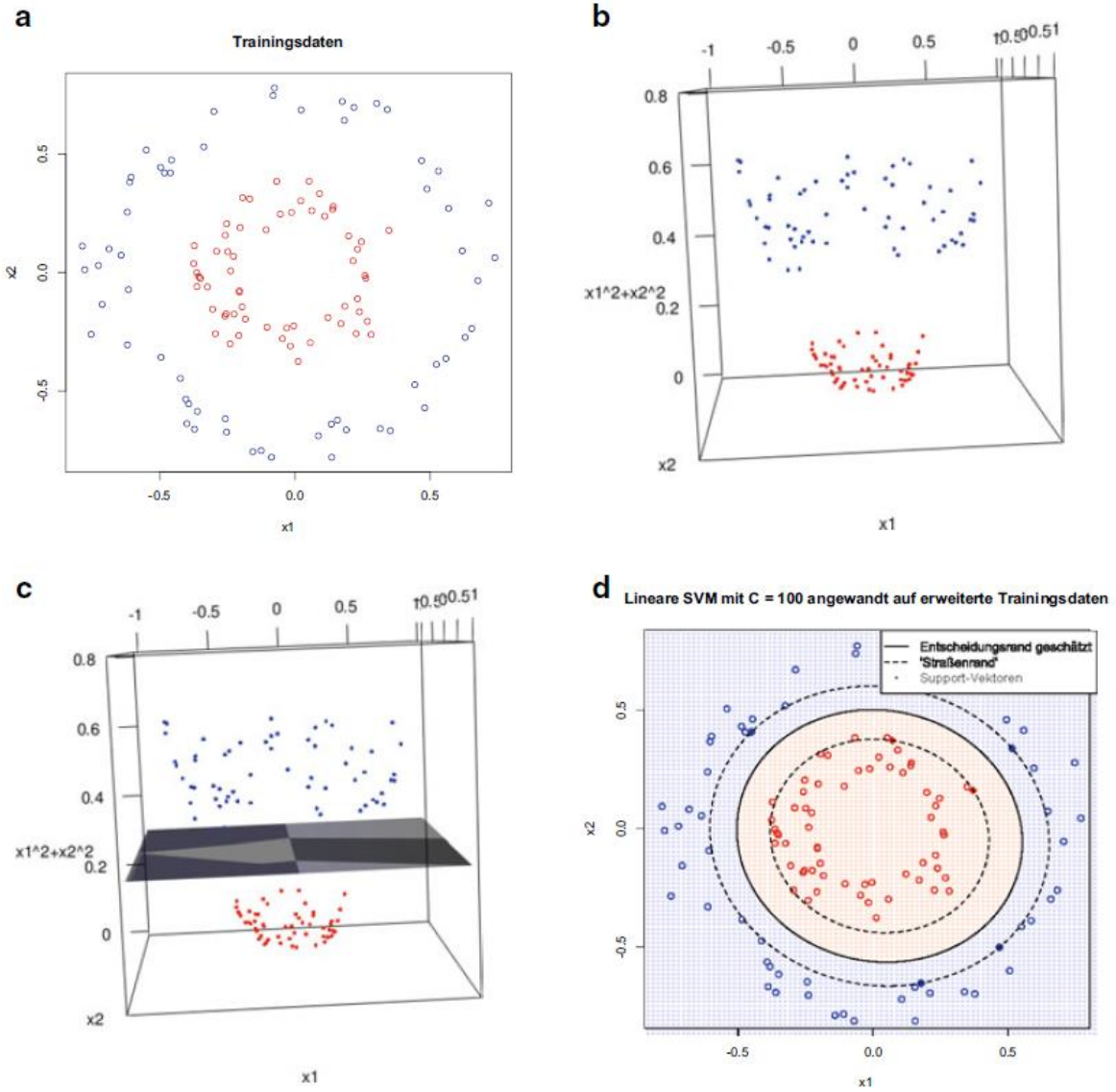
- Fast to train, fast to predict
- Work well with sparse data
- Relatively easy to understand how predictions are made
- Work well with large number of features

Weaknesses

- Coefficients hard to interpret, especially if features are highly correlated
- Sometimes fail with small datasets
- Perform bad with non-linear features and datasets that are not linearly separable

Source: Müller, A. C., Guido, S. (2016) Introduction to Machine Learning with Python : A Guide for Data Scientists, O'Reilly Media

SVM: Motivation for Polynomial Kernels



Source: Richter, S. (2019). Statistisches und maschinelles Lernen. Springer Spektrum.

SVM: Polynomial basis expansion

Input variables

$$x = (x_1, x_2, x_3)$$

Extended input variables (degree p=2)

$$\phi(x) = \left(x_1, x_2, x_3, x_1^2, x_2^2, x_3^2, x_1x_2, x_1x_3, x_2x_3\right)$$

Extended input variables (degree p=3)

$$\phi(x) = \left(x_1, x_2, x_3, x_1^2, x_2^2, x_3^2, x_1x_2, x_1x_3, x_2x_3, x_1^3, x_2^3, x_3^3, x_1^2x_2, x_1^2x_3, x_2^2x_1, x_2^2x_3, x_3^2x_1, x_3^2x_2, x_1x_2x_3\right)$$

Kernel trick

$$\phi(x) \cdot \phi(y) = (1 + x \cdot y)^p$$

SVM: Gauß kernel

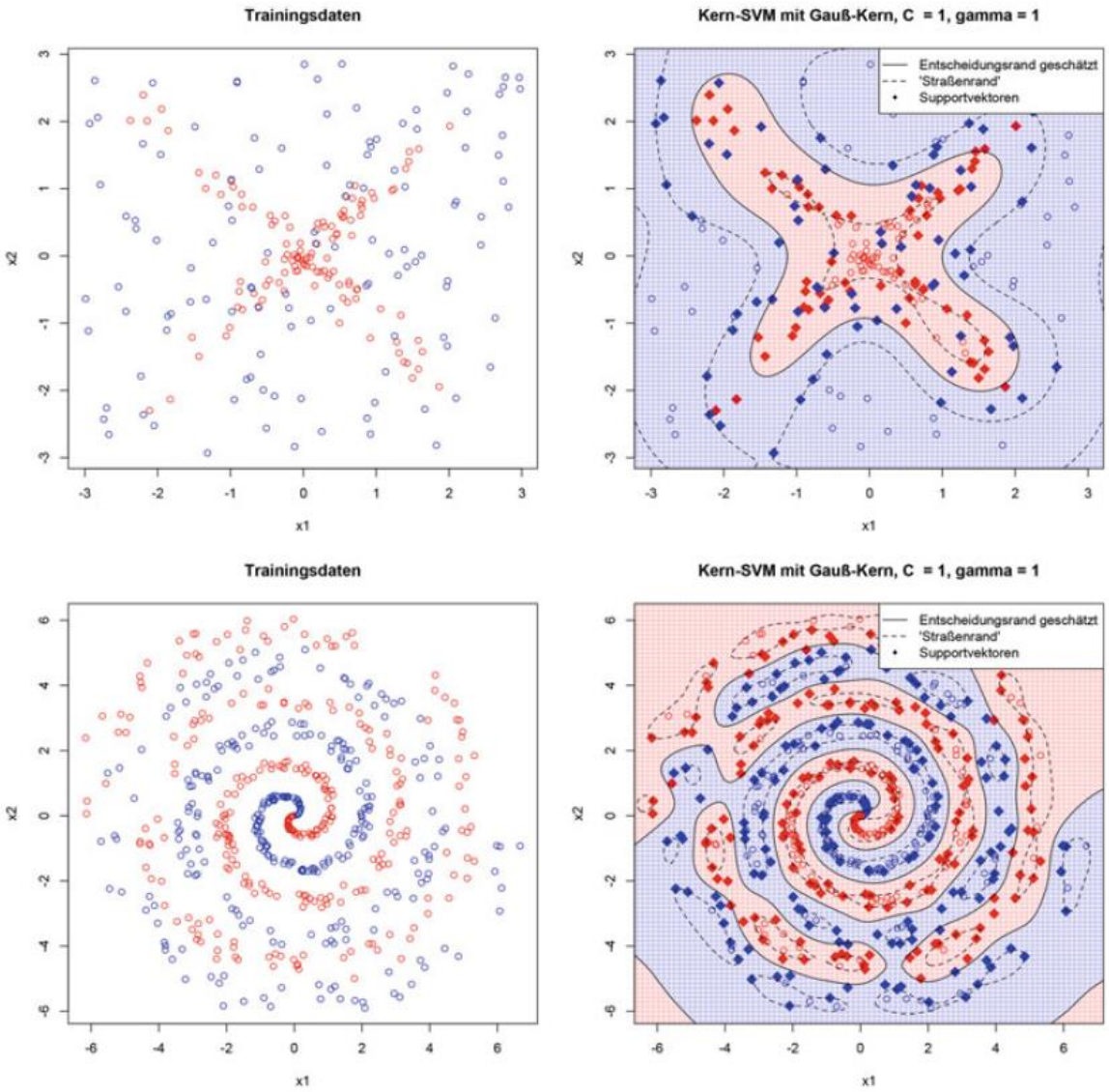
Polynomial kernel

$$\boldsymbol{\phi}(\boldsymbol{x}) \cdot \boldsymbol{\phi}(\boldsymbol{y}) = (\mathbf{1} + \boldsymbol{x} \cdot \boldsymbol{y})^{\boldsymbol{p}}$$

Gaussian (RBF) kernel

$$\boldsymbol{\phi}(\boldsymbol{x}) \cdot \boldsymbol{\phi}(\boldsymbol{y}) = \boldsymbol{e}^{-\boldsymbol{\gamma}\|\boldsymbol{x}-\boldsymbol{y}\|^2}$$

SVM: Gauß Kernel Graphics



Source: Richter, S. (2019). Statistisches und maschinelles Lernen. Springer Spektrum.

Kernelized Support Vector Machines – Summary

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Parameters

- Regularization parameter C
- Kernel “poly” or “rbf”
- Kernel specific parameters “degree” or “gamma”

Strengths

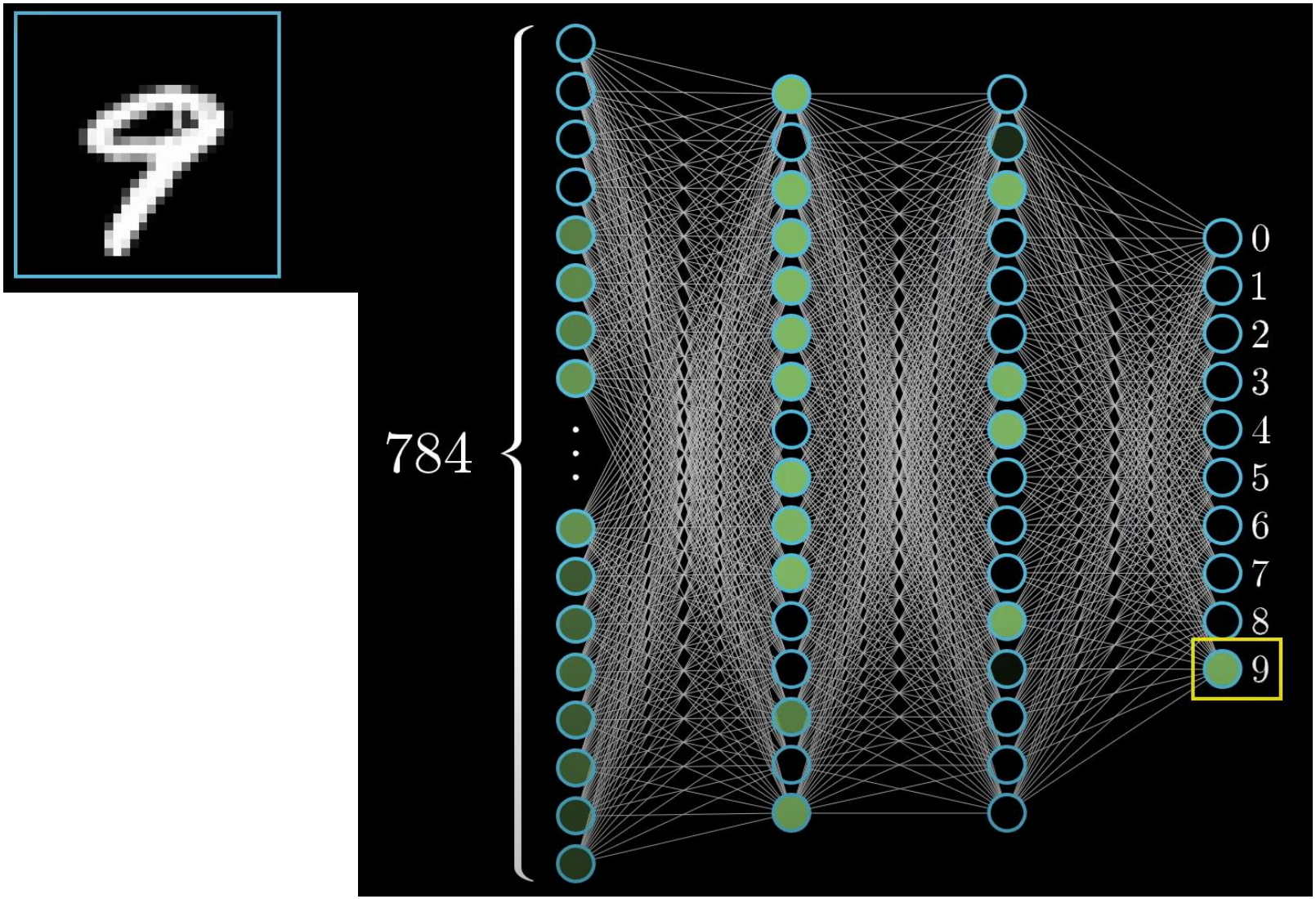
- Complex decision boundaries
- Work well with few and also many features
- Work well, if all features are on same scale / in same units

Weaknesses

- Runtime and memory usage challenges with high number of samples
- Require preprocessing / scaling of data to get good results
- Results hard to interpret, difficult to explain to non-experts

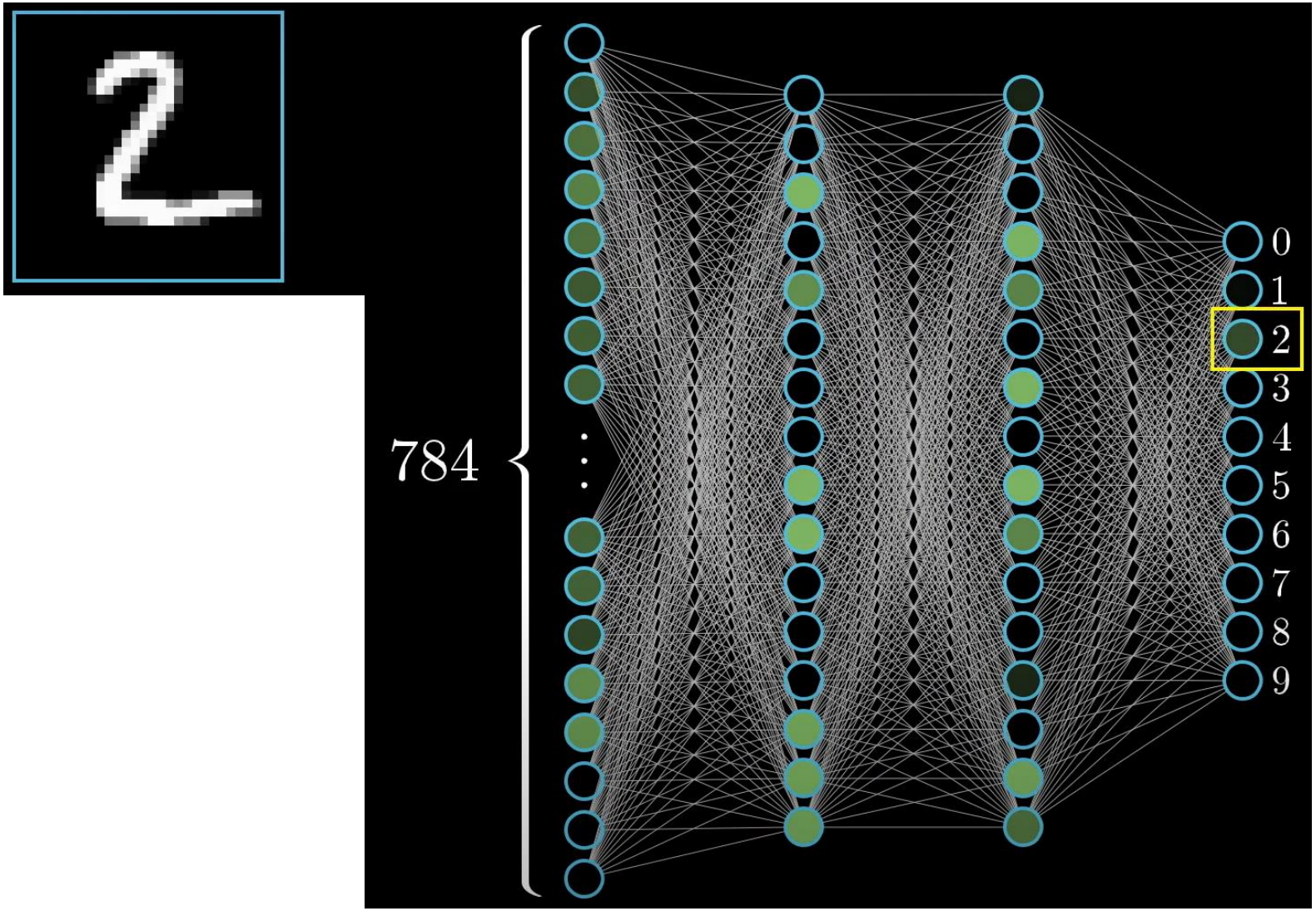
Source: Müller, A. C., Guido, S. (2016) Introduction to Machine Learning with Python : A Guide for Data Scientists, O'Reilly Media

Neural Networks



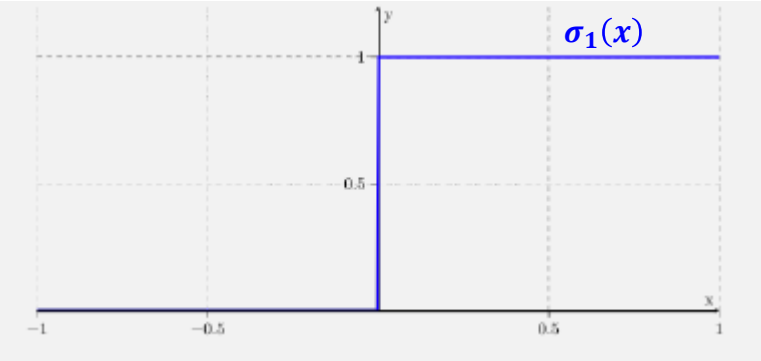
Source: https://ki-campus.org/node/209 / https://www.youtube.com/watch?v=aircAruvnKk

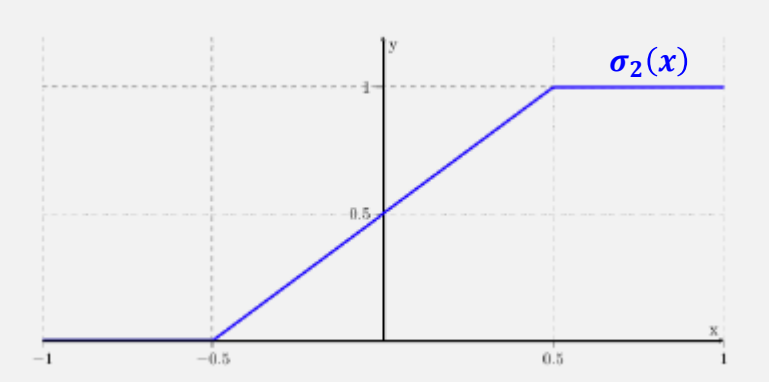
Neural Networks

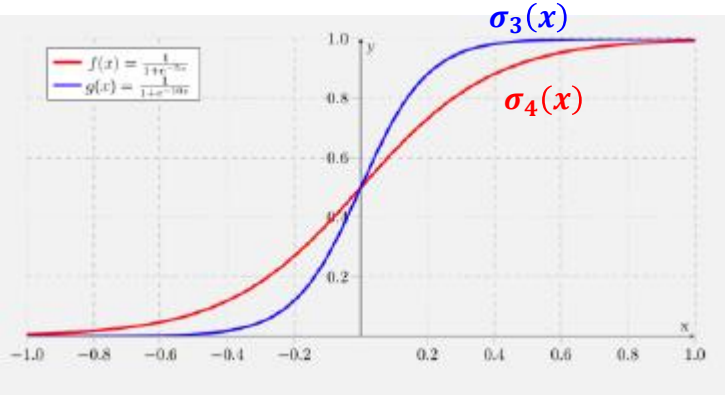


Source: https://ki-campus.org/node/209 / https://www.youtube.com/watch?v=aircAruvnKk

Neural Networks – Activation Functions

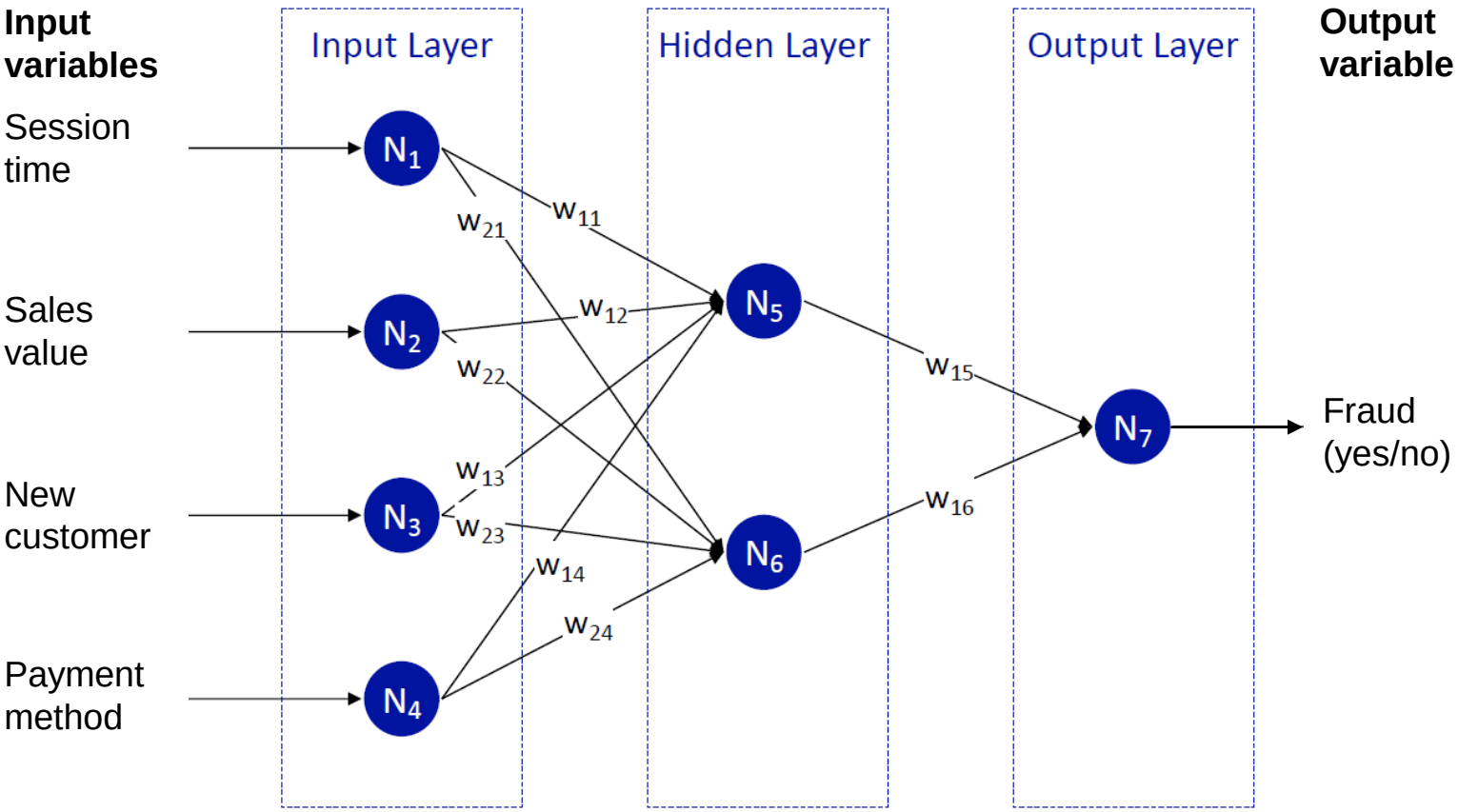






Source: Prof. Dr. Michael Bücker – Data Mining

Neural Networks – Online Retail Fraud Detection



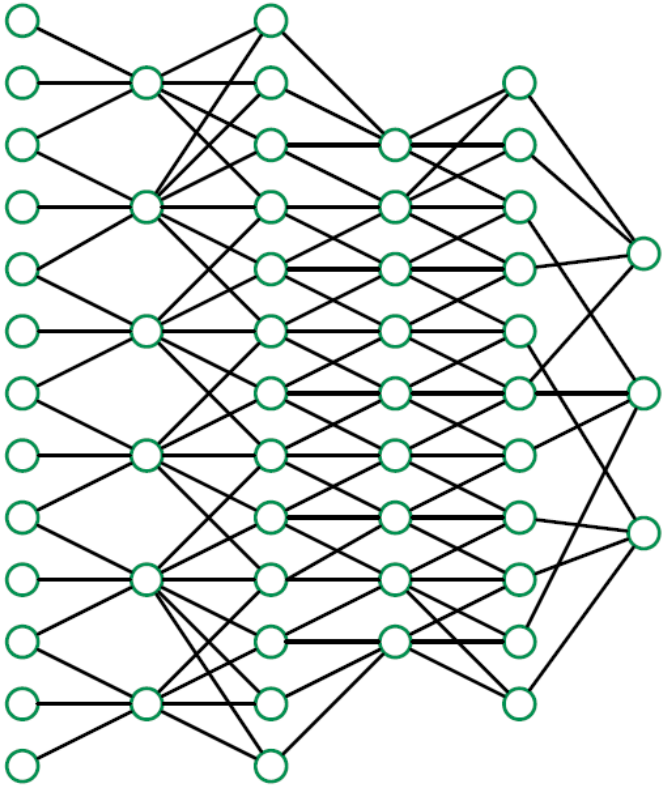
$$N_5 = \sigma(w_{11}N_1 + w_{12}N_2 + w_{13}N_3 + w_{14}N_4 + b_5)$$

$$N_6 = \sigma(w_{21}N_1 + w_{22}N_2 + w_{23}N_3 + w_{24}N_4 + b_6)$$

$$N_7 = \sigma(w_{15}N_5 + w_{16}N_6 + b_7)$$

Source: Prof. Dr. Michael Bücker – Data Mining

Neural Networks – Complexity



Question for discussion

A neural network has 6 layers, each consisting of 100 nodes, and each fully connected to the previous layer. Roughly how many parameters ($\boldsymbol{w_{ij}}$) does this network have?

Source: UCSanDiegoX DSE220x – Machine Learning Fundamentals

Neural networks – Summary

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Parameters

- Activation function, number and size of layers
- Many more

Strengths

- State-of-the-art in many applications
- Able to build very complex models

Weaknesses

- Black box – difficult to interpret and explain results
- Careful preprocessing and scaling of data needed
- Very long computation time for large datasets
- Difficulties with mixed kinds of features on different scales

Source: Müller, A. C., Guido, S. (2016) Introduction to Machine Learning with Python : A Guide for Data Scientists, O'Reilly Media