Werkzeuge für das wissenschaftliche Arbeiten

Python for Machine Learning and Data Science

Magnus Bender
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Wintersemester 2022/23

Inhaltsübersicht

1. Programmiersprache Python
   a) *Einführung, Erste Schritte*
   b) *Grundlagen*
   c) *Fortgeschritten*
2. Auszeichnungssprachen
   a) *LaTeX, Markdown*
3. Benutzeroberflächen und Entwicklungsumgebungen
   a) *Jupyter Notebooks lokal und in der Cloud (Google Colab)*
4. Versionsverwaltung
   a) *Git, GitHub*
5. Wissenschaftliches Rechnen
   a) *NumPy, SciPy*
6. Datenverarbeitung und -visualisierung
   a) *Pandas, matplotlib, NLTK*
7. Machine Learning (scikit-learn)
   a) **Grundlegende Ansätze (Datensätze, Auswertung)**
   b) Einfache Verfahren (Clustering, …)
8. DeepLearning
   a) TensorFlow, PyTorch, HuggingFace Transformers

Themen

I. Projektaufgabe 4

   1. Herangehensweise & Tipps

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    1. „Künstliche Intelligenz“, Data Science & Machine Learning

    2. Agenten

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III. Clustering

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„Datenverarbeitung und -darstellung“

1. Hellinger-Distanz zwischen zwei Matrizen P, Q

   - Distanz jeweils zeilenweise in Ergebnisvektor H

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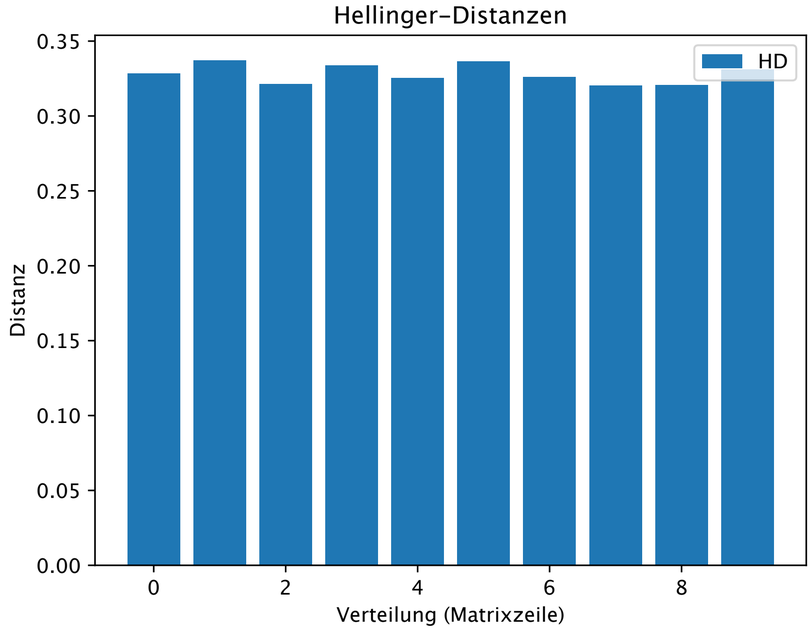

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- Rückgabe des `plt`-Moduls

II.
Begrifflichkeiten

1. „Künstliche Intelligenz“, Maschinelles Lernen & Data Science

Danksagung

- Nachfolgende Folien sind teilweise übernommen aus folgenden Vorlesungen und Vorträgen
  - Prof. Ralf Möller: „Non-Standard Datenbanken und Data-Mining“
  - Dr. Marcel Gehrke, Prof. Ralf Möller: „Einführung in Web und Data Science“
  - Prof. Ralf Möller: „Von AlphaZero zur Mars-Rover-Autonomie“

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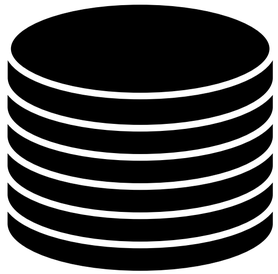

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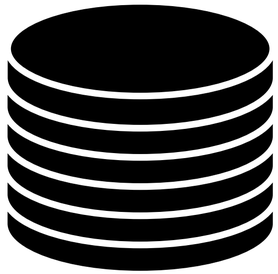

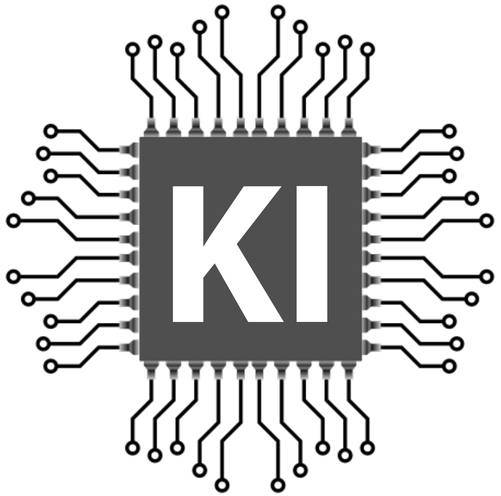

„Die KI”

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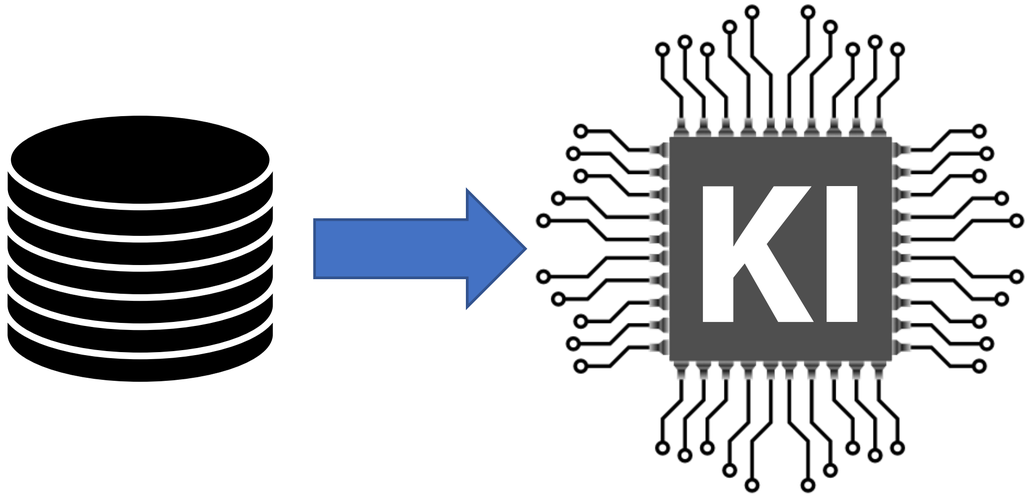

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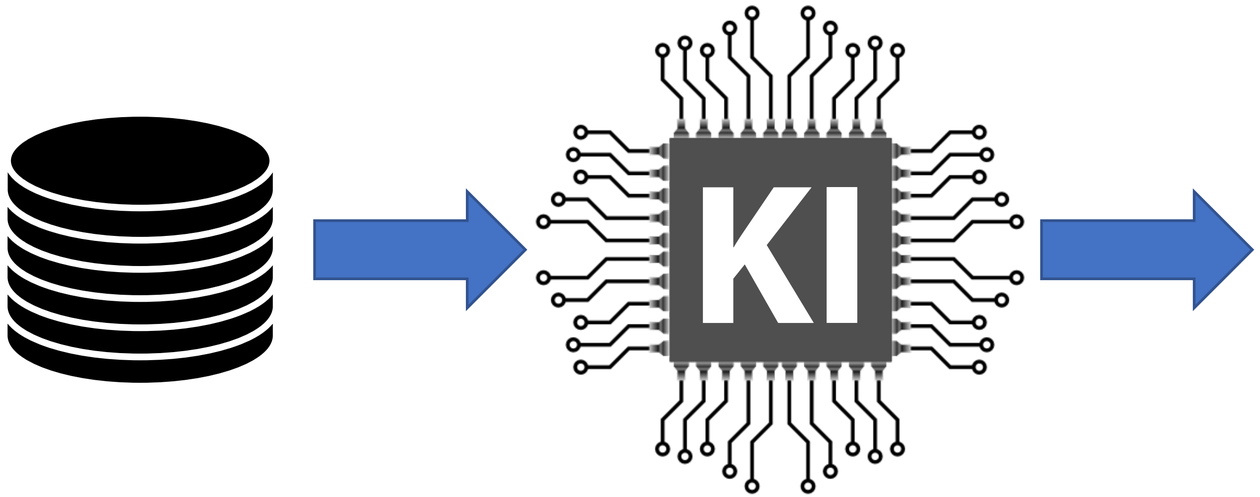

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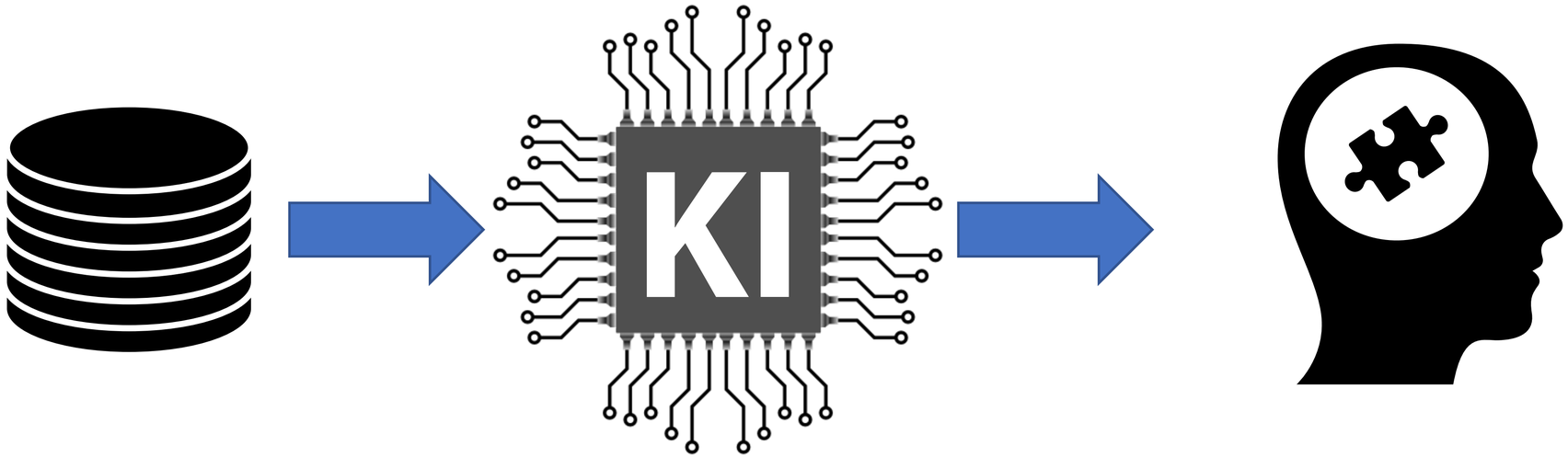

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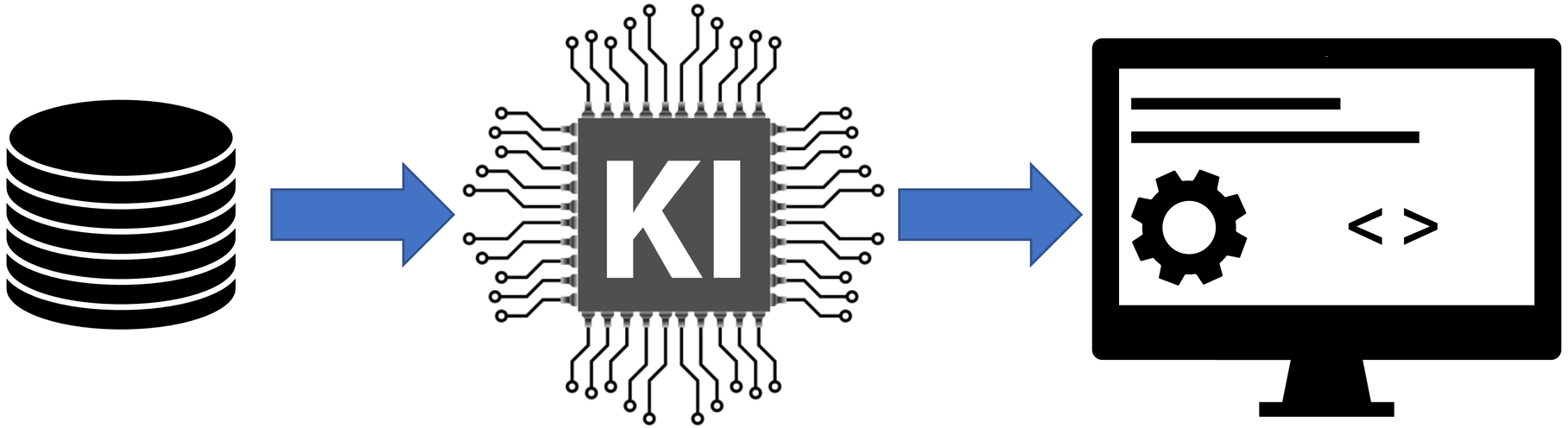

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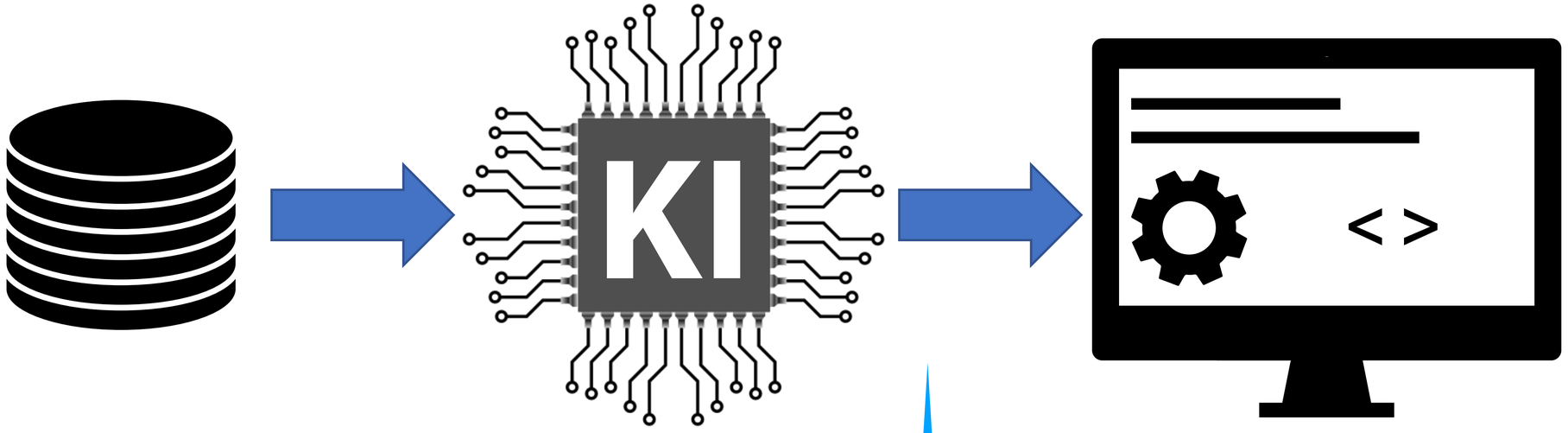

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Zum Beispiel:

Klassifikation, Regression, Prädiktion, Diagnose, …

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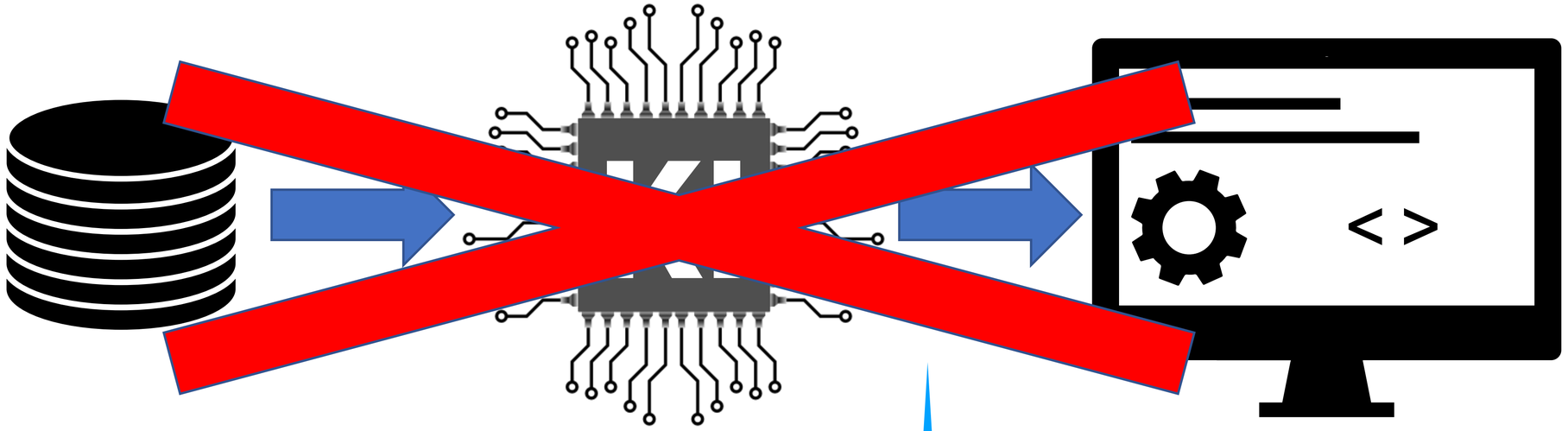

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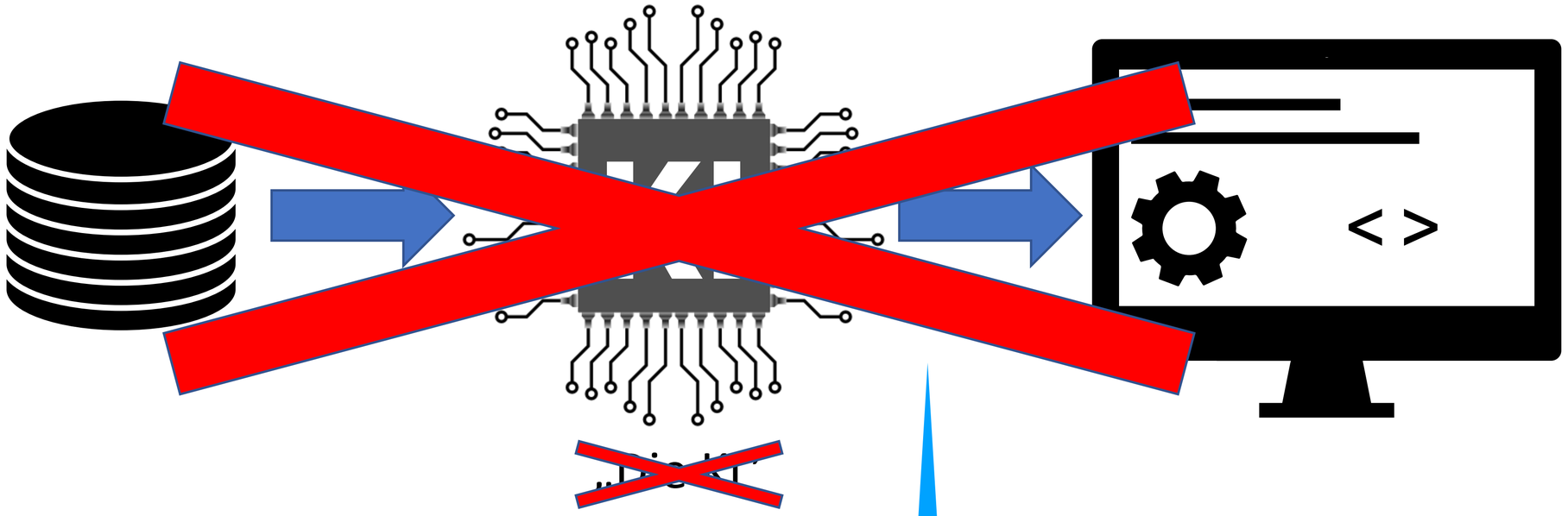

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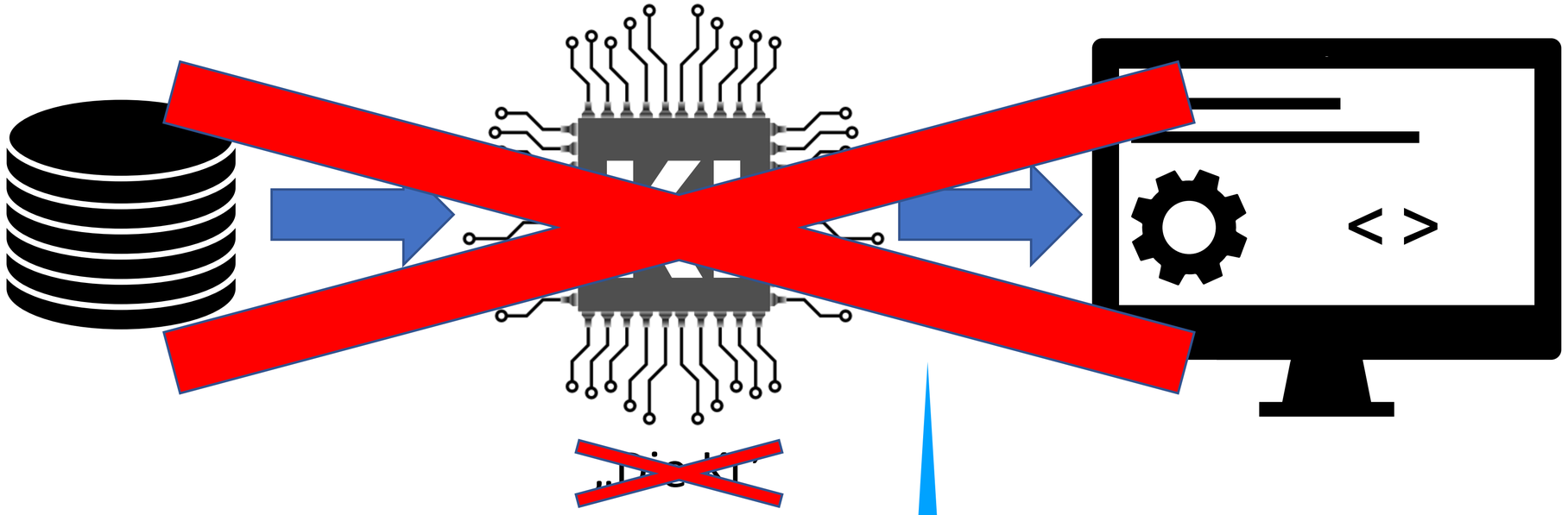
„Künstliche Intelligenz“ Märchen



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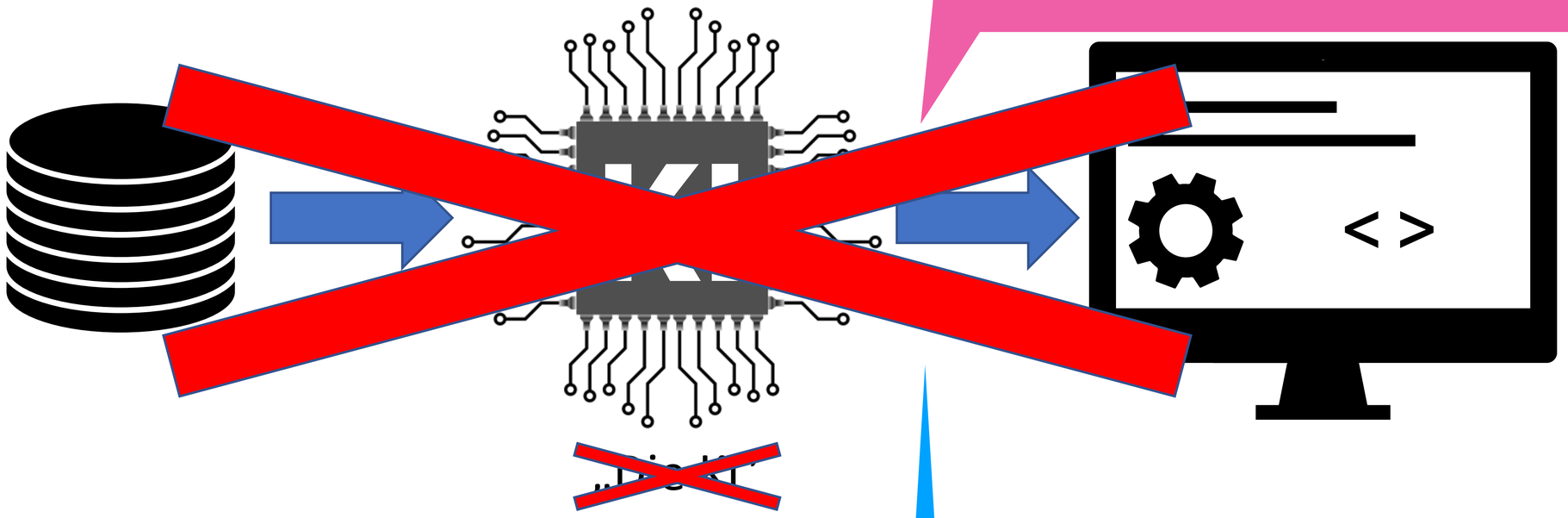
„Künstliche Intelligenz“ Märchen

„KI“ als ein Baustein, der wie im Kopf funktioniert, und dann die „Intelligenz“ auf einen Computer bringt.



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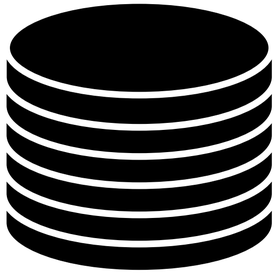

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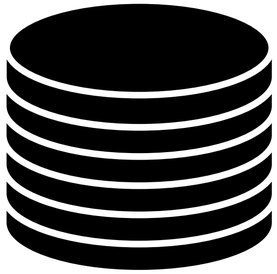

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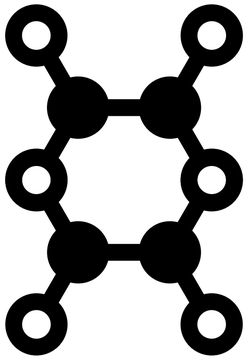
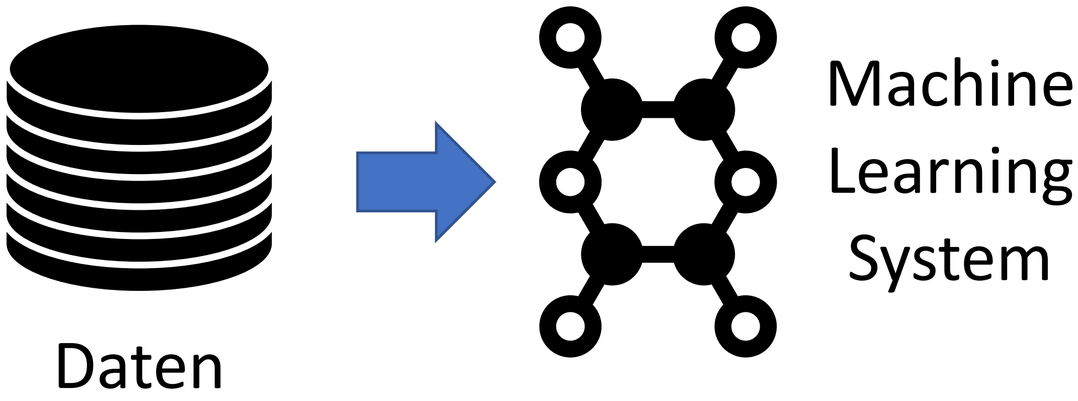


Machine Learning System


Daten
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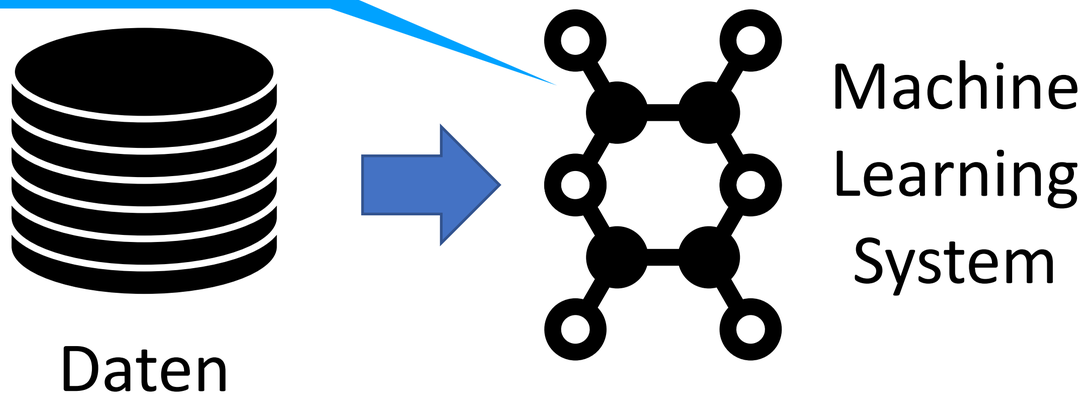
TensorFlow, PyTorch



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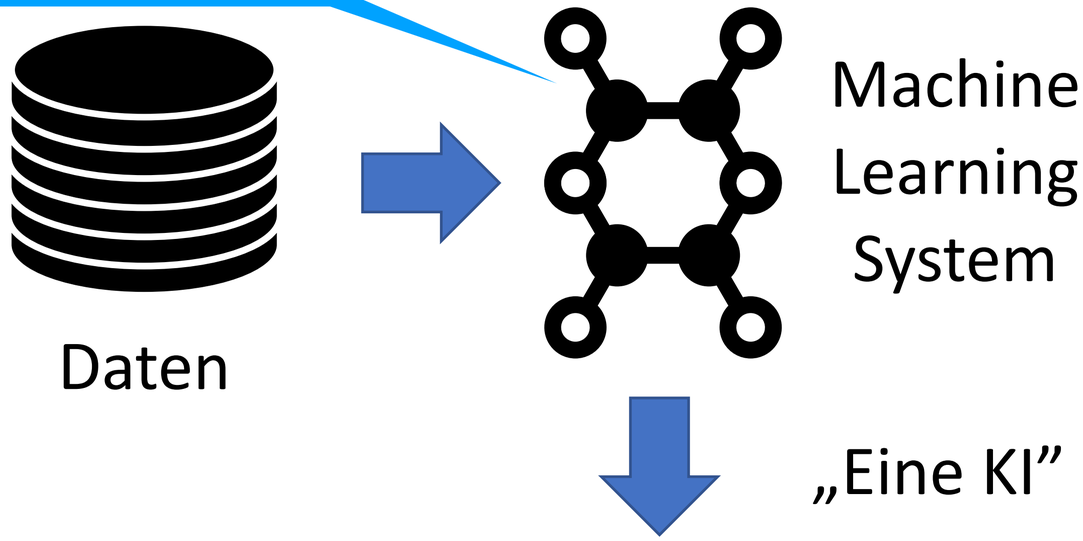

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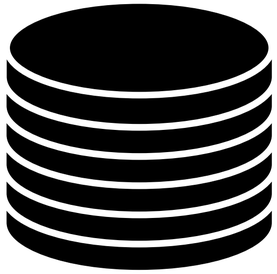

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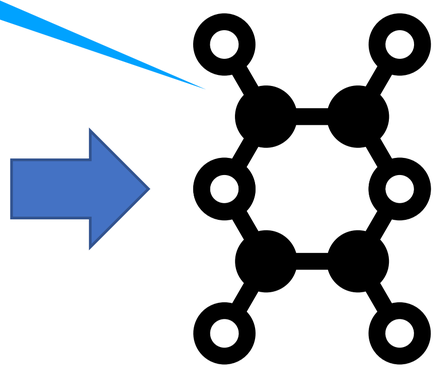

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„Eine KI”

Programm:
Entscheidungsbaum-evaluator,
Kaskade von linearen und stückweise linearen Funktionen

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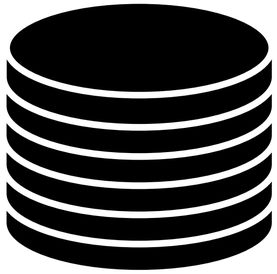

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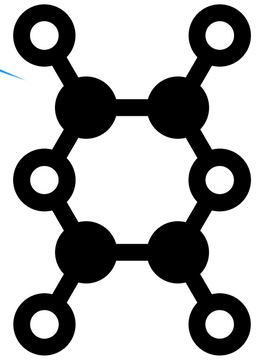

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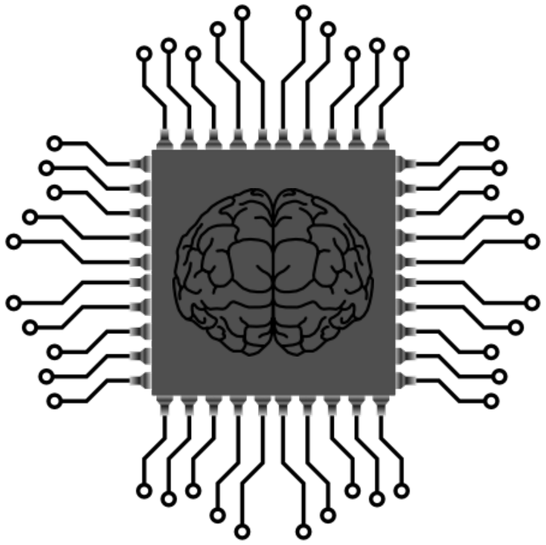

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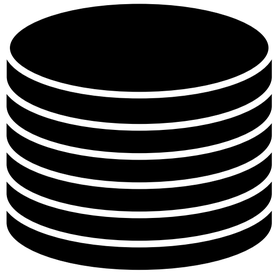

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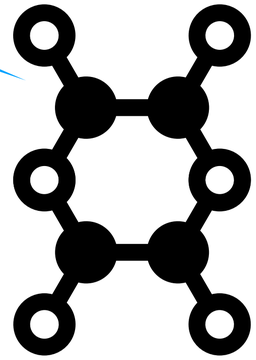

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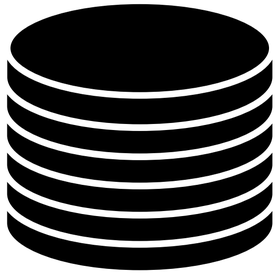

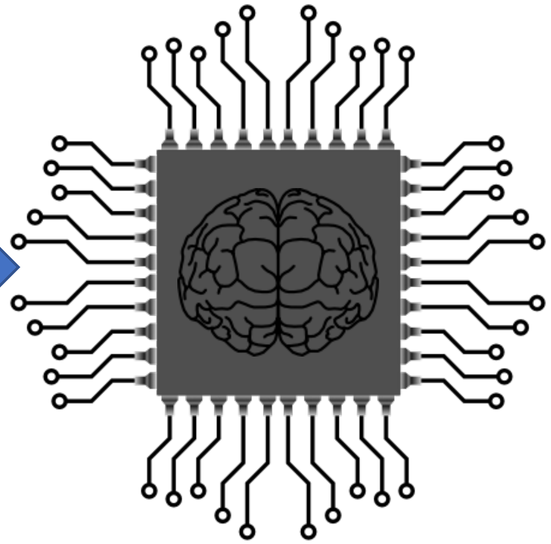

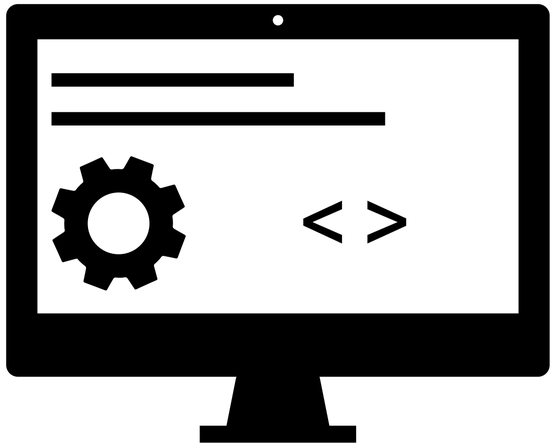

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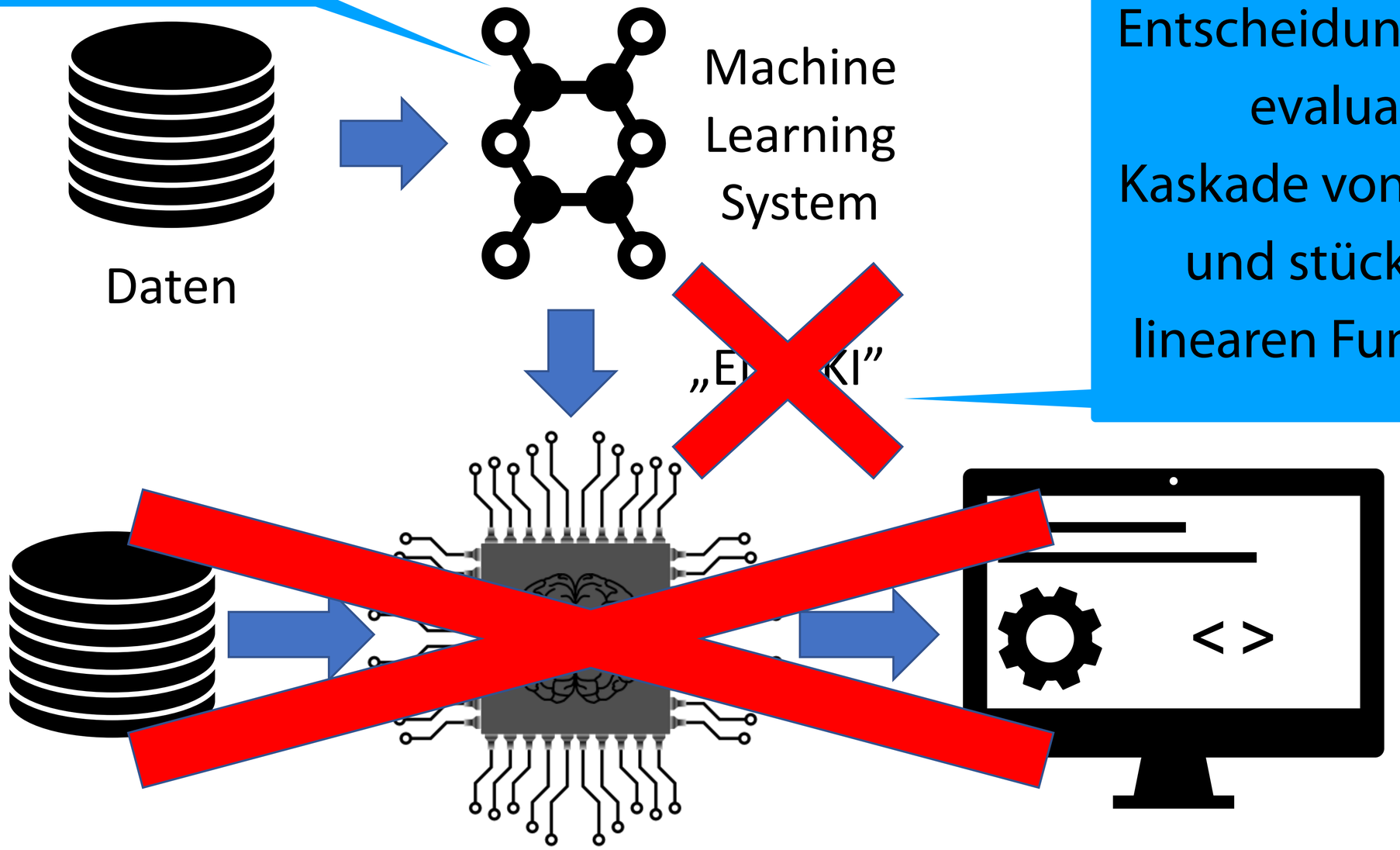

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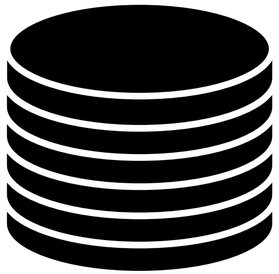

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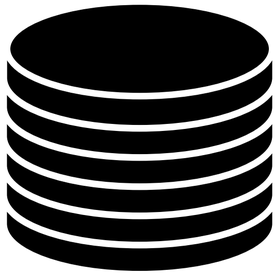

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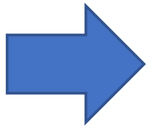

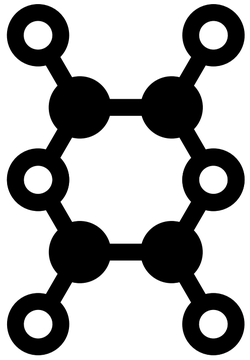

Training

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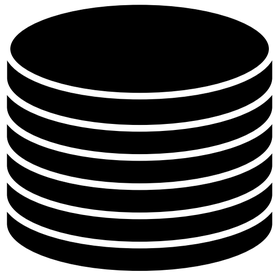

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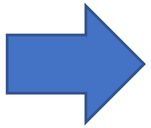

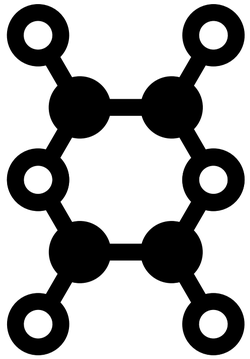

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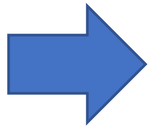
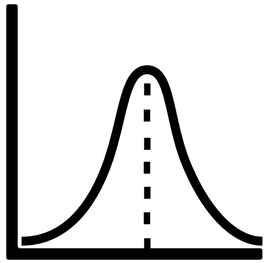
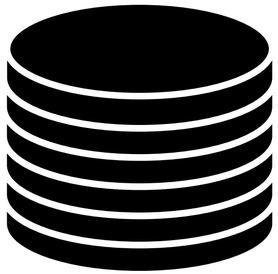




Modell (Programm)

Maschinelles Lernen



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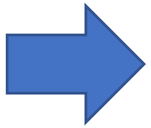
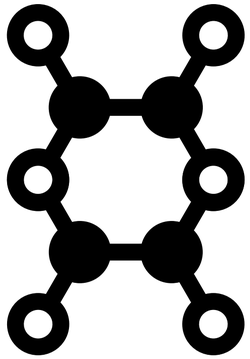
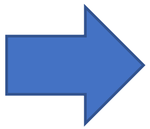
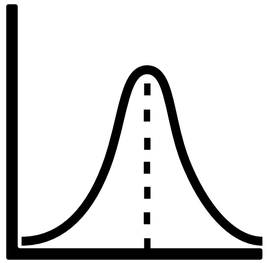


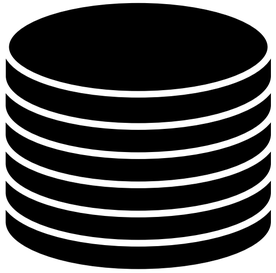


Training



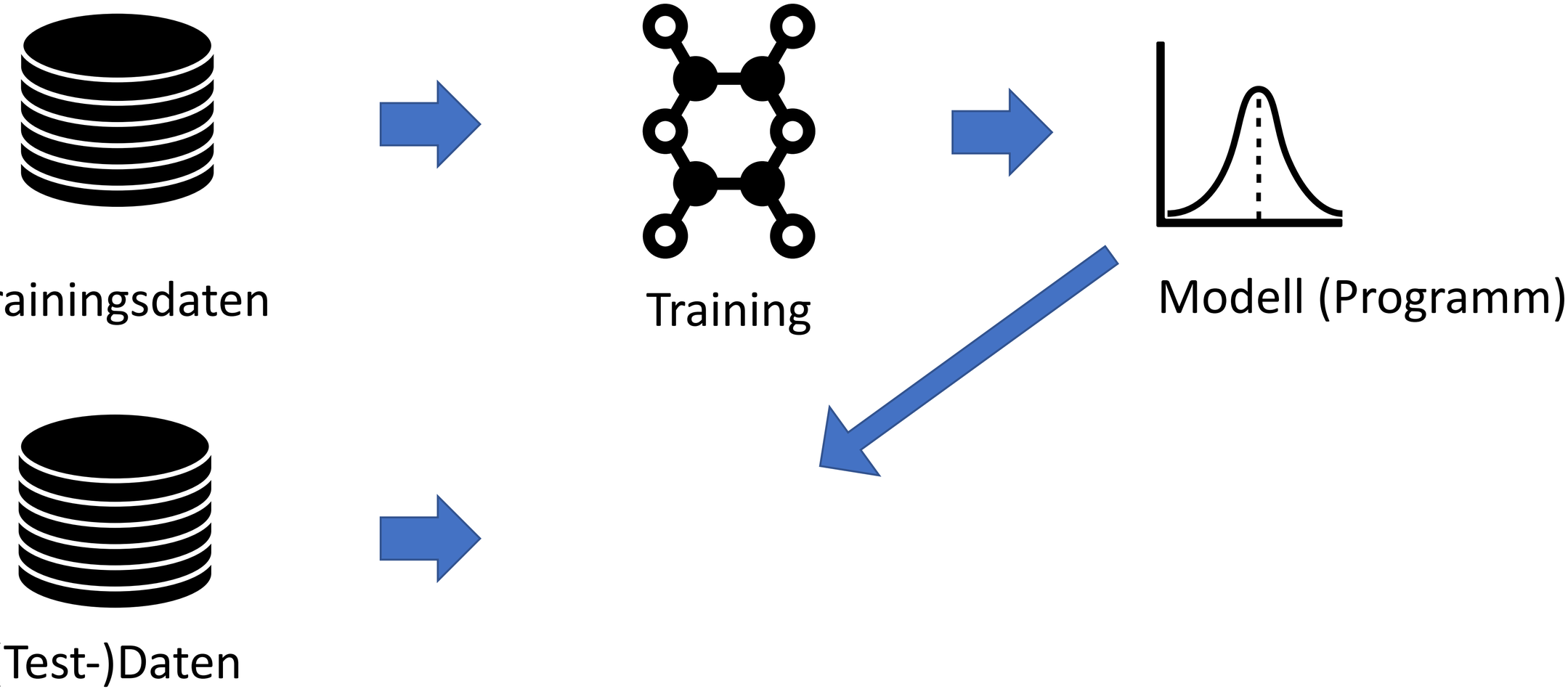


Modell (Programm)

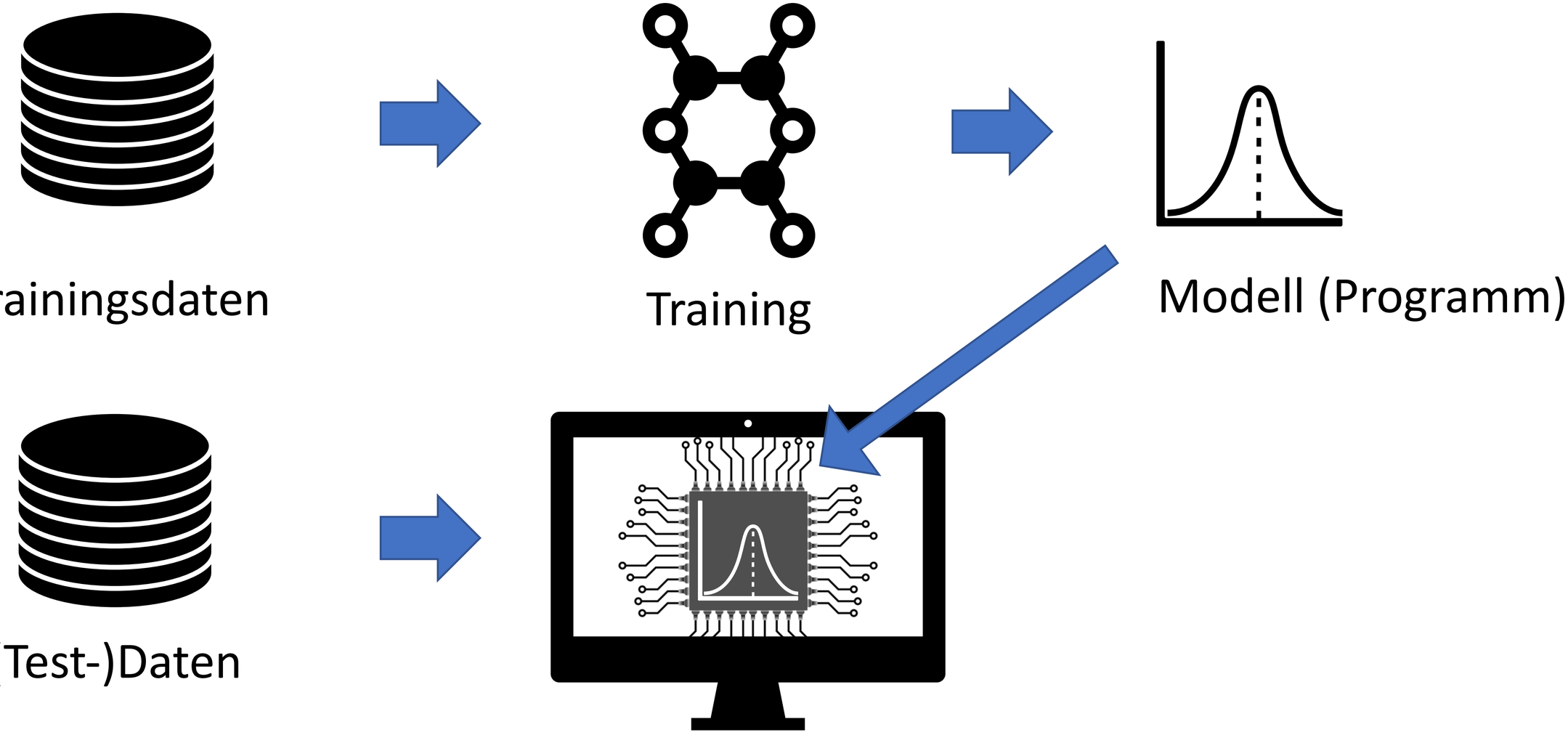


(Test-)Daten

Maschinelles Lernen



Maschinelles Lernen



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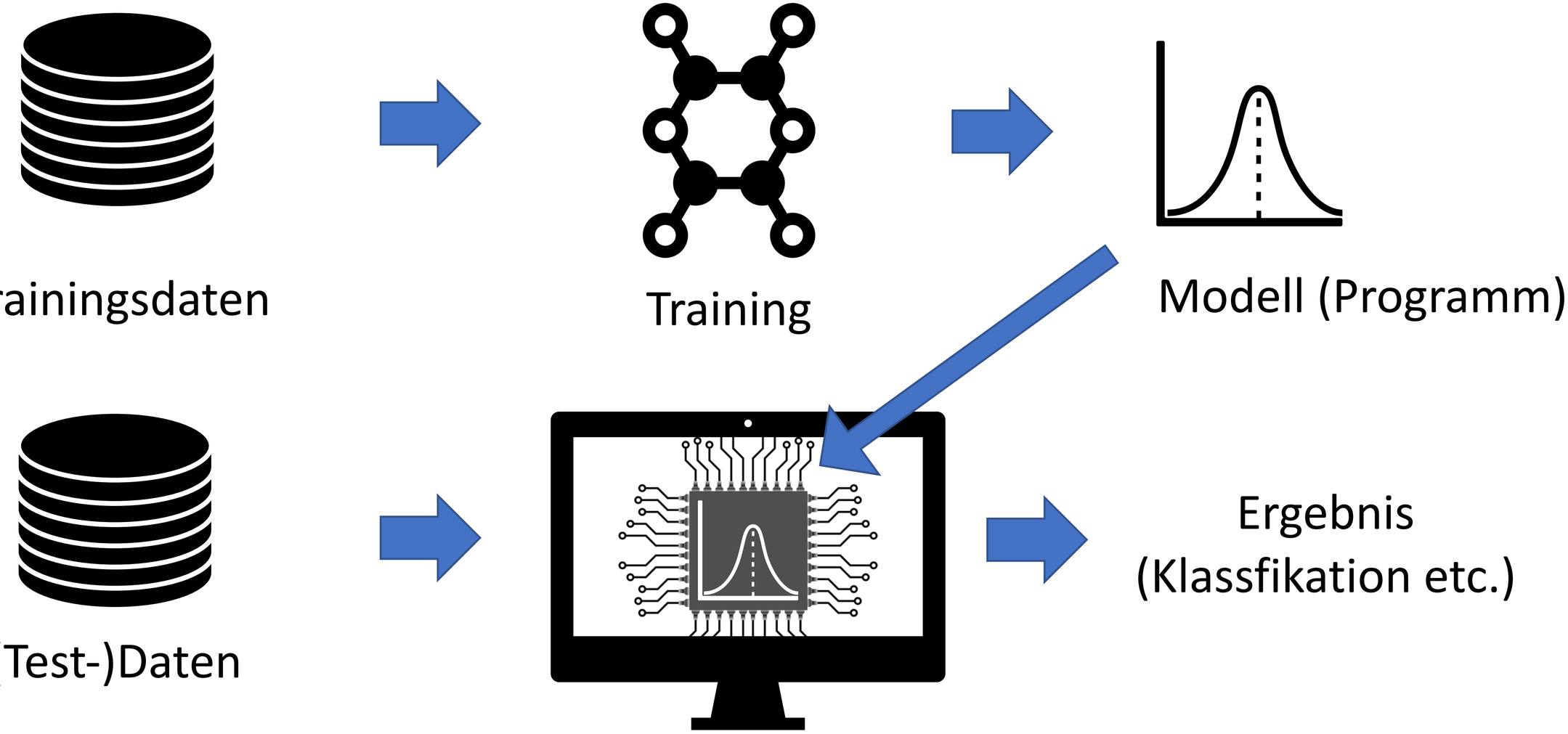

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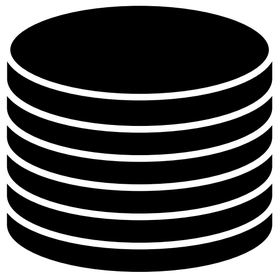
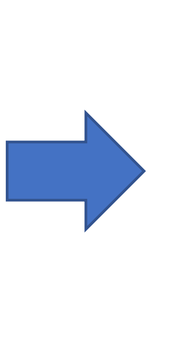
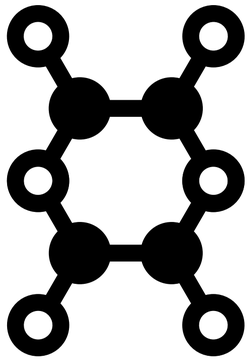
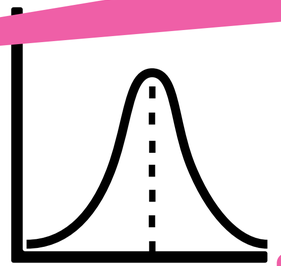


Trainingsdaten





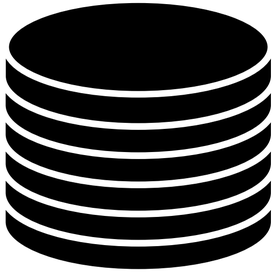
Training



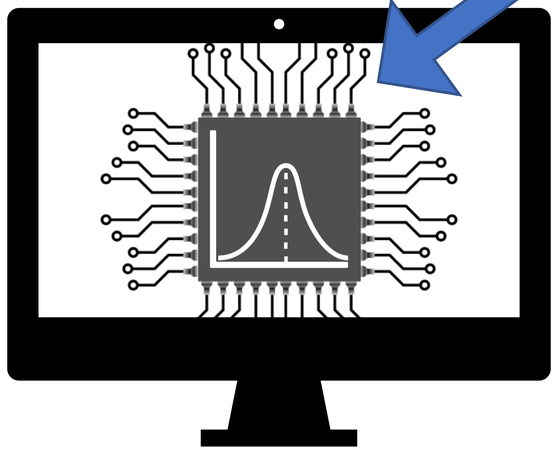
Modell (P

Ein Modell aus den Trainigsdaten „lernen“ (berechnen).

Modell (Programm) mit anderen Daten nutzen.



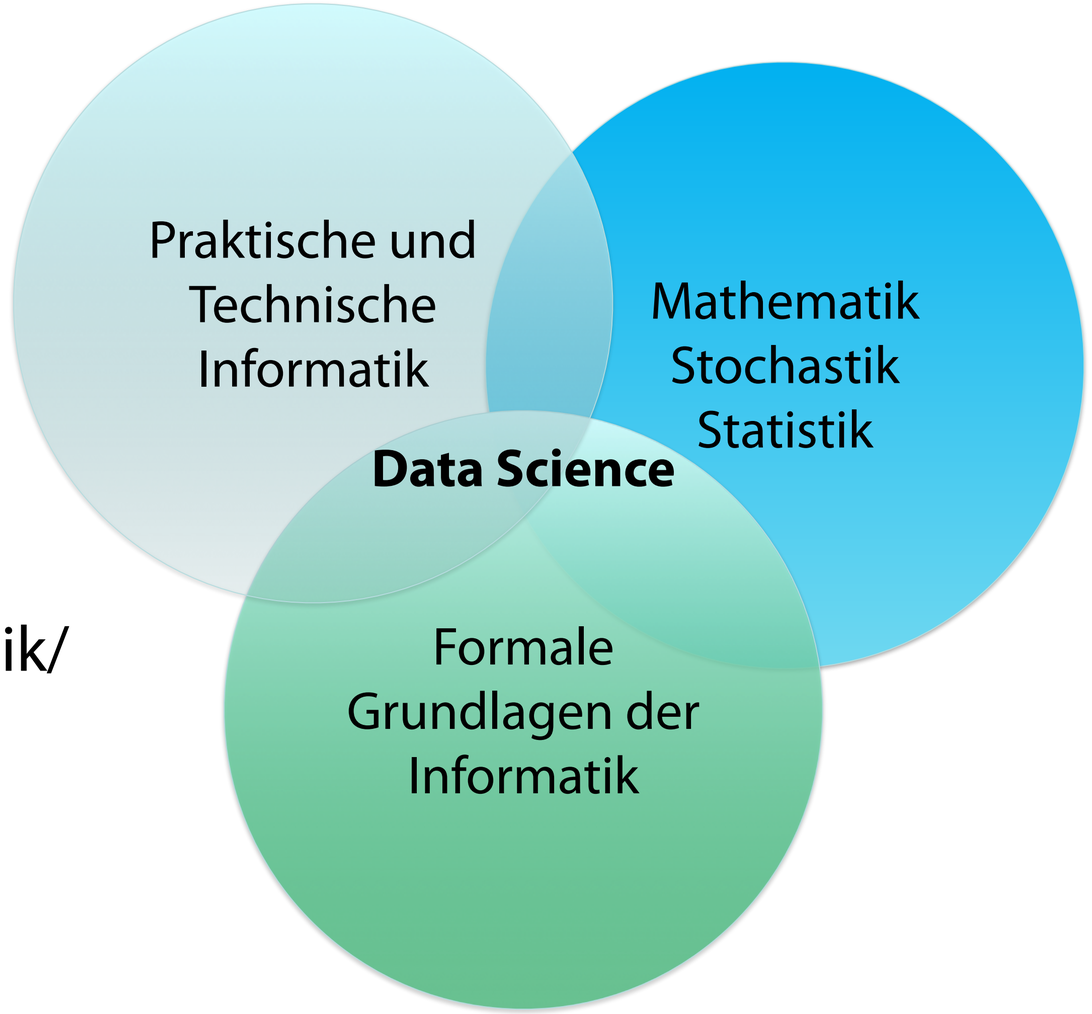
(Test-)Daten



Ergebnis
(Klassfikation etc.)

Data Science

- Extraktion von Wissen aus Daten (u.a. Graphdaten)
- Begriff schon vor 60 Jahren für Informatik vorgeschlagen
- Entwicklung innovativer Konzepte in den Bereichen Logik, Datenbanken und Stochastik/ Statistik (Datenanalyse und Wissensentdeckung)
- Verwendung von LADS und Analysis



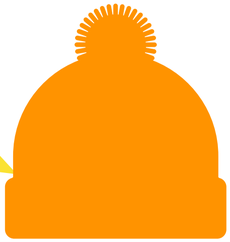
II.
Begrifflichkeiten

2. Agenten

II.
Begrifflichkeiten

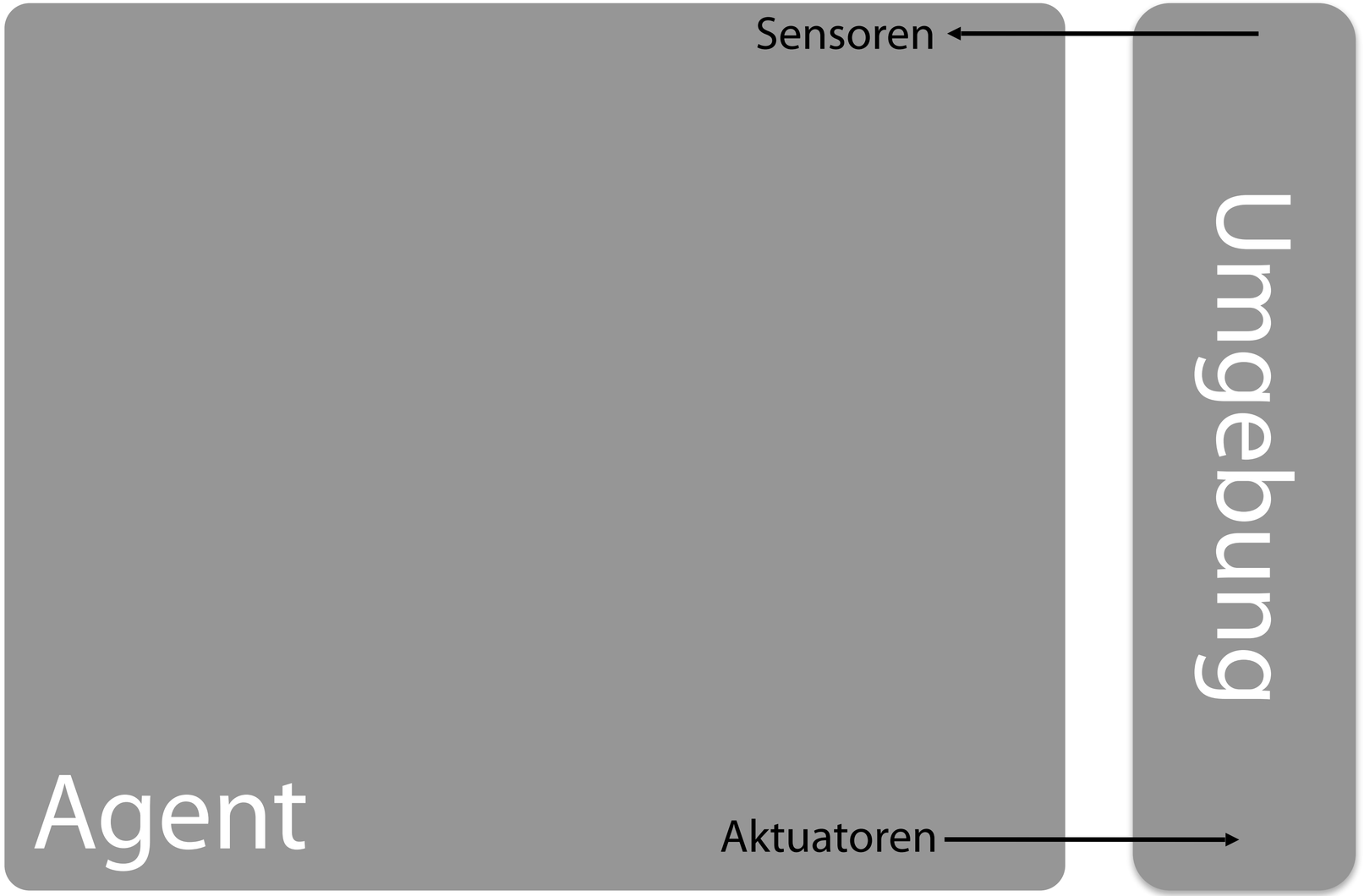
2. Agenten

Und wo ist jetzt das, was man häufig unter „KI“ versteht?

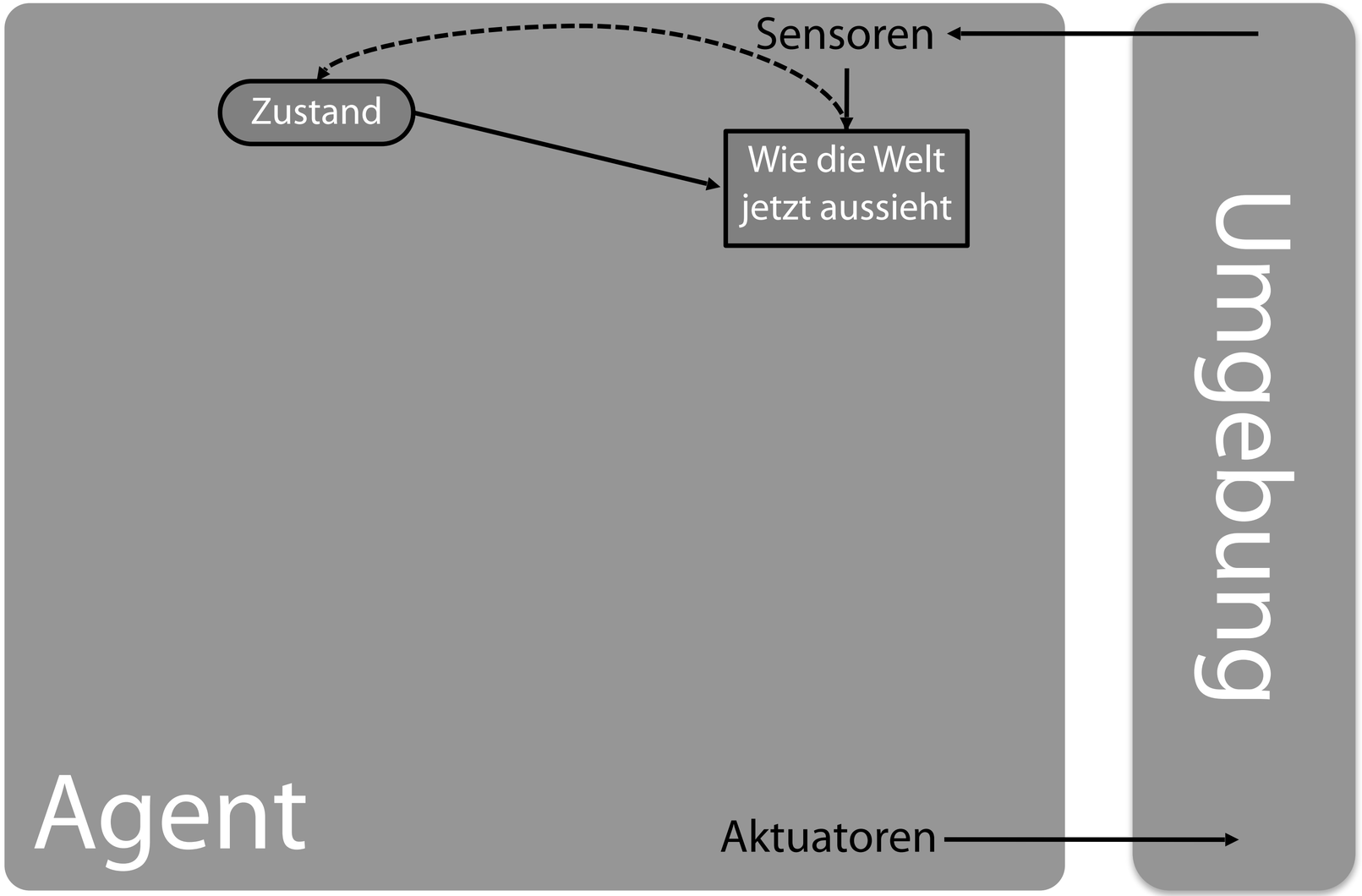


Agenten

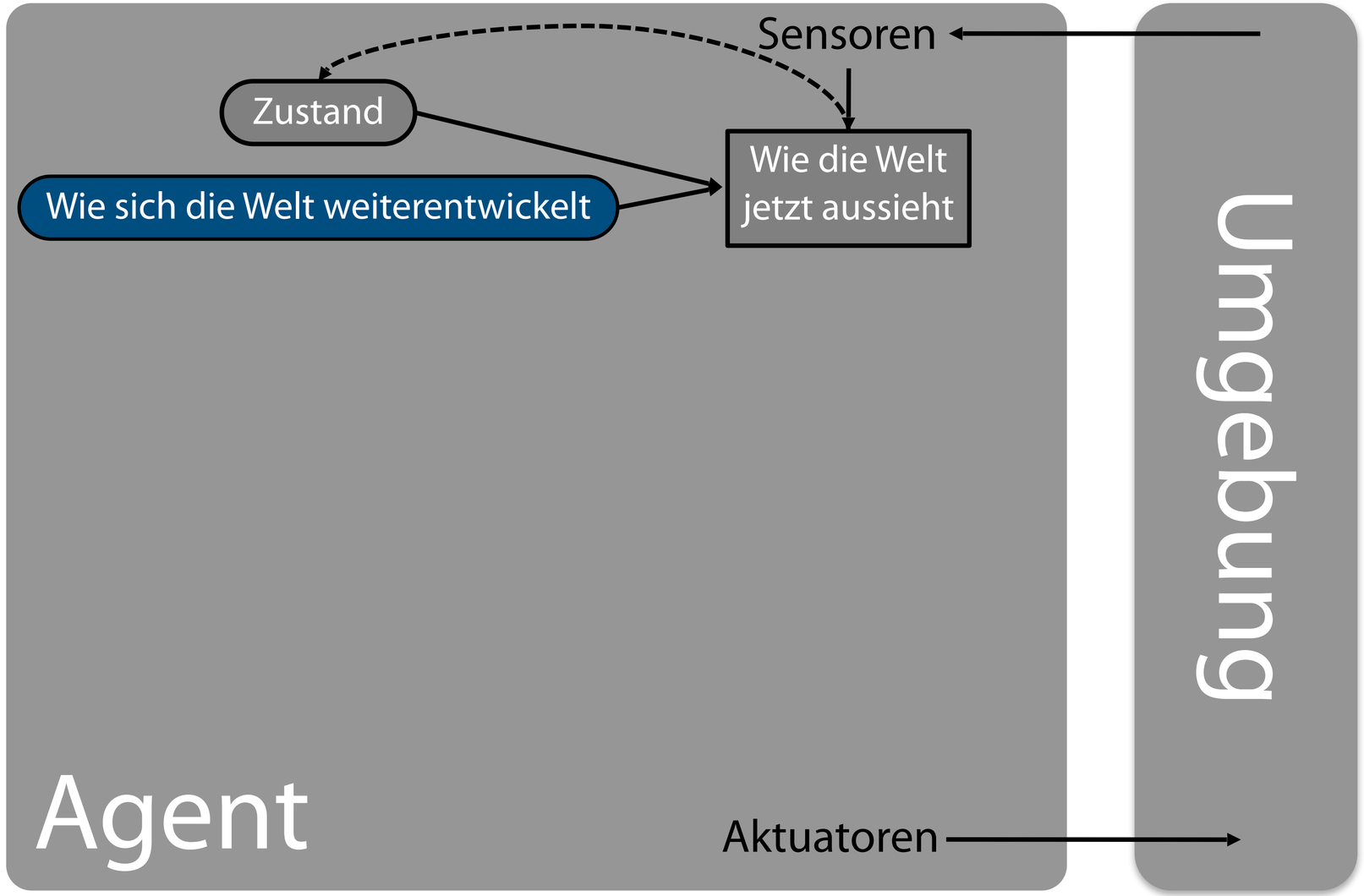
Agenten



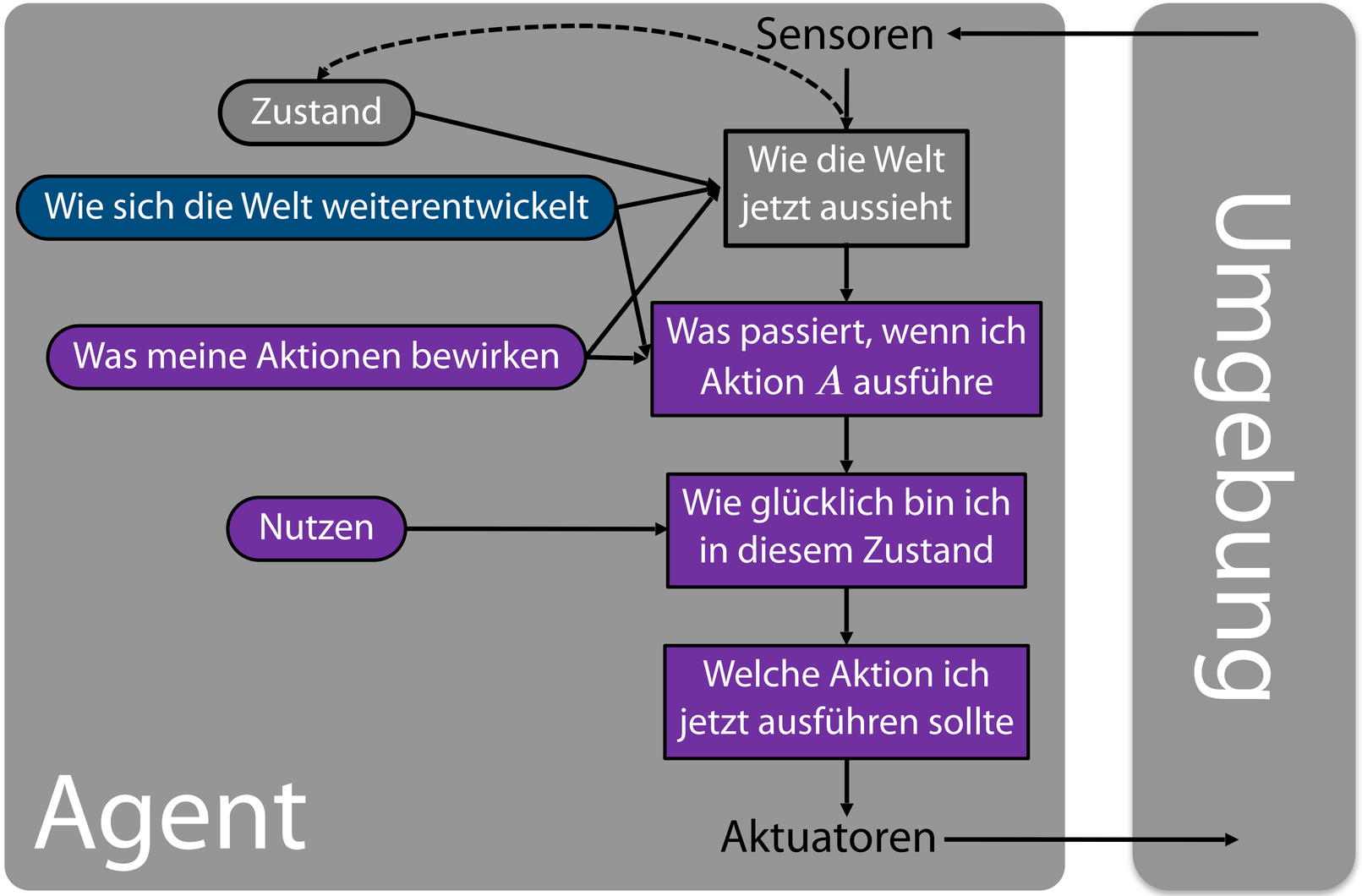
Agenten


Sensoren
Zustand
Wie die Welt jetzt aussieht
Agent
Aktuatoren
Umgebung

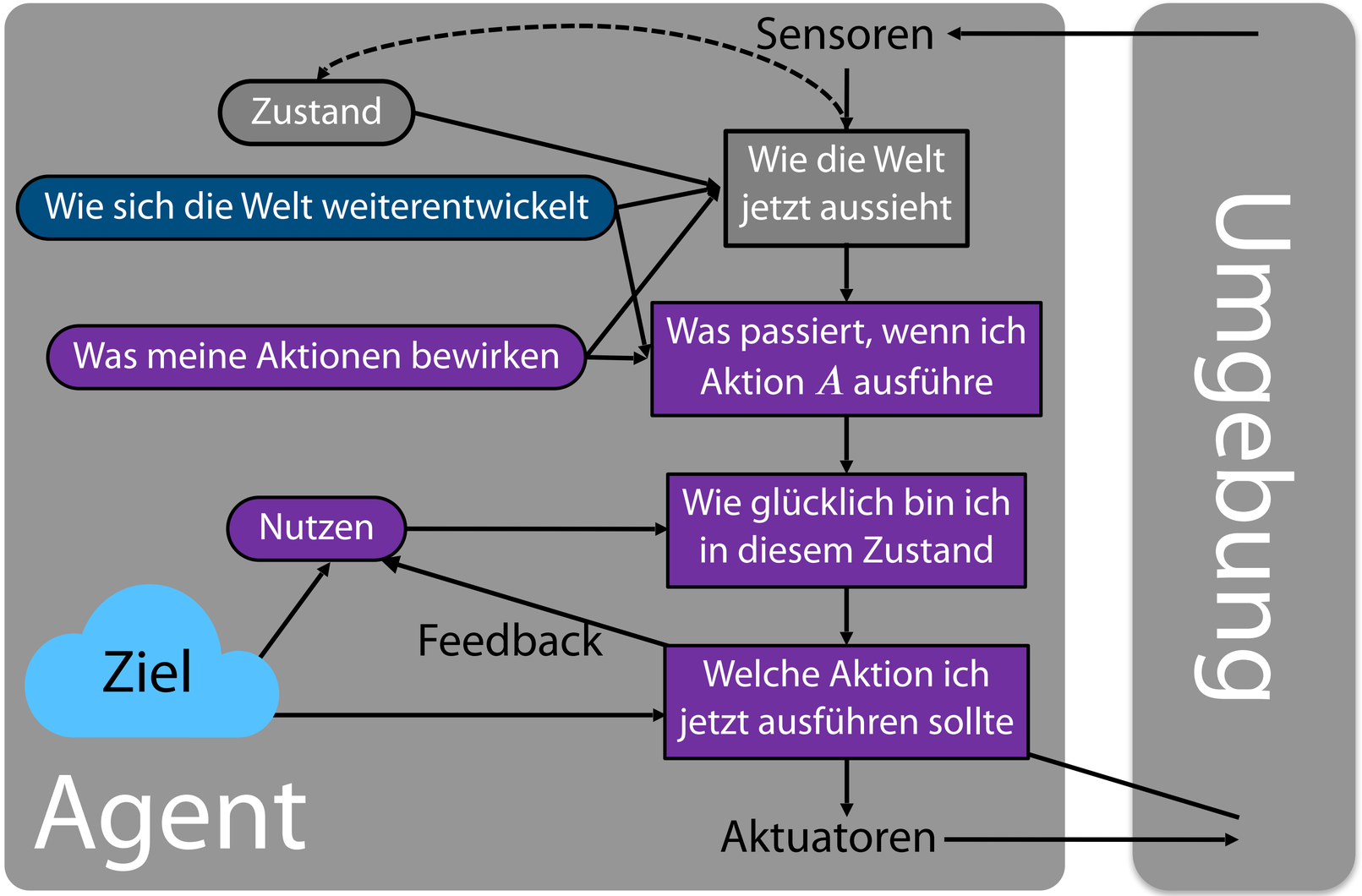
Agenten


Sensoren
Zustand
Wie die Welt jetzt aussieht
Wie sich die Welt weiterentwickelt
Agent
Aktuatoren
Umgebung

Agenten

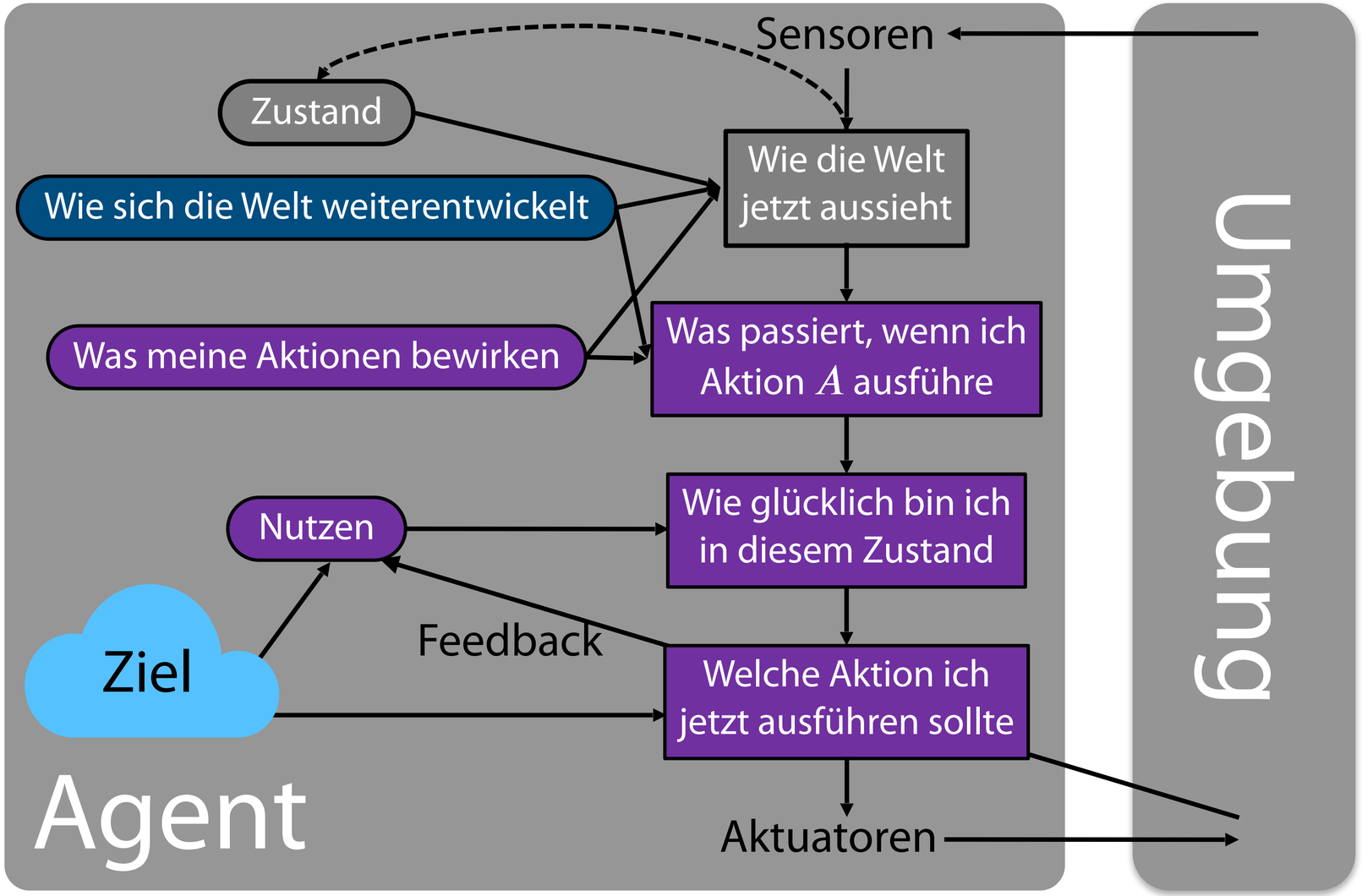

Sensoren
Zustand
Wie die Welt jetzt aussieht
Wie sich die Welt weiterentwickelt
Was meine Aktionen bewirken
Was passiert, wenn ich Aktion A ausführe
Nutzen
Wie glücklich bin ich in diesem Zustand
Welche Aktion ich jetzt ausführen sollte
Aktuatoren
Agent
Umgebung

Agenten


Sensoren
Zustand
Wie die Welt jetzt aussieht
Wie sich die Welt weiterentwickelt
Was meine Aktionen bewirken
Was passiert, wenn ich Aktion A ausführe
Wie glücklich bin ich in diesem Zustand
Nutzen
Feedback
Ziel
Welche Aktion ich jetzt ausführen sollte
Agent
Aktuatoren
Umgebung

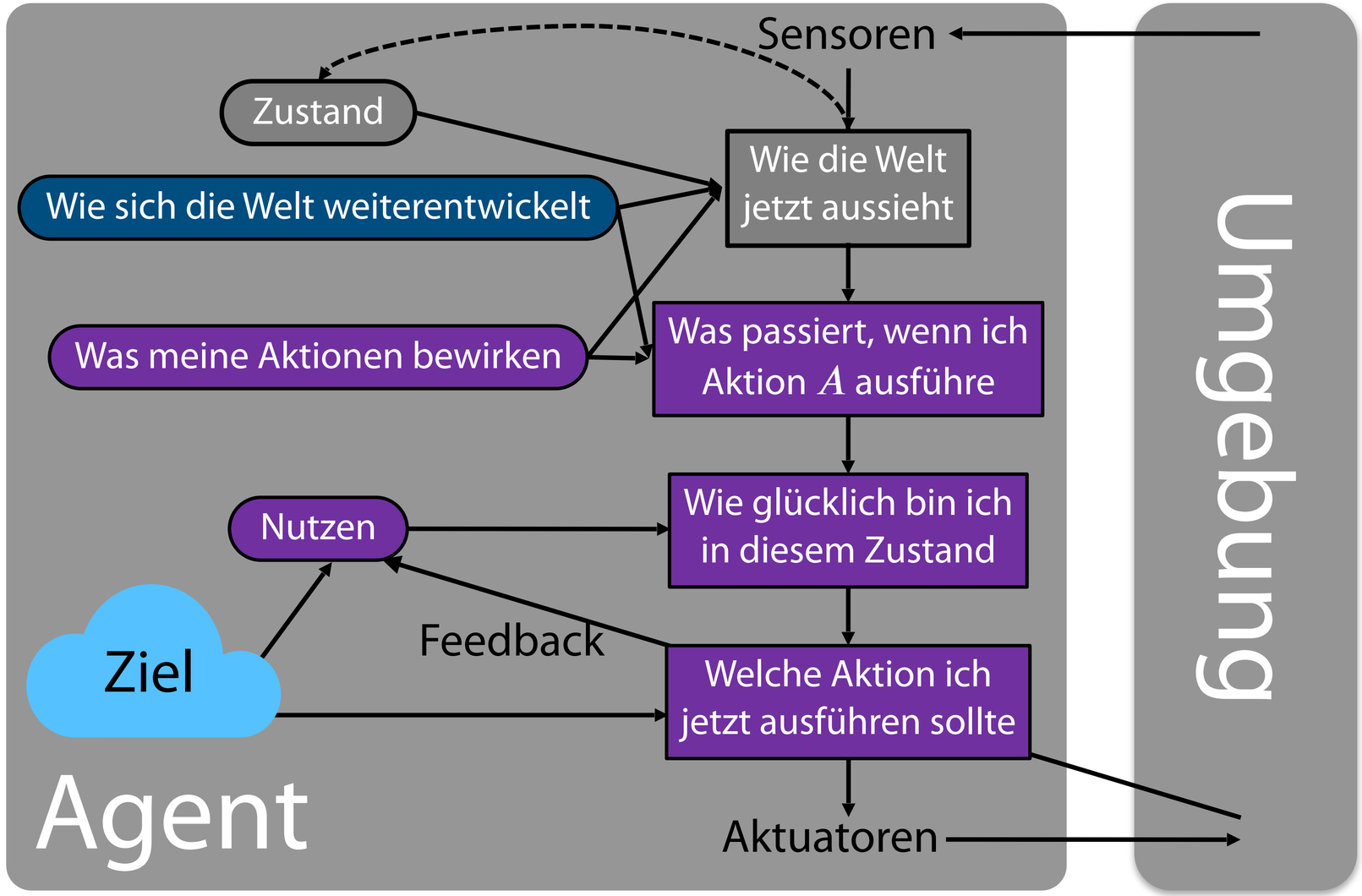
Agenten

- Wissenschaft der intelligenten Systeme



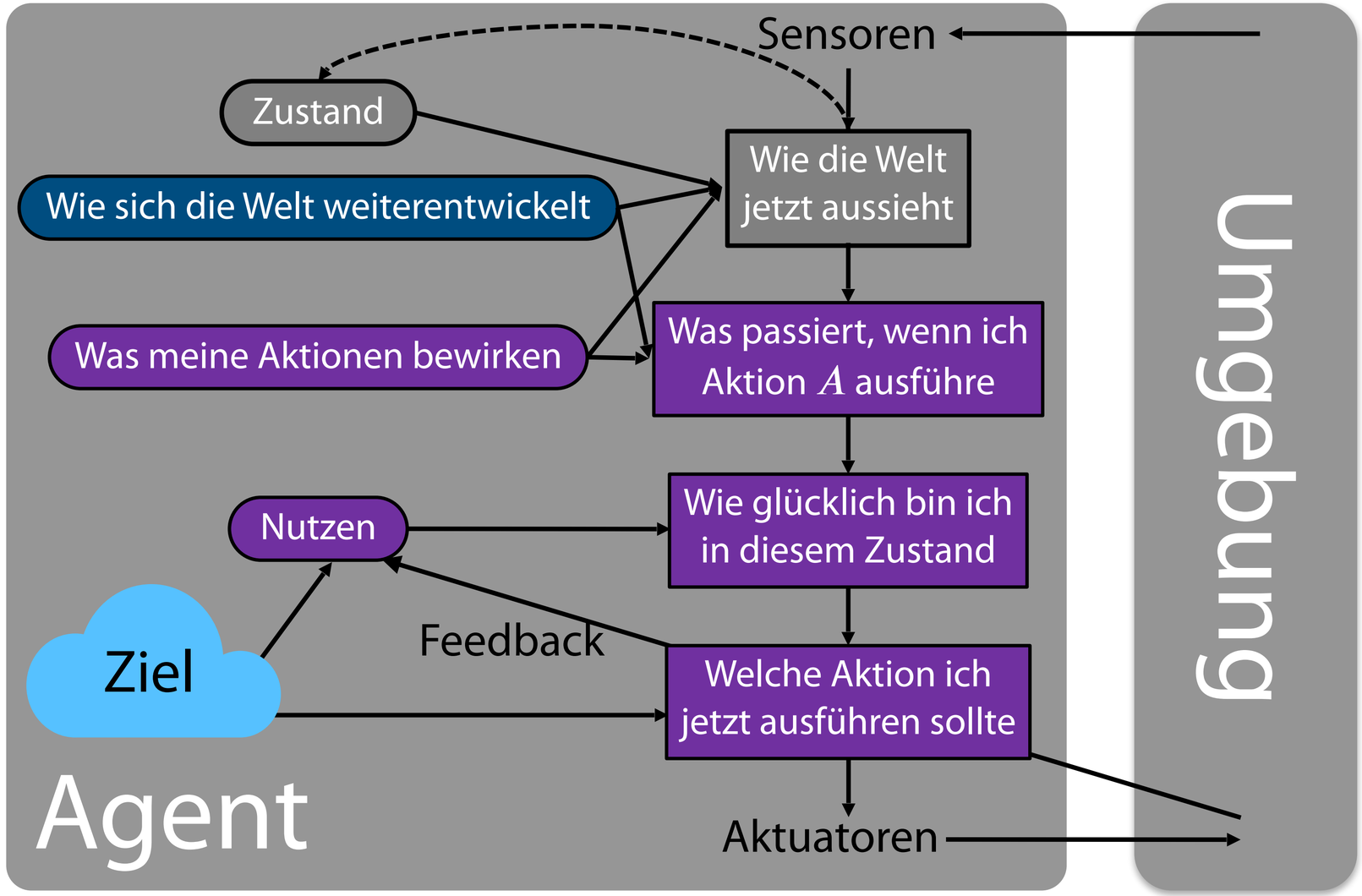
Agenten

- Wissenschaft der intelligenten Systeme
- Agenten
  - Haben/bilden Ziele
  - Sensoren/Aktoren
  - Handlungsplanung
  - Lernen zur Laufzeit

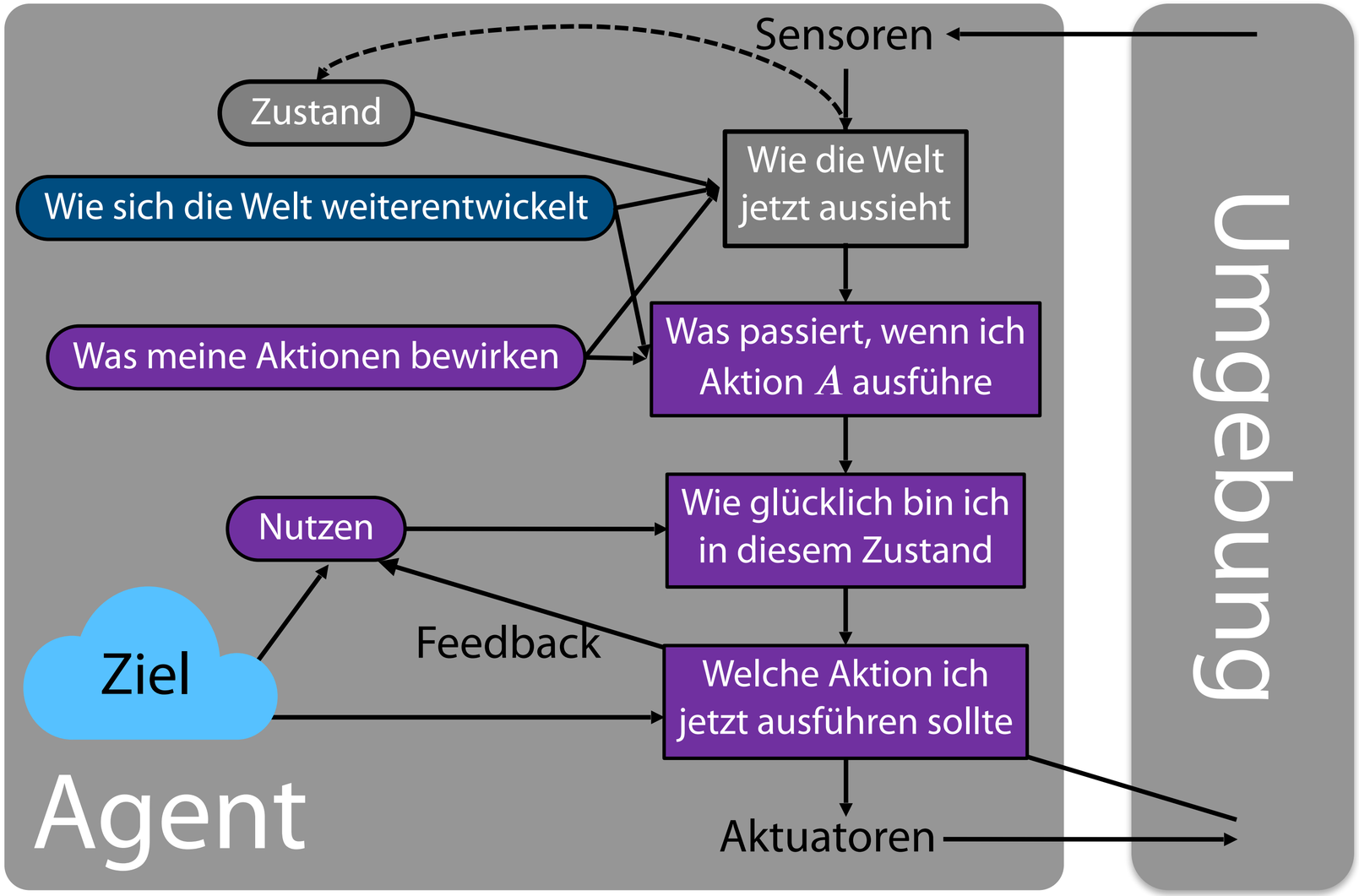


Agenten

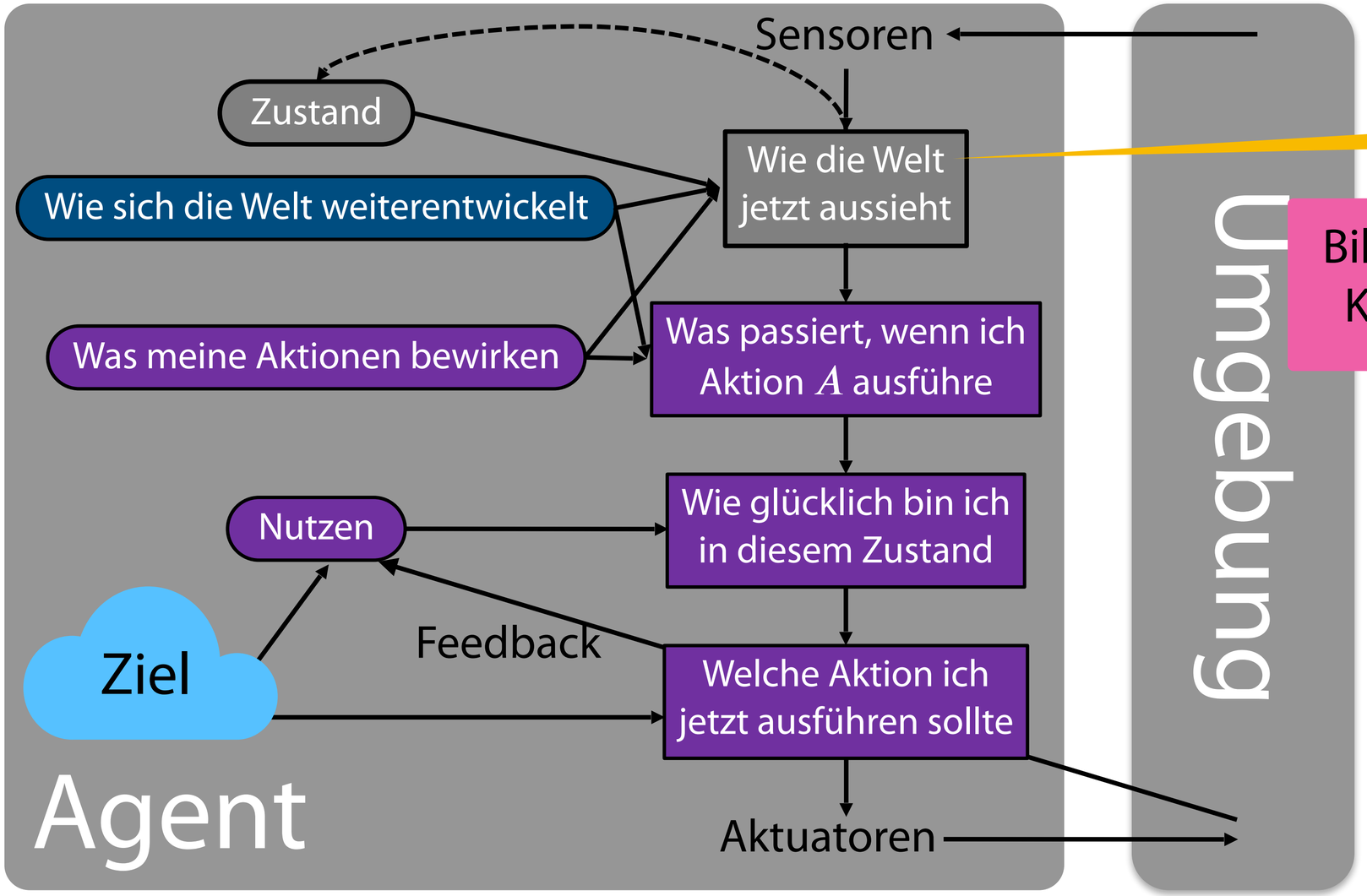
- Wissenschaft der intelligenten Systeme
- Agenten
  - Haben/bilden Ziele
  - Sensoren/Aktoren
  - Handlungsplanung
  - Lernen zur Laufzeit
- Agenten interagieren mit Menschen (and anderen Agenten)
  - Ziele der Agenten beeinflussbar



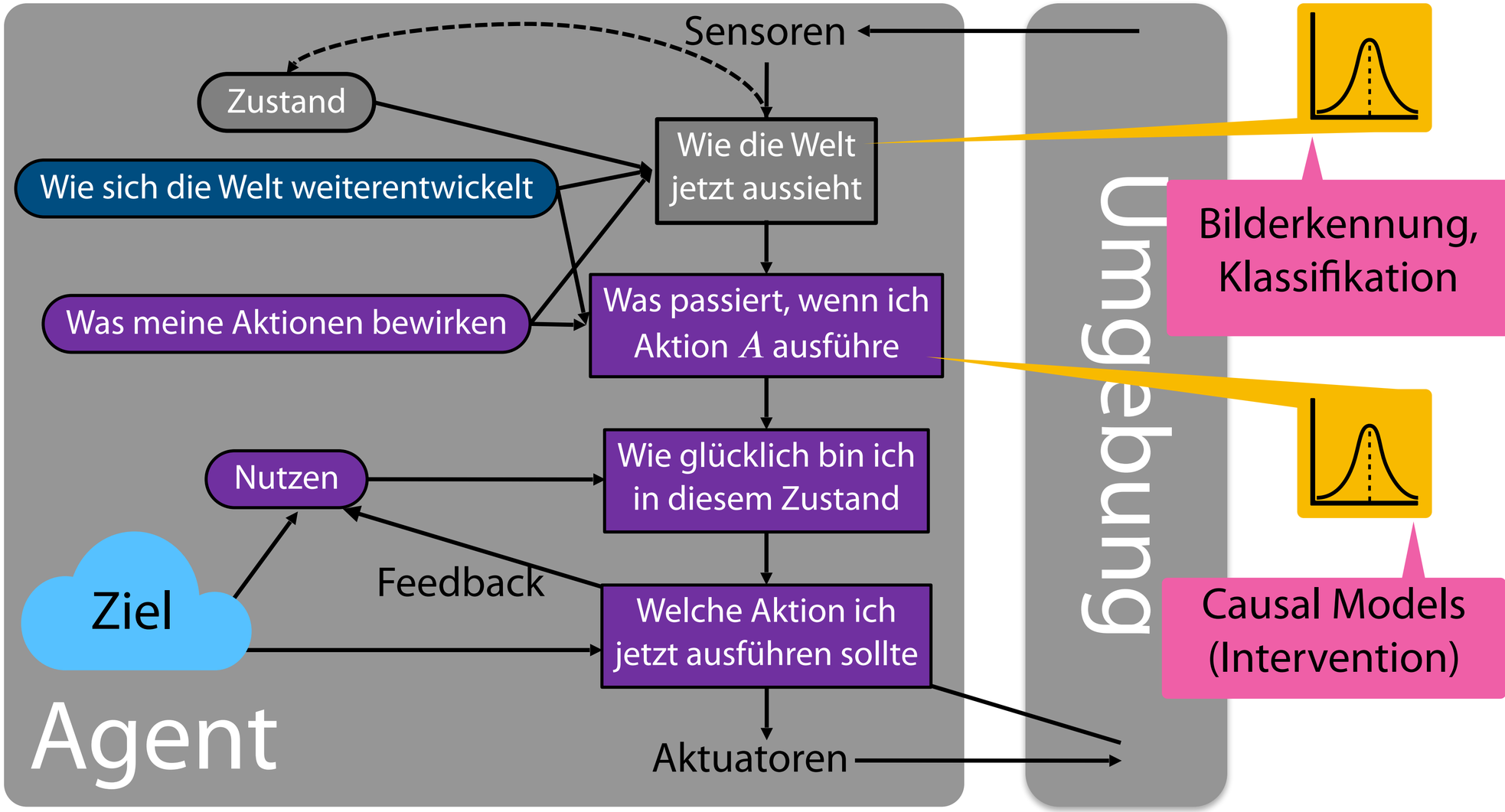
Agent: Maschinelles Lernen



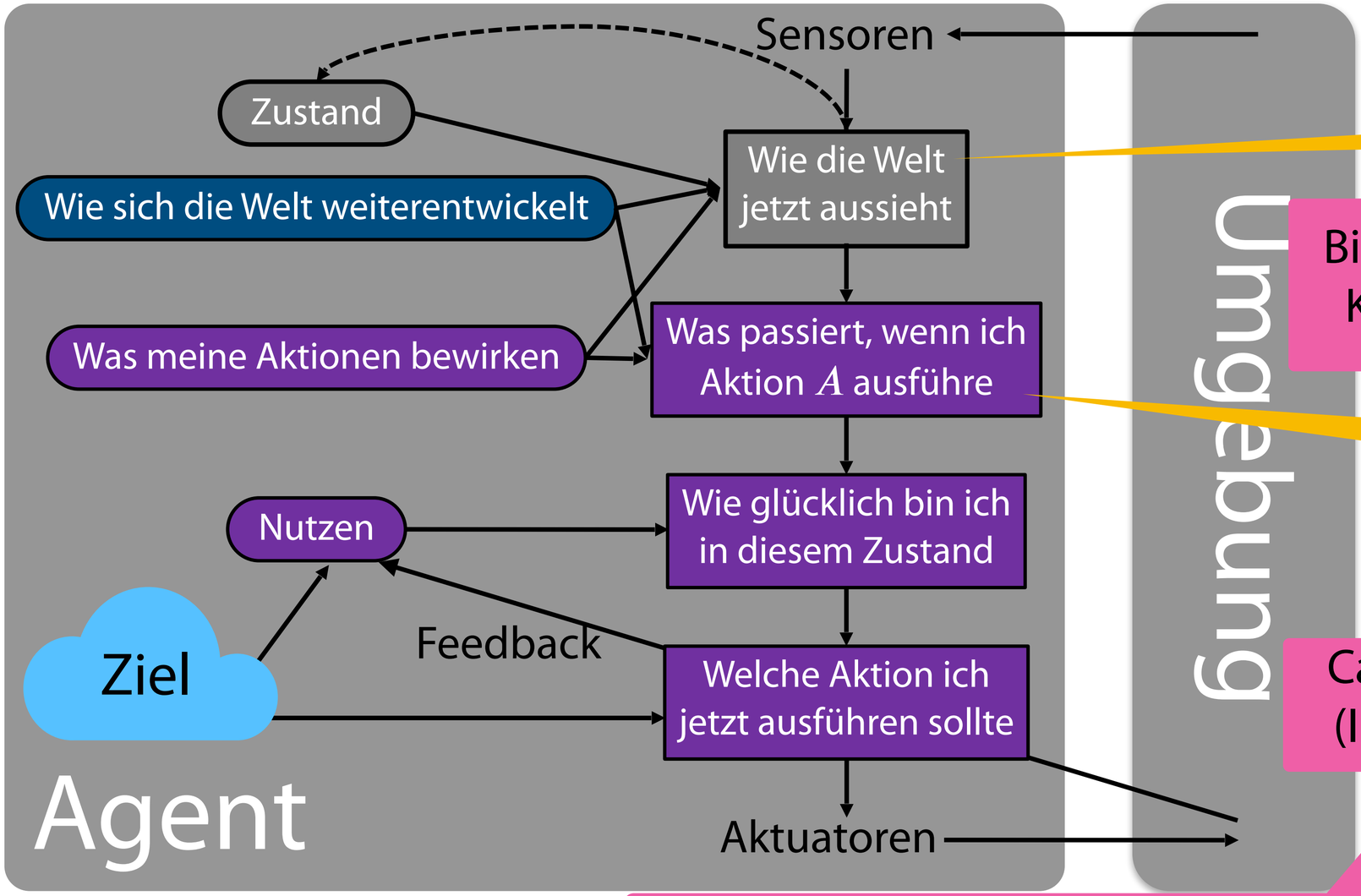
Agent: Maschinelles Lernen



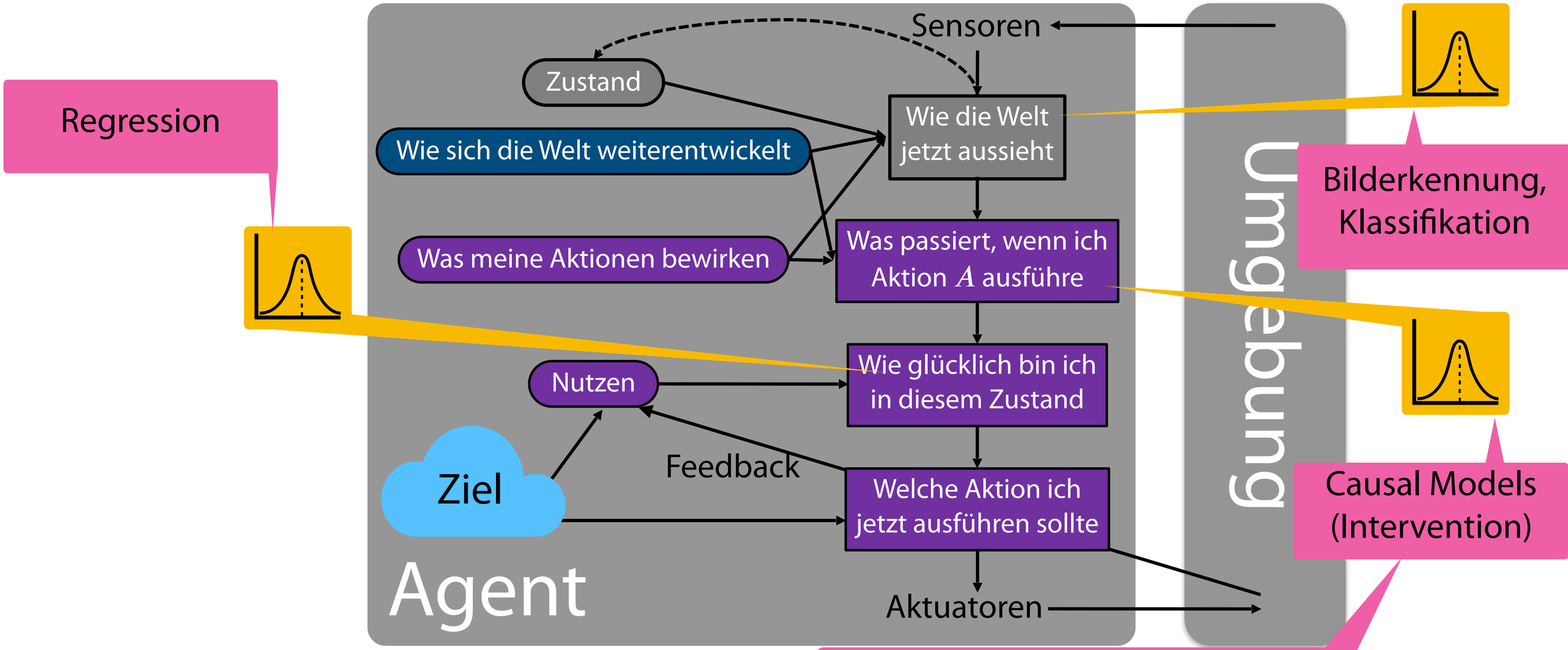
Agent: Maschinelles Lernen



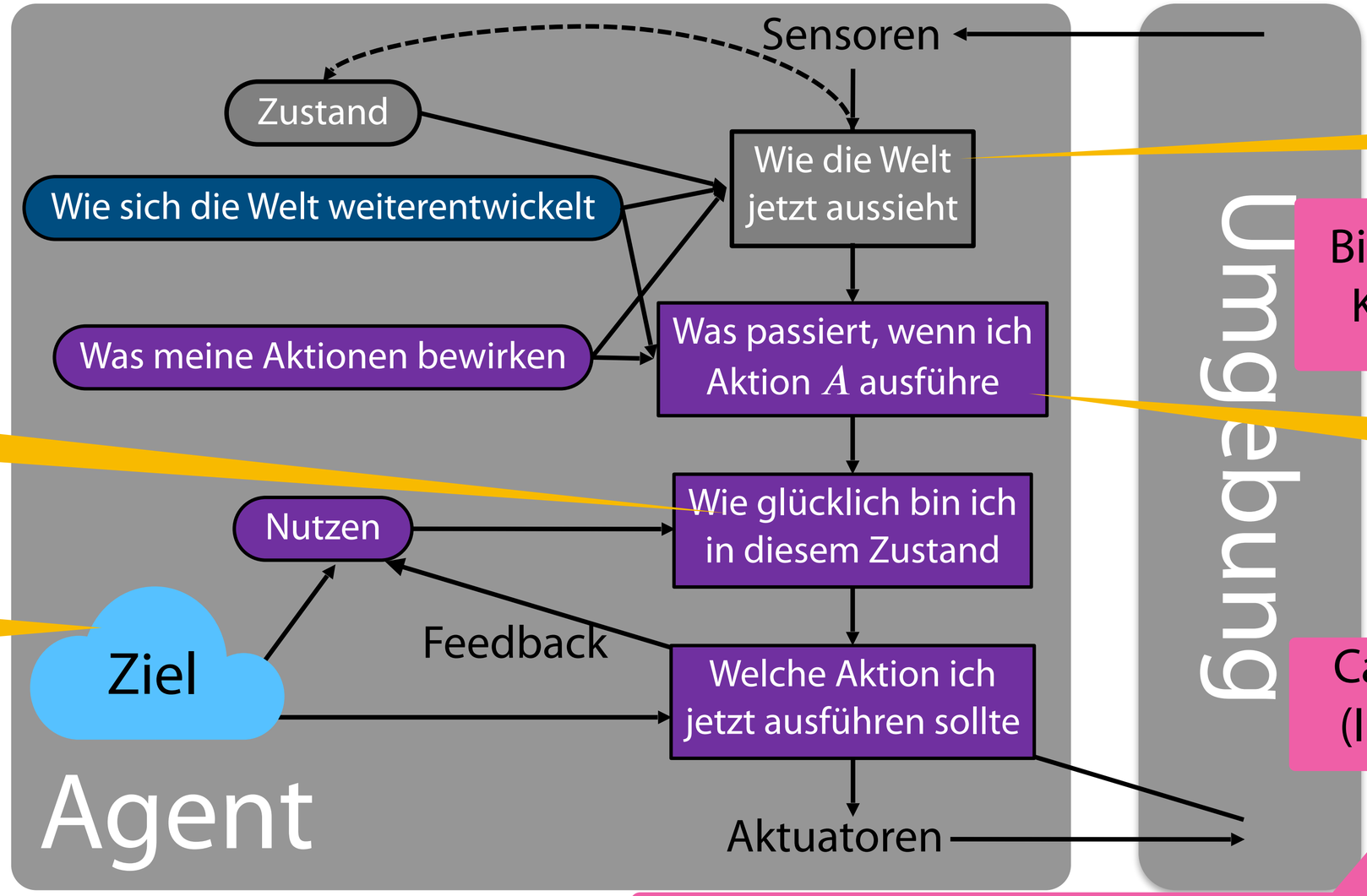
Agent: Maschinelles Lernen



Agent: Maschinelles Lernen



Agent: Maschinelles Lernen



Regression

Bilderkennung, Klassifikation

Causal Models (Intervention)

Reinforcement Learning (Ziel und Nutzen aus Feedback „lernen“)

Causal Models (Counterfactuals) „Was wäre, wenn ich x getan hätte?“

Konzept

Konzept

- „Werkzeuge“ für das wissenschaftliche Arbeiten
  - Fokus auf Werkzeug *Python*
  - Anwendung *Machine Learning* und *Data Science*

Konzept

- „Werkzeuge“ für das wissenschaftliche Arbeiten
  - Fokus auf Werkzeug *Python*
  - Anwendung *Machine Learning* und *Data Science*
- Vorstellung einer Auswahl
- Verfahren des *Machine Learning* und *Data Science*
  1. Problematik
  2. Idee der Theorie
  3. Lösung mittels Python & Paketen

Vorlesungen zu den Themen

- Bachelor
  - **Einführung in Web und Data Science** (CS1800)
  - **Non-Standard Datenbanken und Data Mining** (CS3130)
  - Logikprogrammierung (CS3055)

Vorlesungen zu den Themen

- Bachelor
  - **Einführung in Web und Data Science** (CS1800)
  - **Non-Standard Datenbanken und Data Mining** (CS3130)
  - Logikprogrammierung (CS3055)
- Master
  - Aktuelle Themen Data Science und KI (CS 5070) (z.B. zum Thema „Probabilistic and Differential Programming“)
  - **Intelligente Agenten** (CS 4514)
  - Informationssysteme (CS4130)

Vorlesungen zu den Themen

Kleine Teilmenge von IFIS-Modulen

- Bachelor
  - **Einführung in Web und Data Science** (CS1800)
  - **Non-Standard Datenbanken und Data Mining** (CS3130)
  - Logikprogrammierung (CS3055)
- Master
  - Aktuelle Themen Data Science und KI (CS 5070) (z.B. zum Thema „Probabilistic and Differential Programming“)
  - **Intelligente Agenten** (CS 4514)
  - Informationssysteme (CS4130)

III.
Clustering

Clustering

Problem	Clustering, Partitionierung
Verfahren	*k*-Means
Art	Unüberwacht
Hyperparameter	Initiale Zentroiden, Anzahl Zentroiden
Python-Paket	SKLearn
Klasse	`sklearn.cluster.KMeans`

Clustering

Problem	Clustering, Partitionierung
Verfahren	*k*-Means
Art	Unüberwacht
Hyperparameter	Initiale Zentroiden, Anzahl Zentroiden
Python-Paket	SKLearn
Klasse	`sklearn.cluster.KMeans`

Unüberwacht:
Daten haben keine Label, es wird hier nach einer „sinnvollen“ Ordnung/ Gruppierung der Daten gesucht.

Dafür gilt es z.B. eine Fehlerfunktion zu minimieren.

k-Means

- Form des unüberwachten Lernens
- Suche nach natürlicher Gruppierungen von Objekten
  - Klassen direkt aus Daten bestimmen
    - Hohe Intra-Klassen-Ähnlichkeit
    - Kleine Inter-Klassen-Ähnlichkeit

k-Means

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- Suche nach natürlicher Gruppierungen von Objekten
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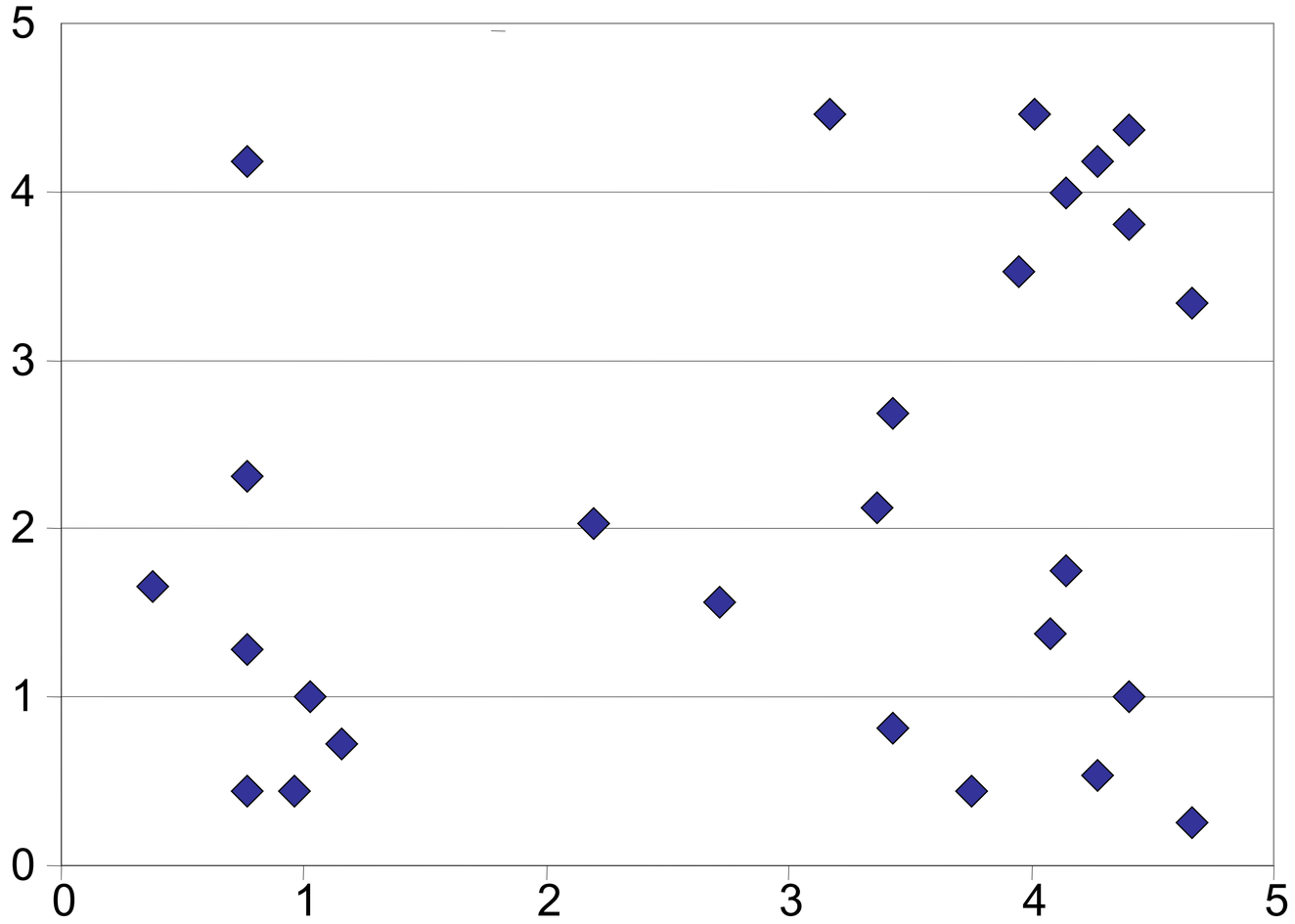
    - Kleine Inter-Klassen-Ähnlichkeit

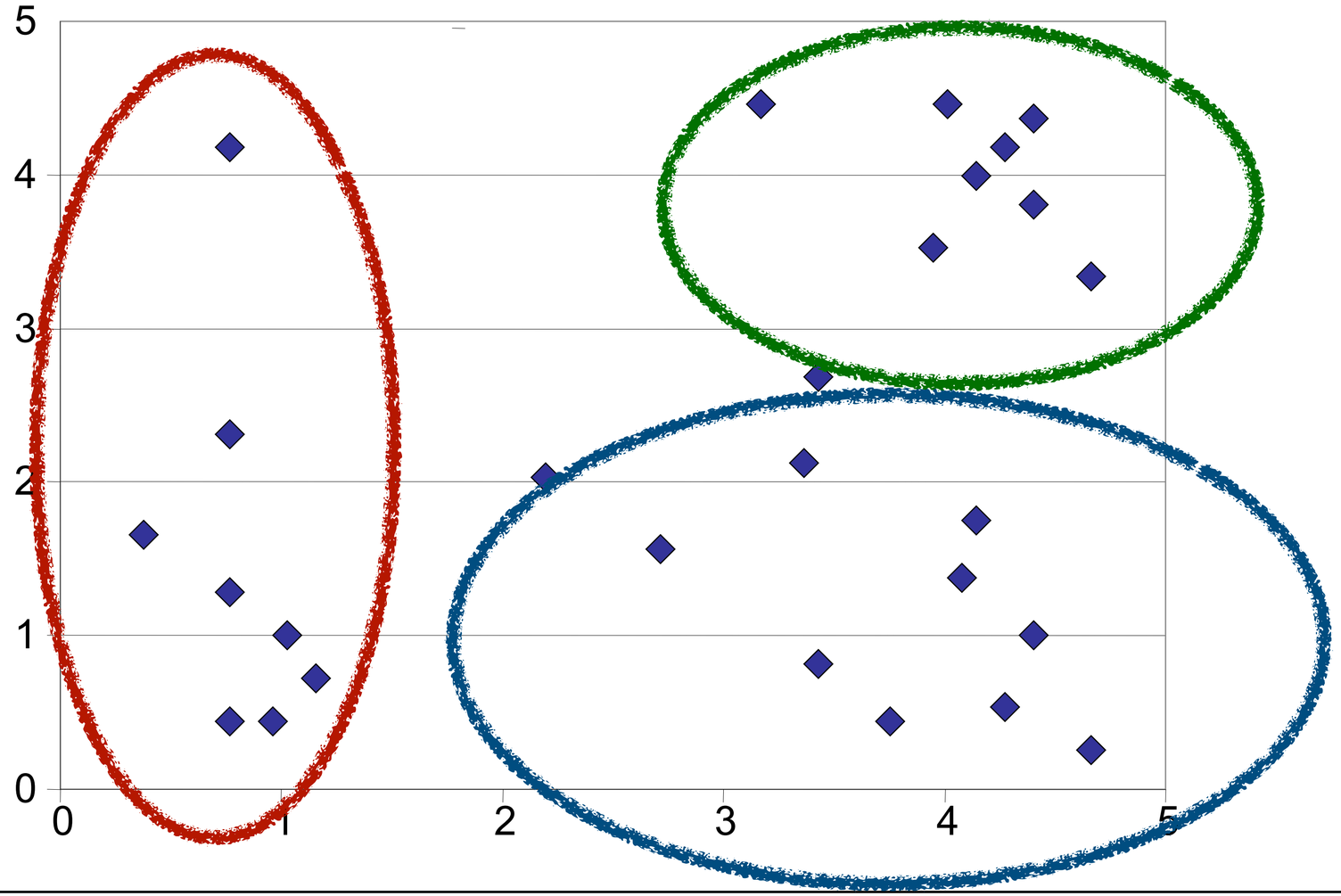
$$\|x - y\|_2 = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

Distanzmaß,
z.B. euklidische Distanz

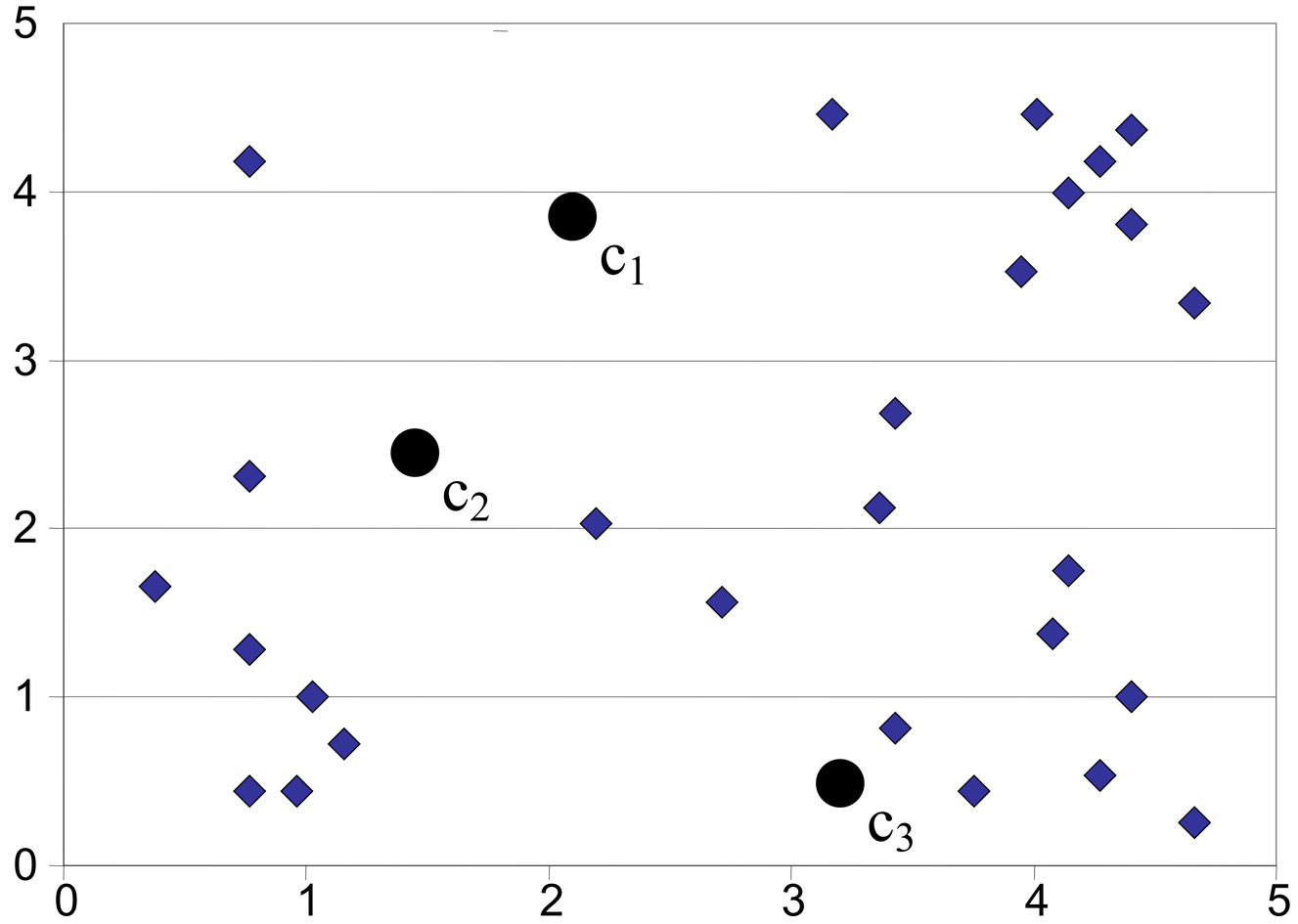
Gruppierungen gesucht!



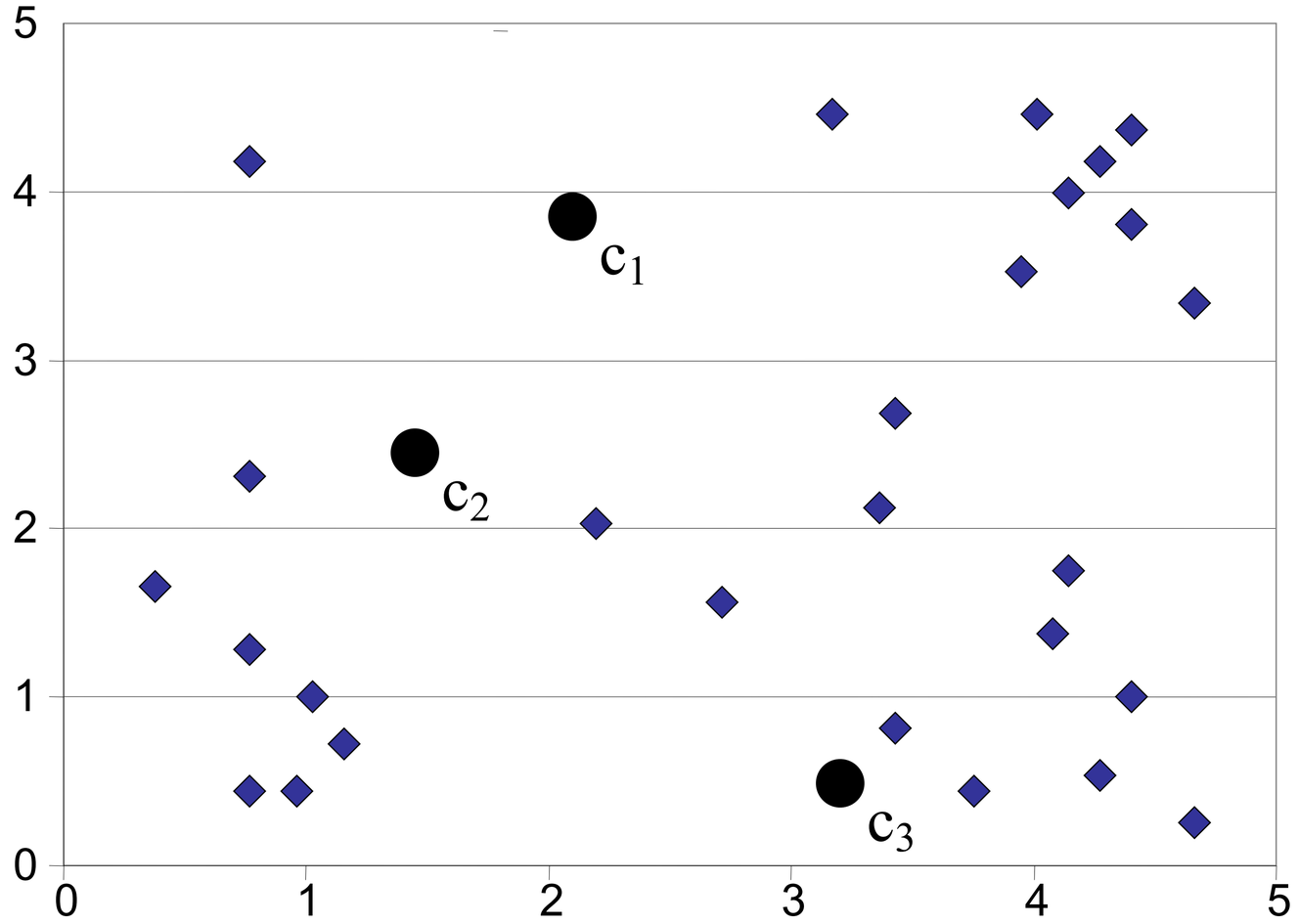
Gruppierungen gesucht!



k-Means; $t = 0$



k-Means; $t = 0$

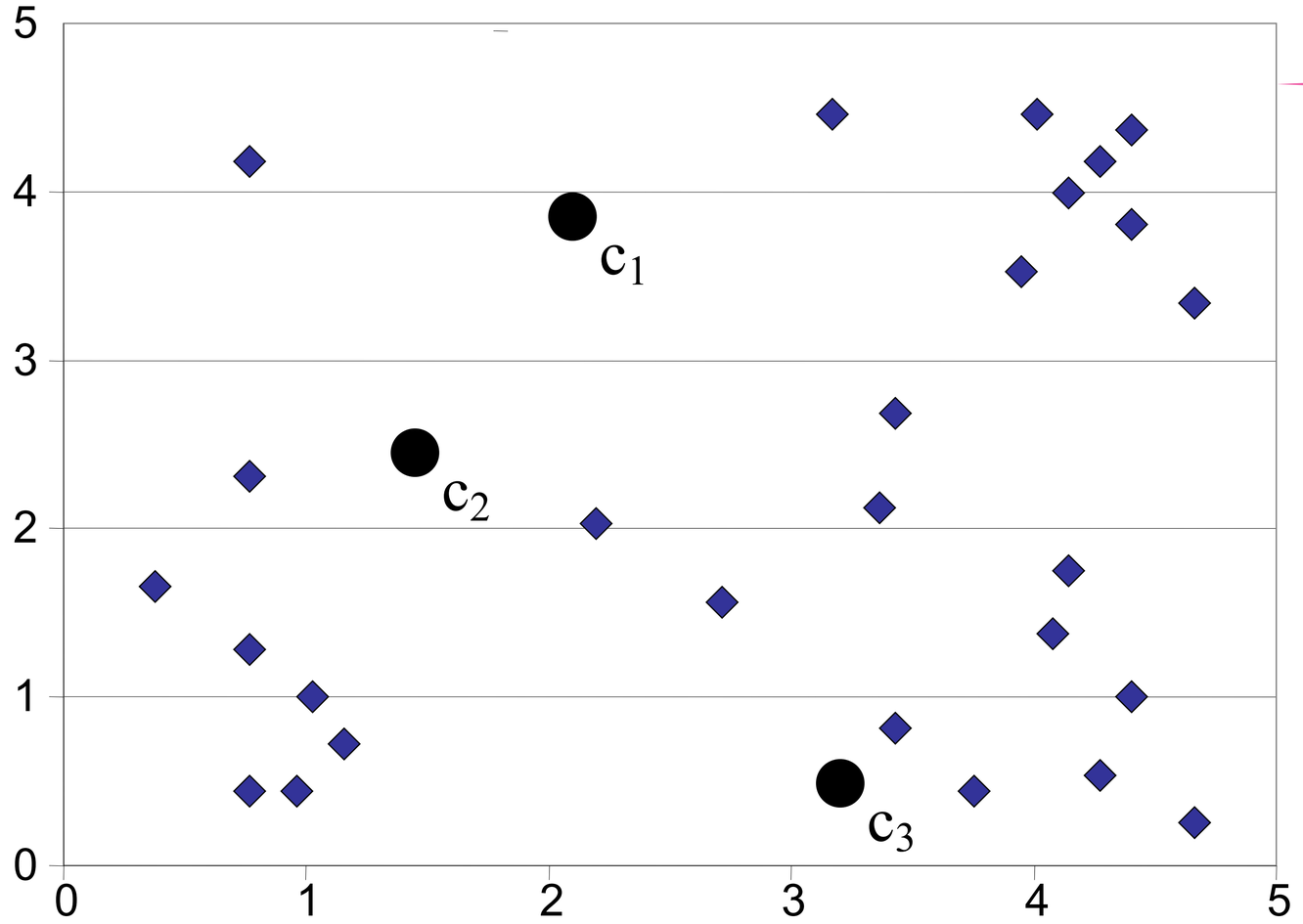


$$C_i^t = \left\{ x_j : \left\| x_j - c_i^t \right\|_2 \leq \left\| x_j - c_r^t \right\|_2 \right.$$

$$\left. \text{for all } r = 1 \ldots k,\ r \neq i \right\}$$

Zentroid $i = 1, \ldots, k$ und Iteration beginnend mit $t = 0$

k-Means; $t = 0$



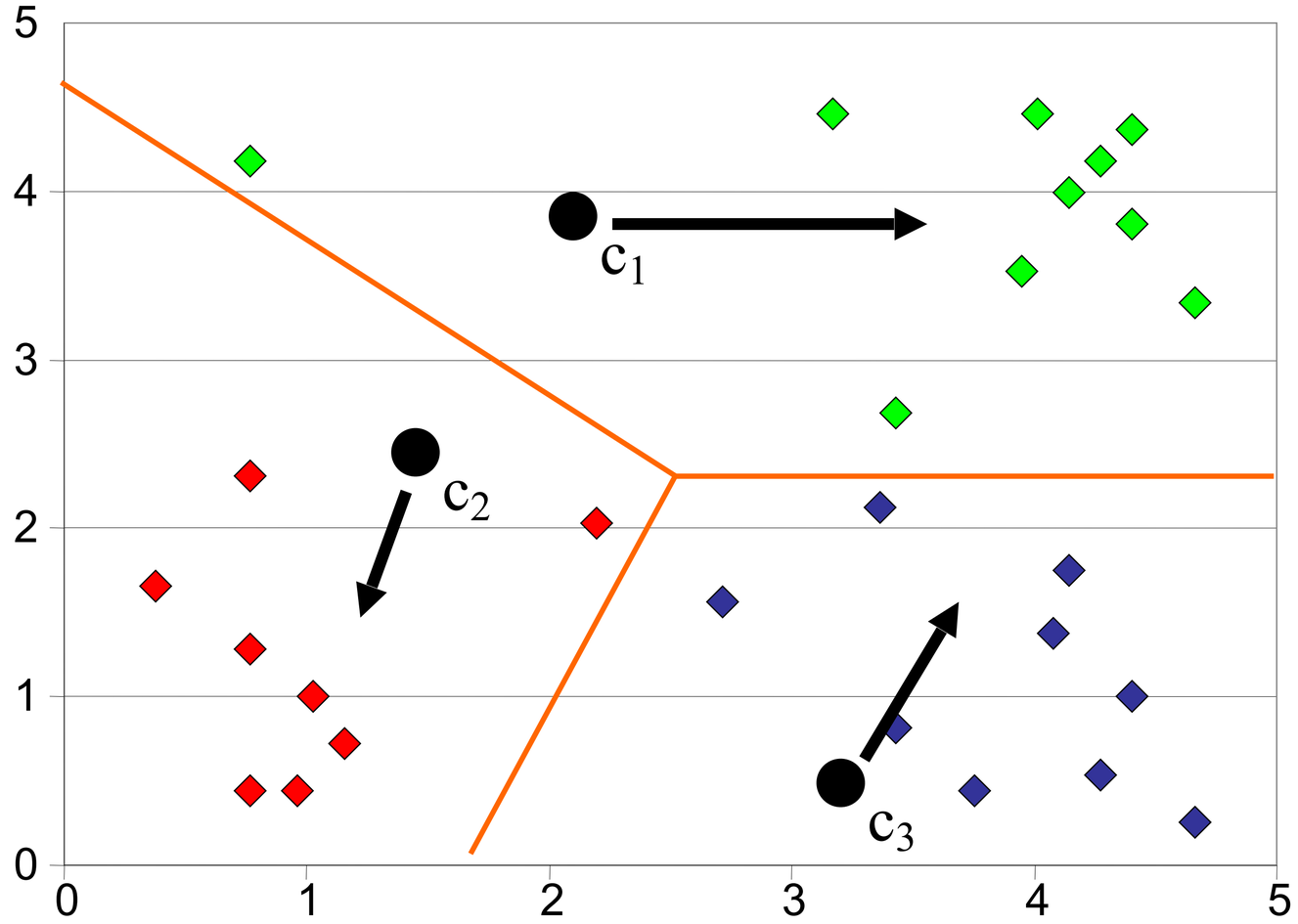
Drei initiale Zentroiden in den Datenpunkten

Zuordnung jedes Datenpunkts zum dichtesten Zentroiden, bilden Cluster *C*.

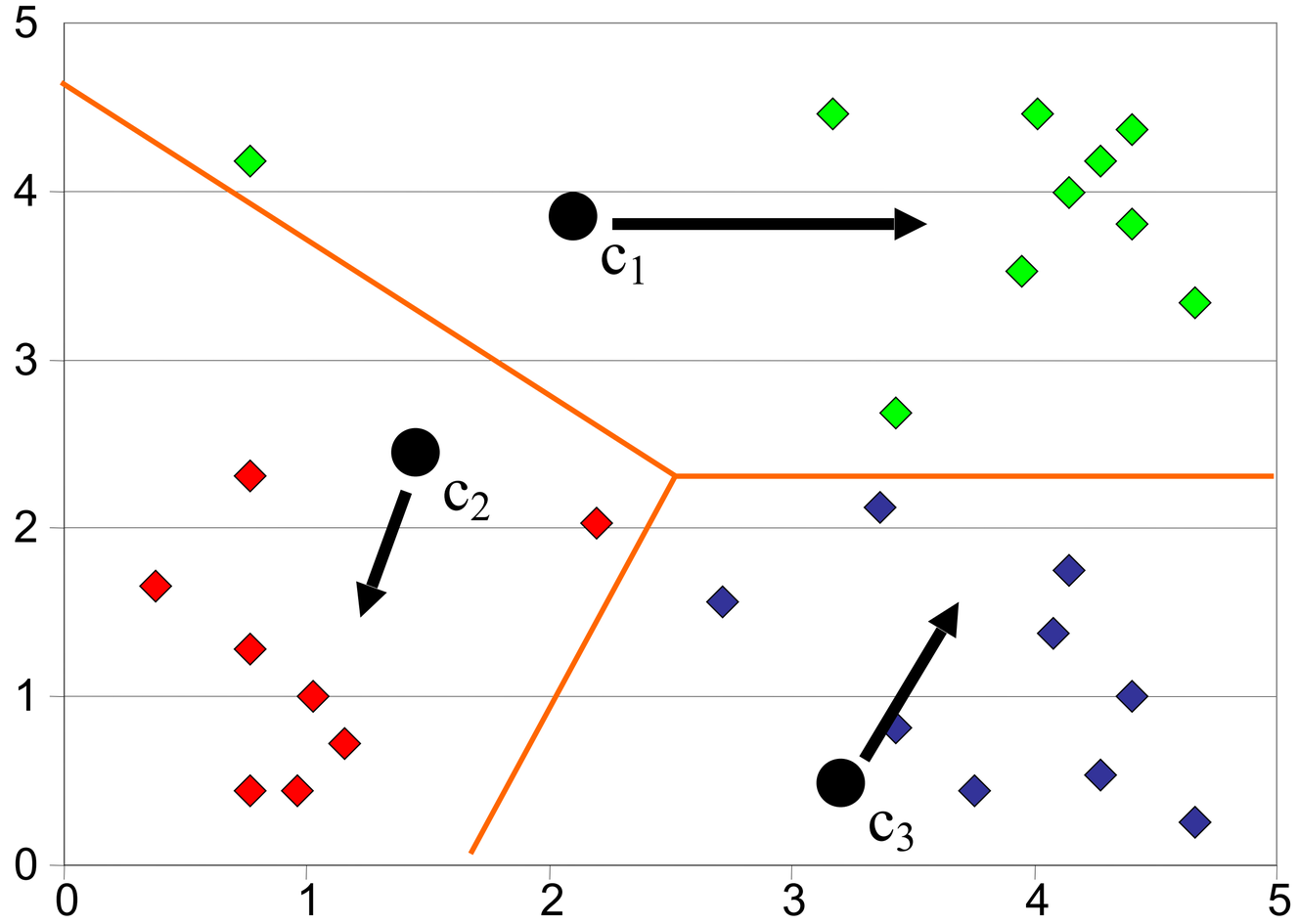
$$C_i^t = \left\{ x_j : \left\| x_j - c_i^t \right\|_2 \leq \left\| x_j - c_r^t \right\|_2 \text{ for all } r = 1 \ldots k,\ r \neq i \right\}$$

Zentroid $i = 1, \ldots, k$ und Iteration beginnend mit $t = 0$

k-Means; $t = 0 + 1$

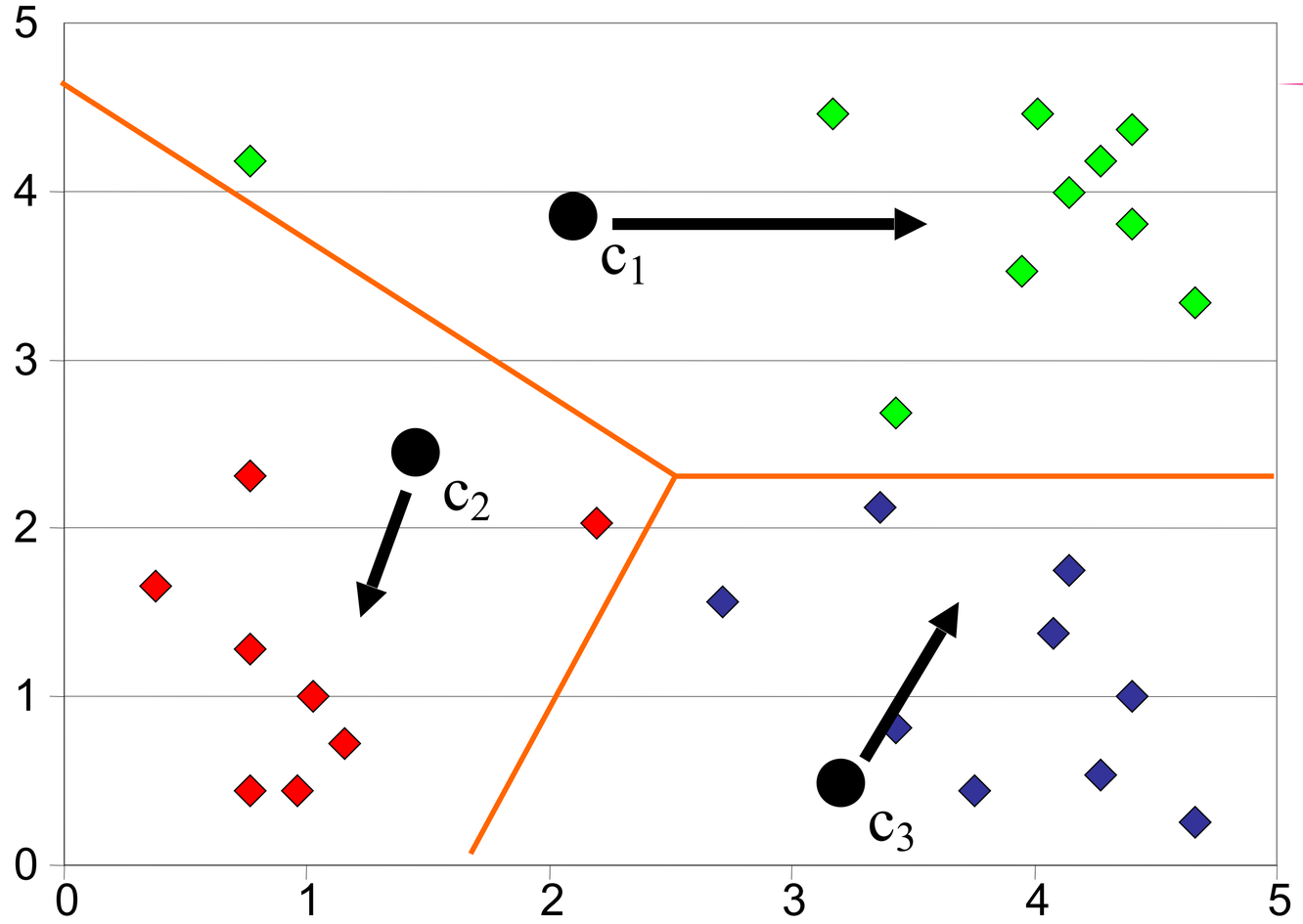


k-Means; $t = 0 + 1$



$$c_i^{t+1} = \frac{1}{\left|C_i^t\right|} \sum_{x_j \in C_i^t} x_j$$

k-Means; $t = 0 + 1$



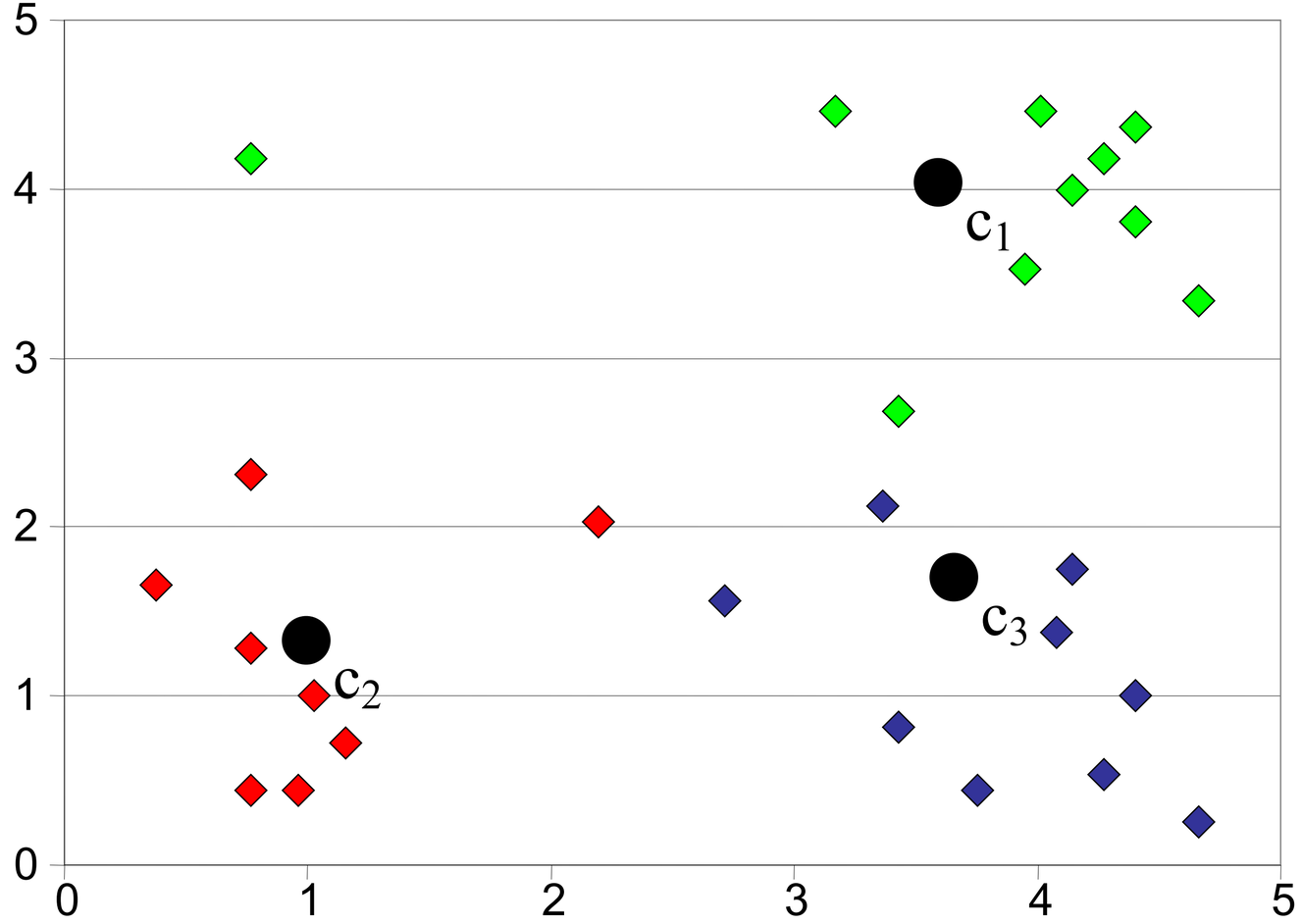
Drei Cluster farblich markiert.

Zentroiden in „Mitte“ jedes Cluster bewegen.

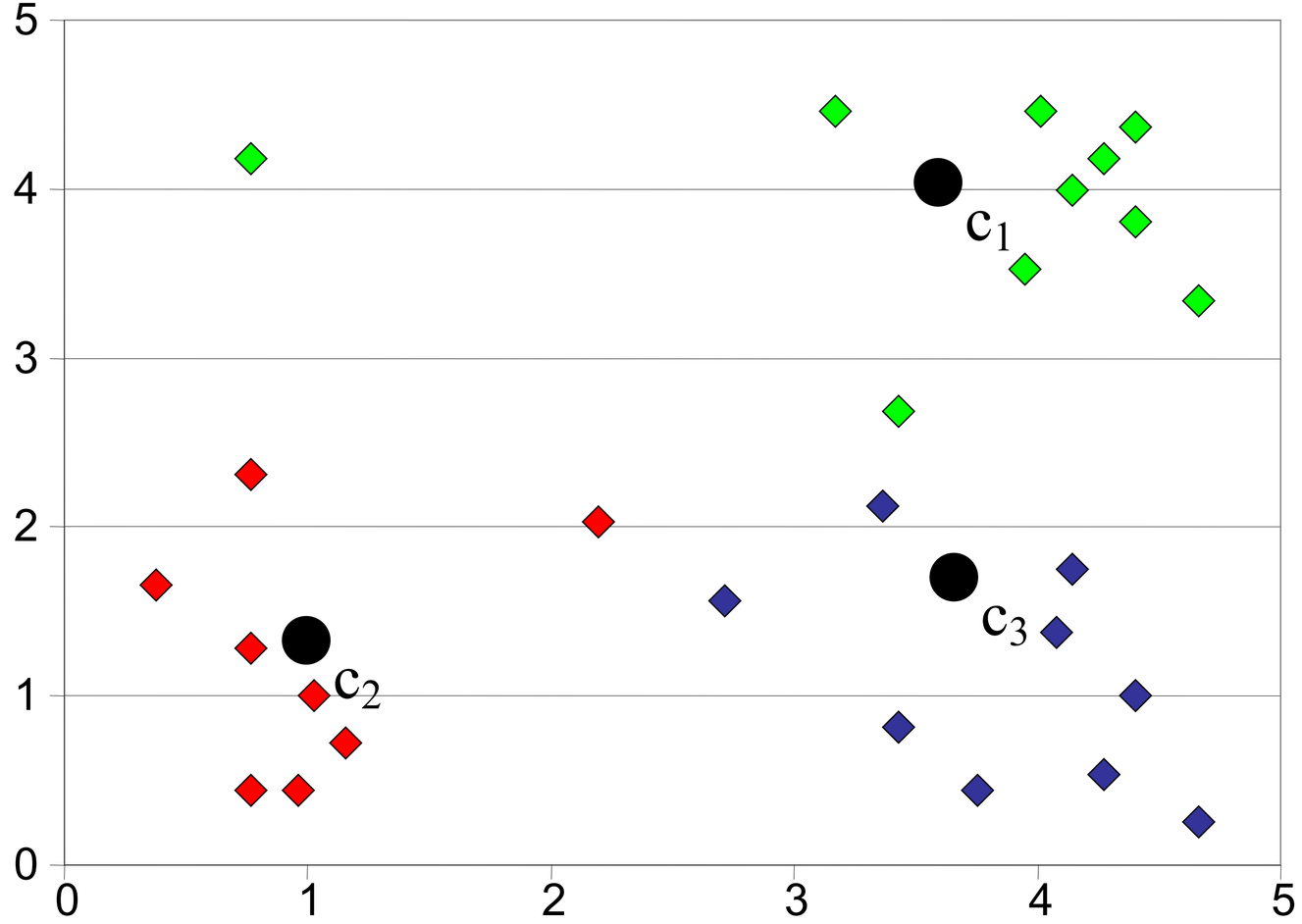
$$c_i^{t+1} = \frac{1}{\left|C_i^t\right|} \sum_{x_j \in C_i^t} x_j$$

Weiter iterieren.

k-Means; *t* = *1*



k-Means; *t* = *1*

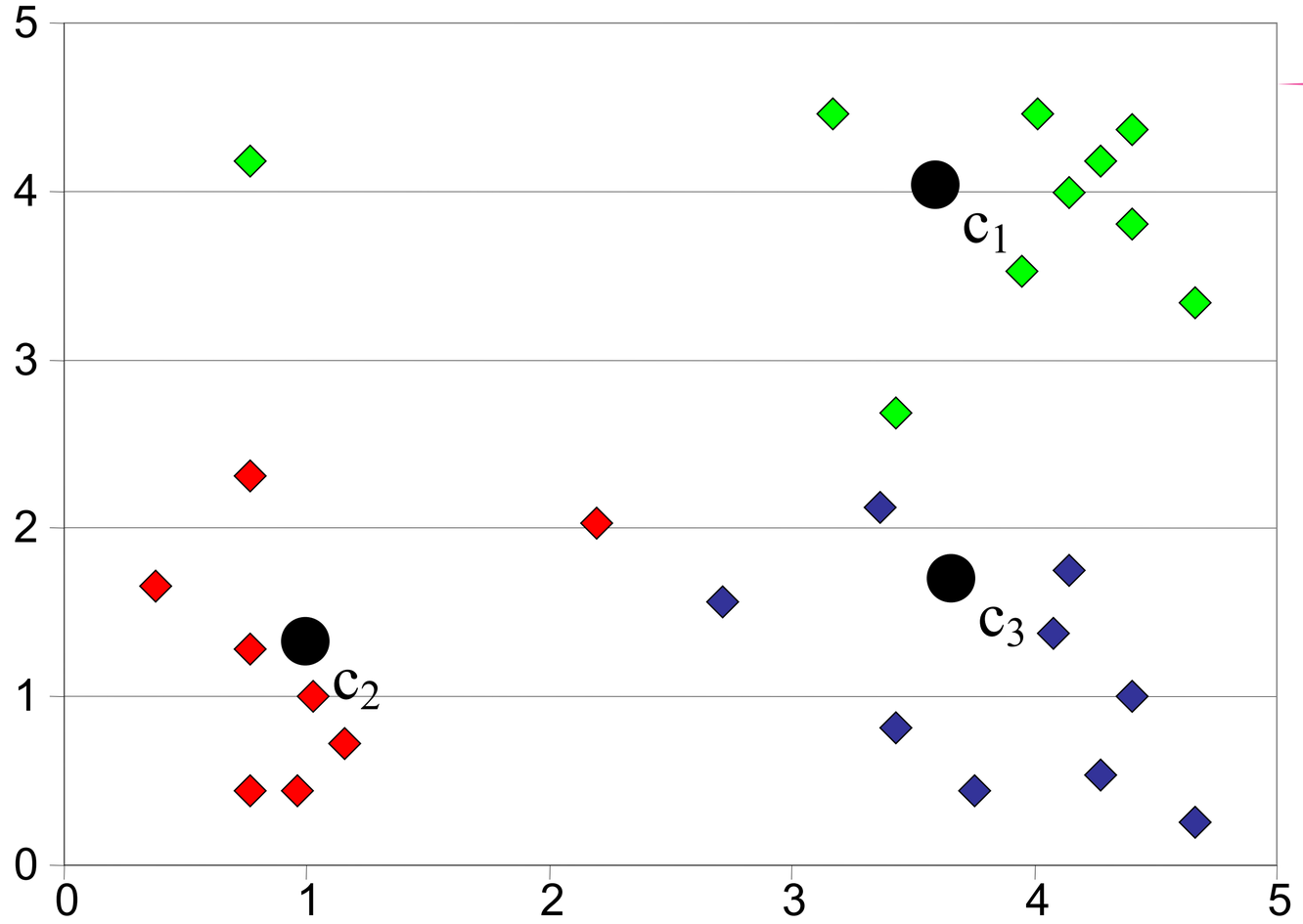


$$C_i^t = \left\{ x_j : \left\| x_j - c_i^t \right\|_2 \leq \left\| x_j - c_r^t \right\|_2 \right.$$

$$\left. \text{for all } r = 1 \ldots k,\ r \neq i \right\}$$

Zentroid $i = 1, \ldots, k$ und Iteration beginnend mit $t = 0$

k-Means; *t* = 1



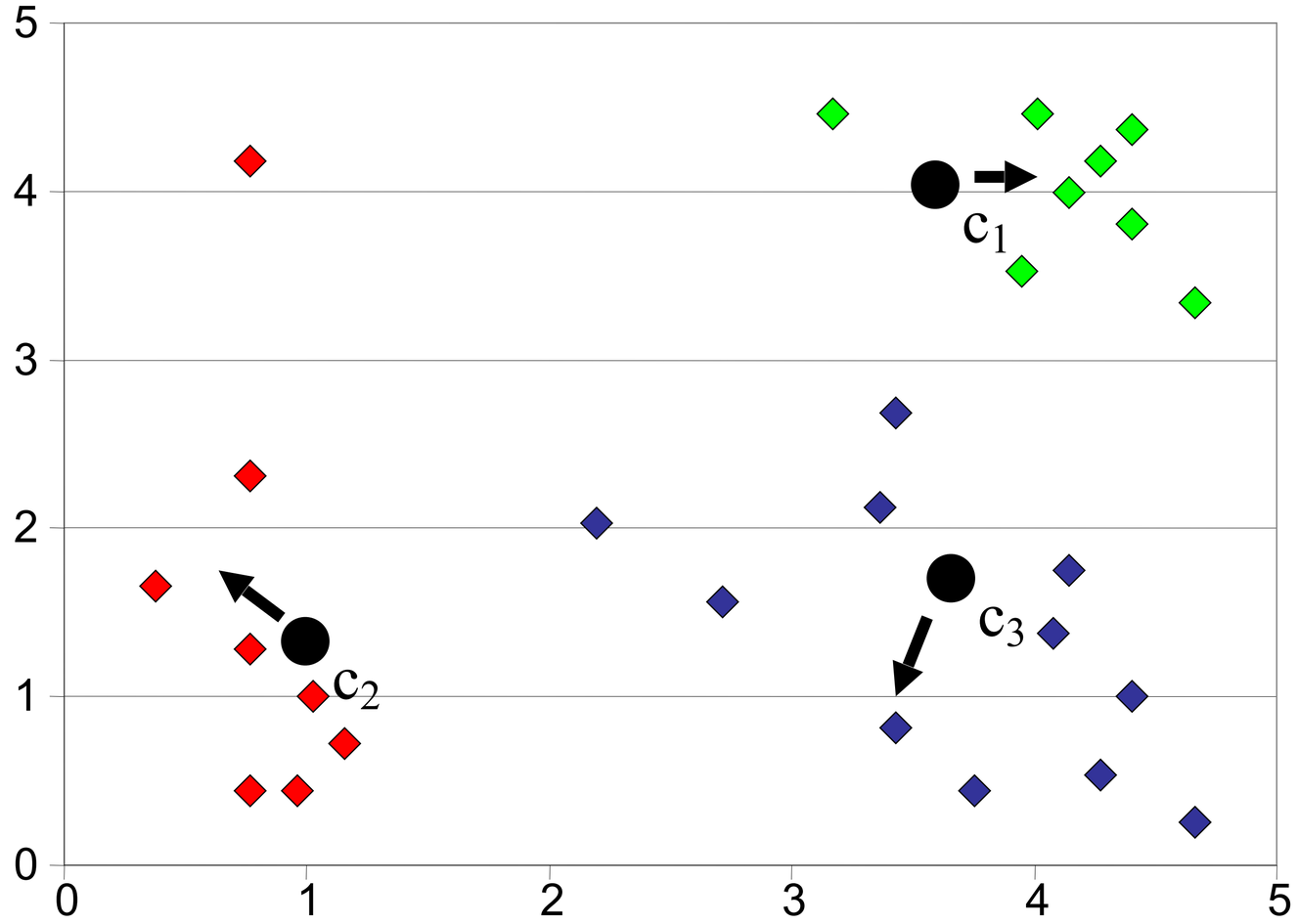
Zentroiden an neuen Positionen

Datenpunkte den Zentroiden neu zuordnen, Cluster verändern sich.

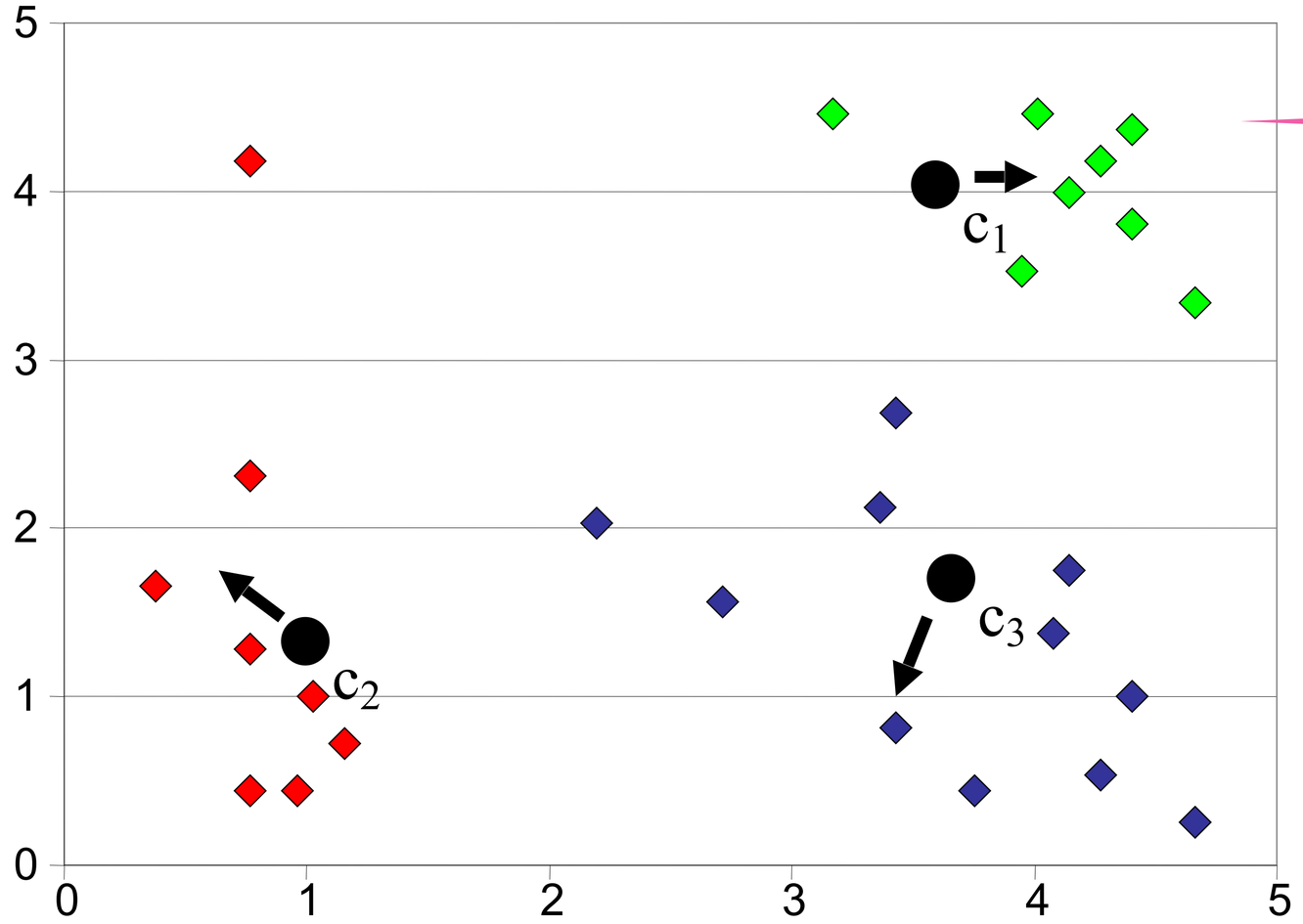
$$C_i^t = \left\{ x_j : \left\| x_j - c_i^t \right\|_2 \leq \left\| x_j - c_r^t \right\|_2 \text{ for all } r = 1 \ldots k,\ r \neq i \right\}$$

Zentroid $i = 1, \ldots, k$ und Iteration beginnend mit $t = 0$

k-Means; $t = 1 + 1$

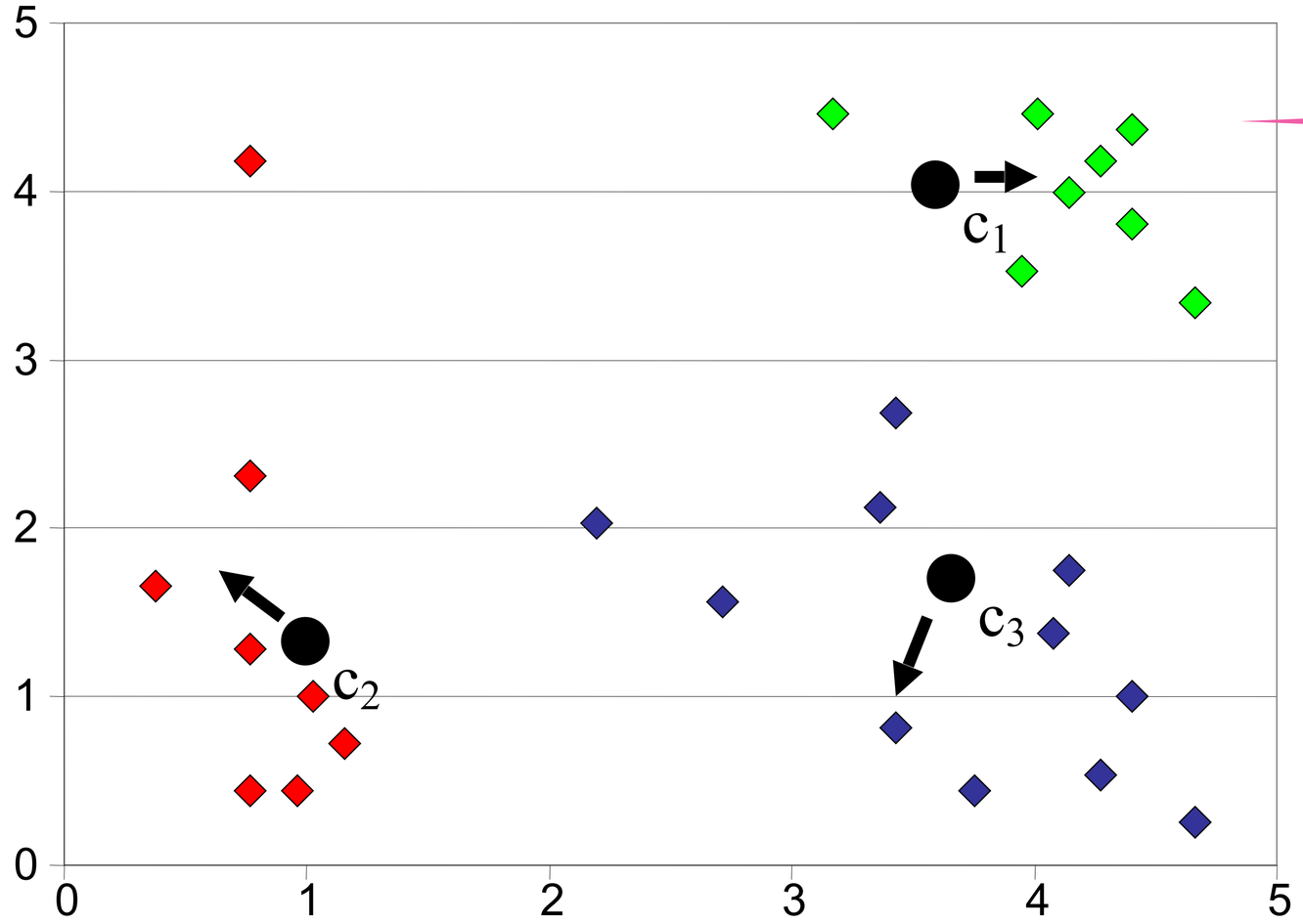


k-Means; $t = 1 + 1$



Erneut Zentroiden in die Mitte schieben.

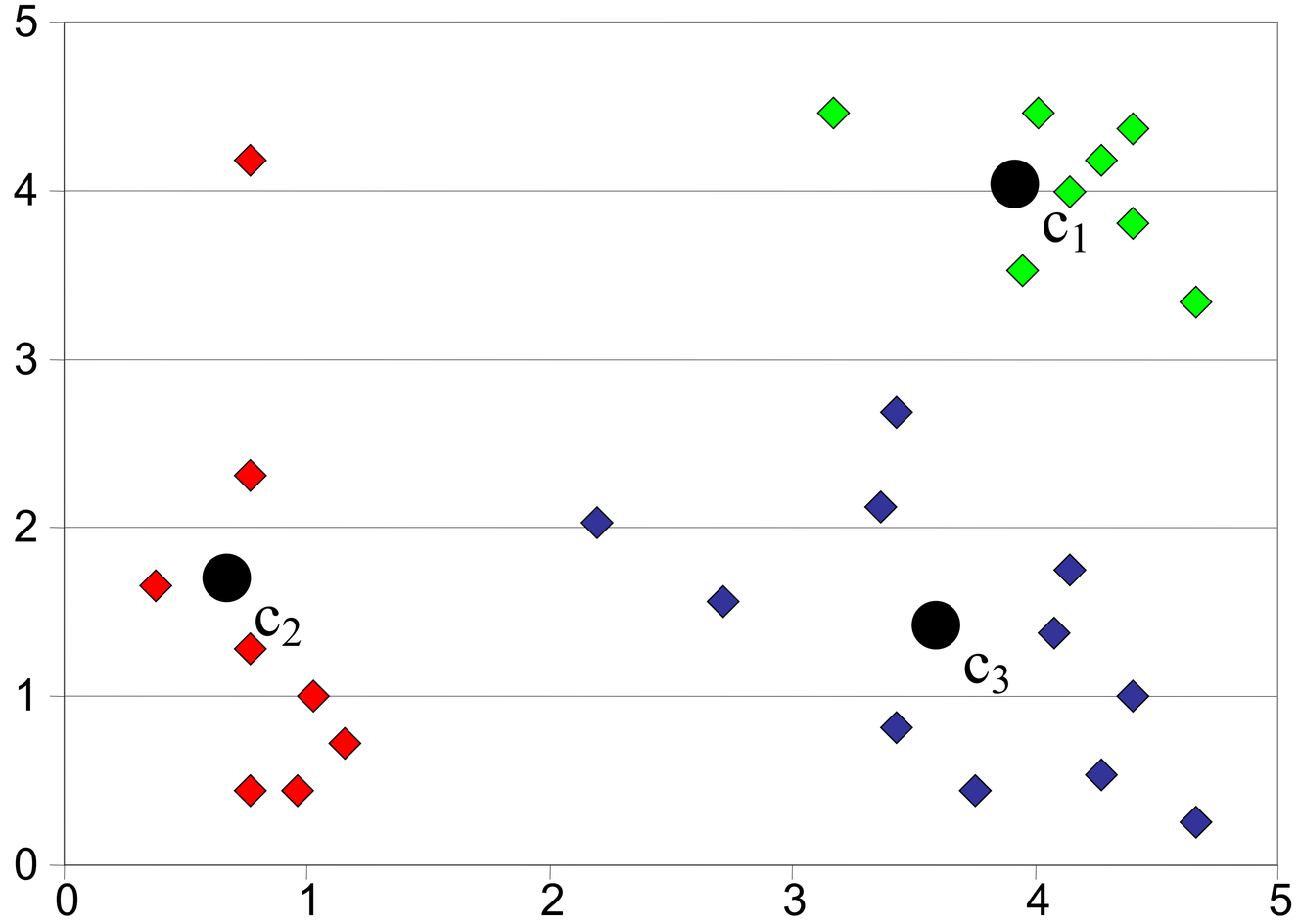
k-Means; $t = 1 + 1$



Erneut Zentroiden in die Mitte schieben.

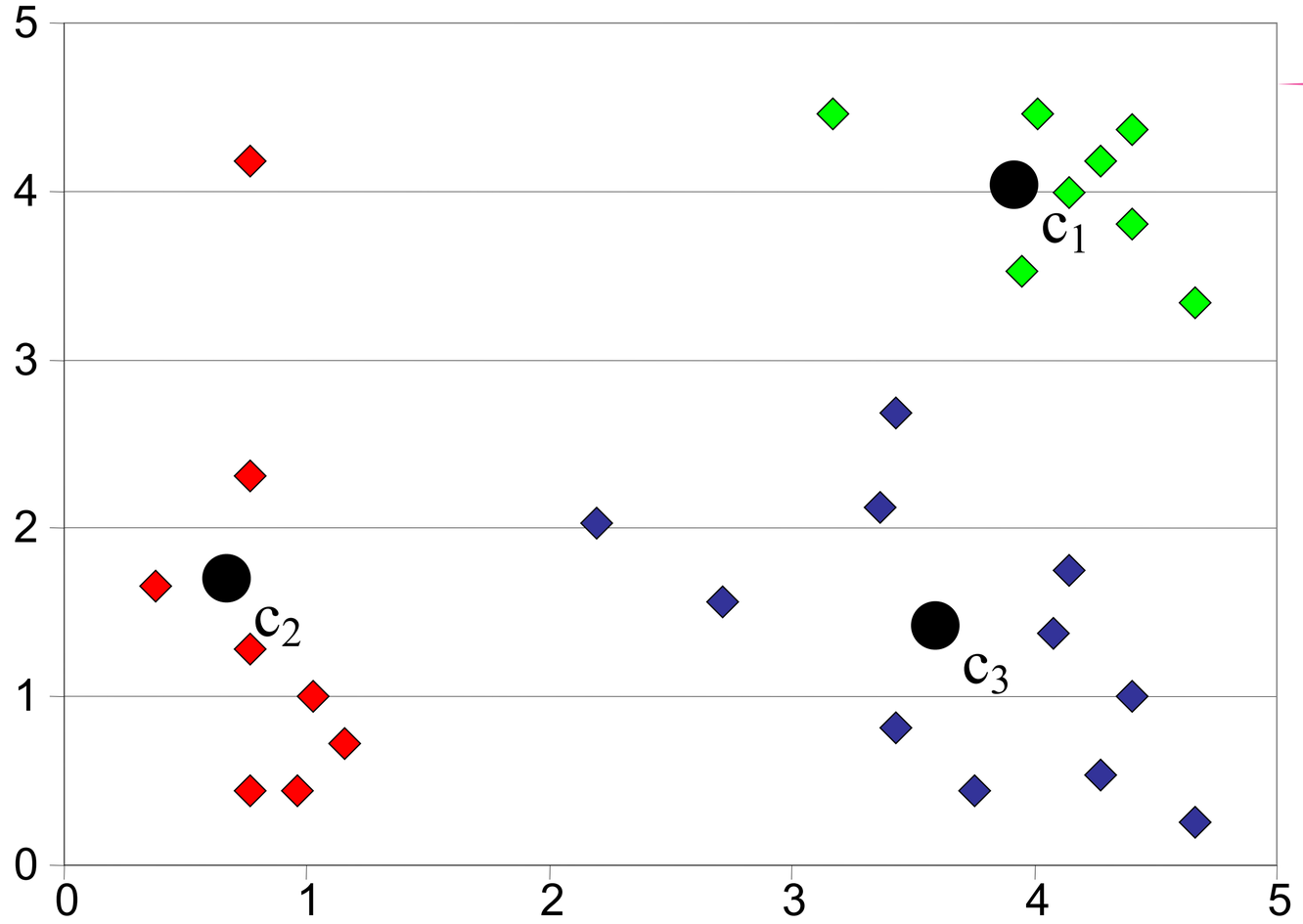
$$c_i^{t+1} = \frac{1}{\left|C_i^t\right|} \sum_{x_j \in C_i^t} x_j$$

k-Means; $t = 2$



J. B. MacQueen: "Some Methods for classification and Analysis of Multivariate Observations, *Proceedings of 5-th Berkeley Symposium on Mathematical Statistics and Probability*", Berkeley, University of California Press, 1:281-297, **1967**

k-Means; $t = 2$



Zentroiden wieder an neuen Positionen

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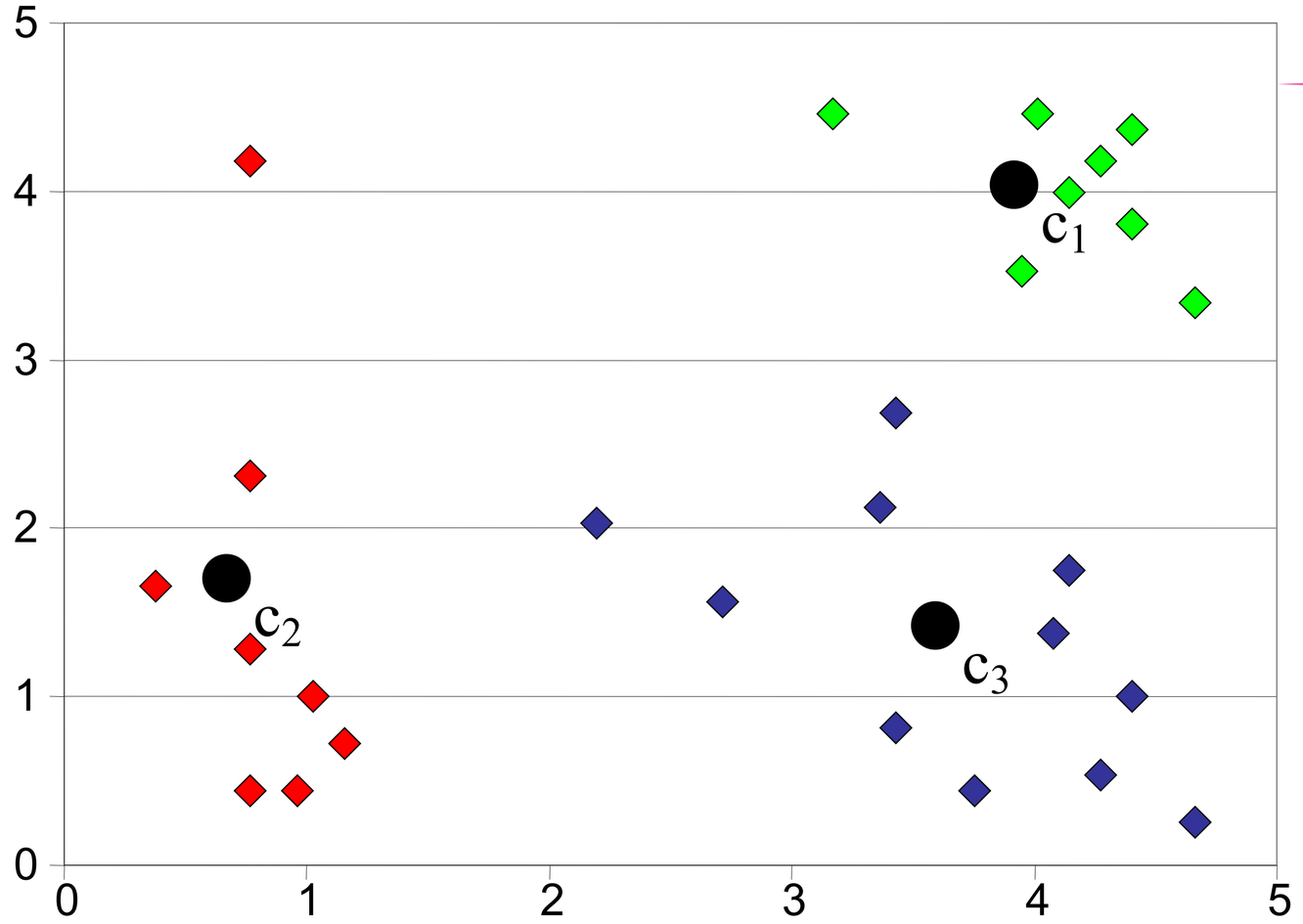


Zentroiden wieder an neuen Positionen

Keine Änderungen den Zugehörigkeiten mehr

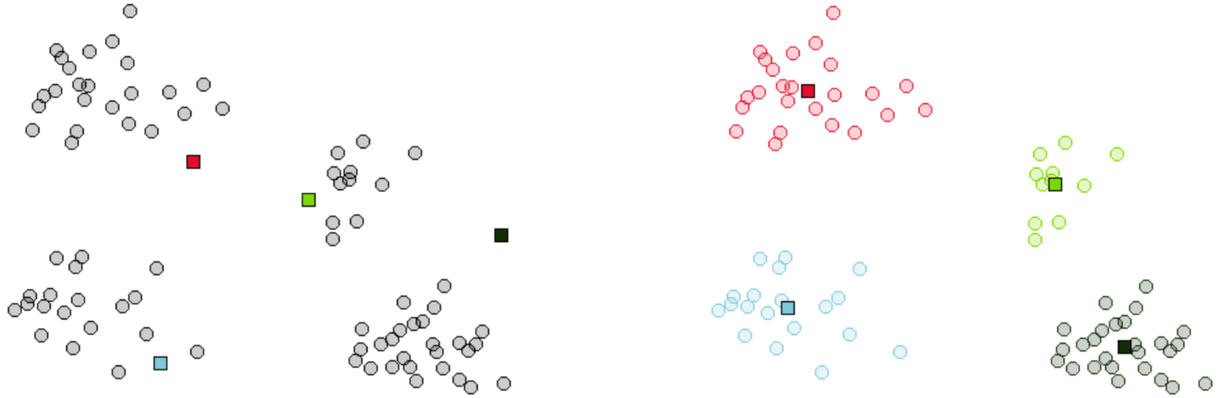
→

Algorithmus beendet

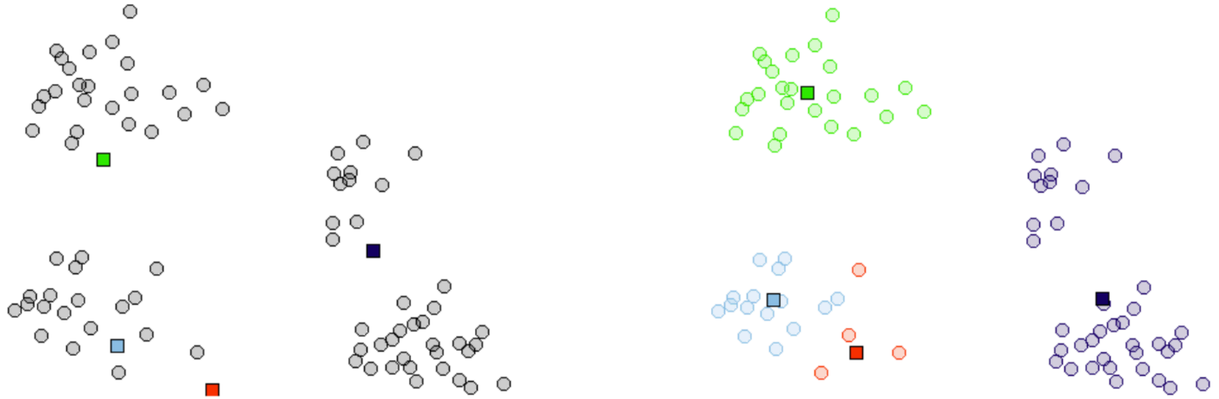
J. B. MacQueen: "Some Methods for classification and Analysis of Multivariate Observations, *Proceedings of 5-th Berkeley Symposium on Mathematical Statistics and Probability*", Berkeley, University of California Press, 1:281-297, **1967**

k-Means: Ergebnis hängt vom Startwert ab

Gutes Ergebnis



Schlechtes Ergebnis



Installation

- Python Paket
  - https://scikit-learn.org/
- Installation z.B. mit `pip3 install scikit-learn`
- Import, z.B.

```
from sklearn.cluster import KMeans
```

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Intern Nutzung von NumPy und C

Integration mit z.B. Matplotlib und Pandas

Installation

- Python Paket
  - https://scikit-learn.org/
- Installation z.B. mit `pip3 install scikit-learn`
- Import, z.B.

Paket `sklearn` und Installation als `scikit-learn`

Intern Nutzung von NumPy und C

Integration mit z.B. Matplotlib und Pandas

```
from sklearn.cluster import KMeans
```

KMeans-Klasse

```
from sklearn.cluster import KMeans
import numpy as np
import matplotlib.pyplot as plt

X = np.array([
  [1, 1], [1, 2], [2, 2],
  [4, 1], [5, 1], [5, 2]
])

plt.scatter(X[:, 0], X[:, 1], s=10)
plt.show()

km = KMeans(n_clusters=2, init='random', tol=1e-4)
km.fit(X)

print(km.cluster_centers_)

print(km.labels_)


print(km.predict([[1, 1.5]]))
```

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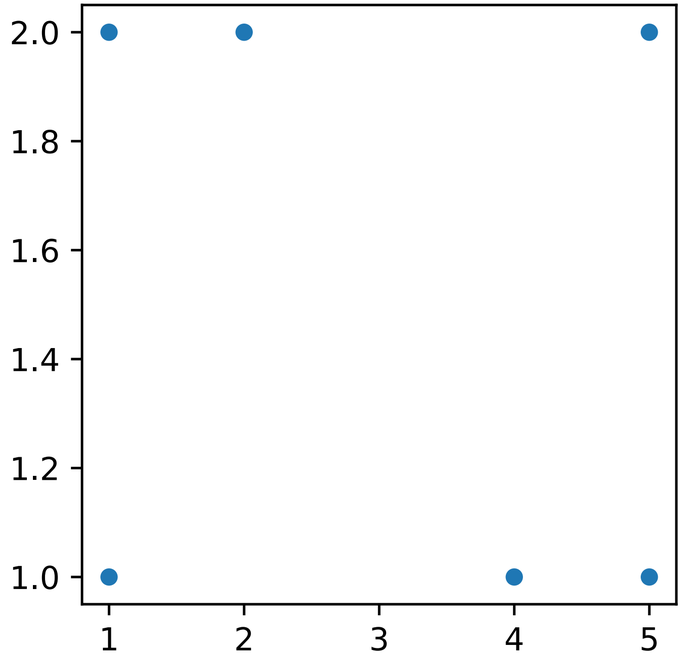

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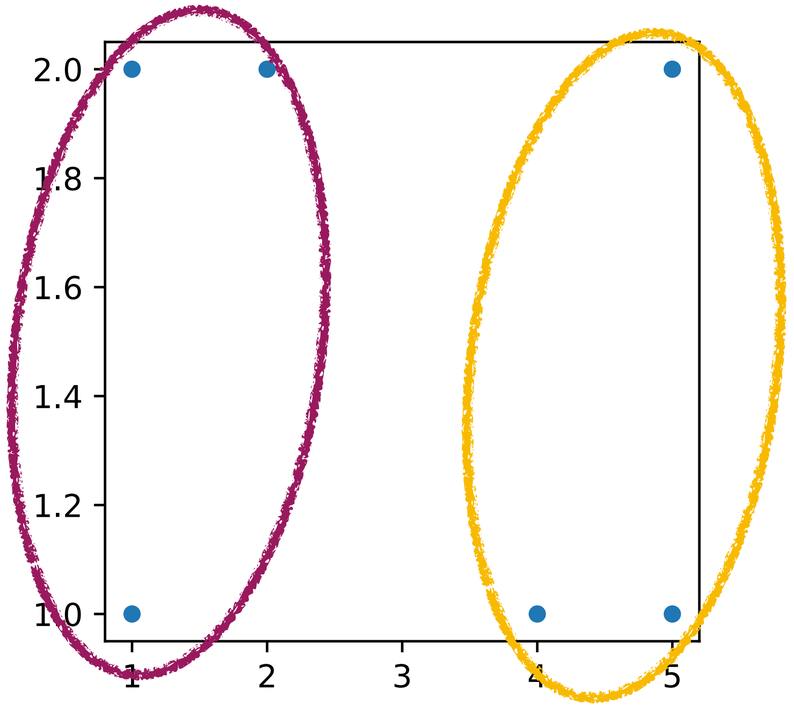

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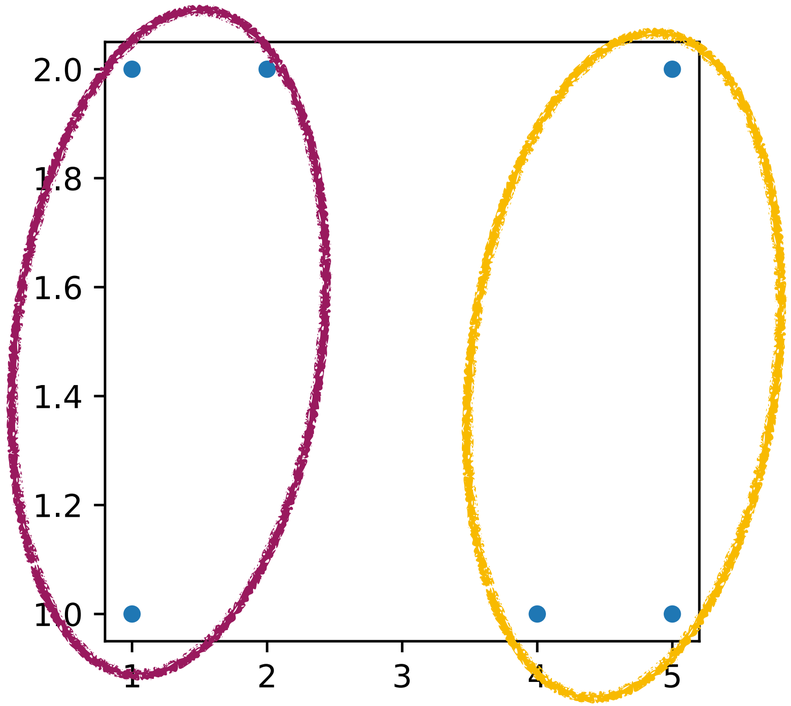
```
[[1.33333333 1.66666667]
 [4.66666667 1.33333333]]
```



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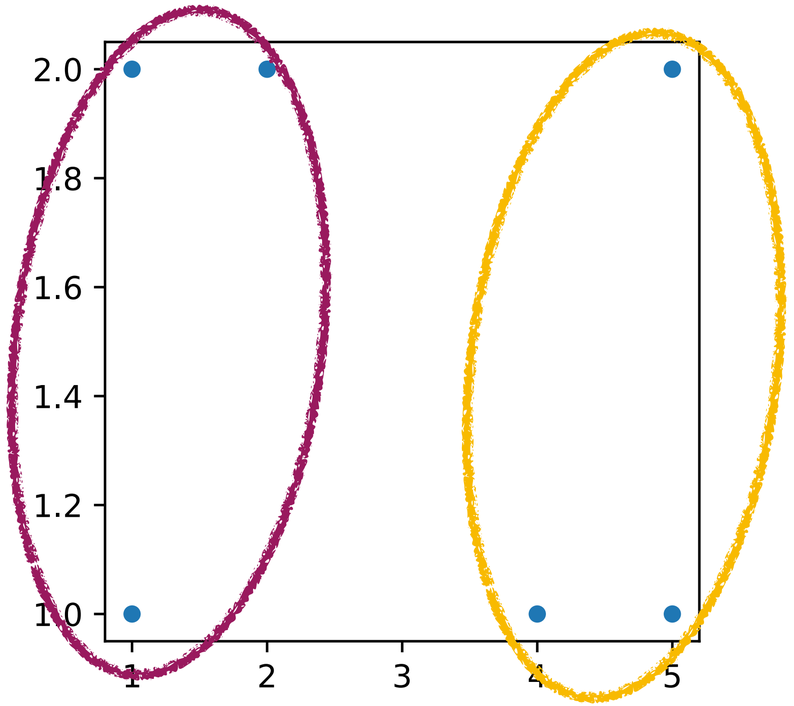

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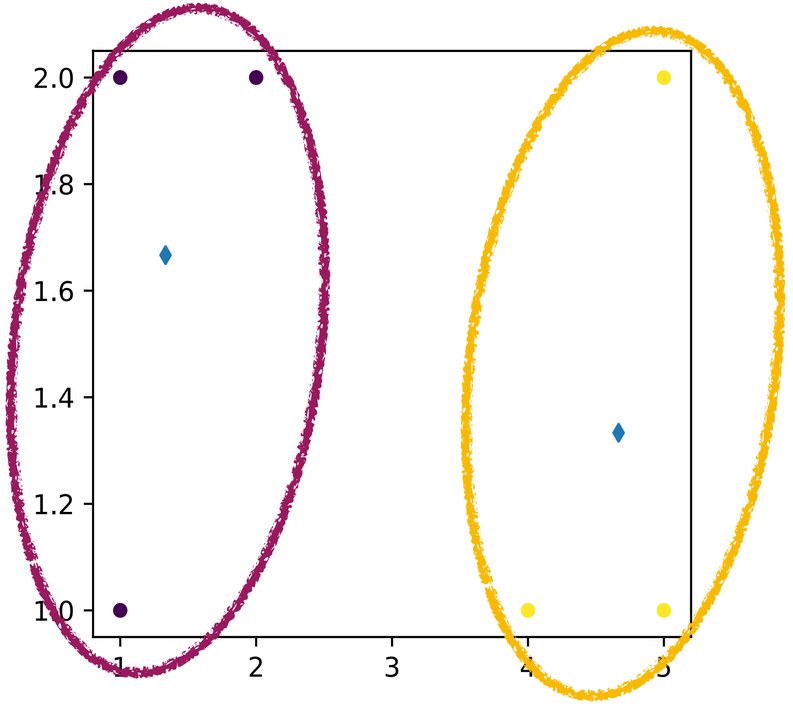

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```
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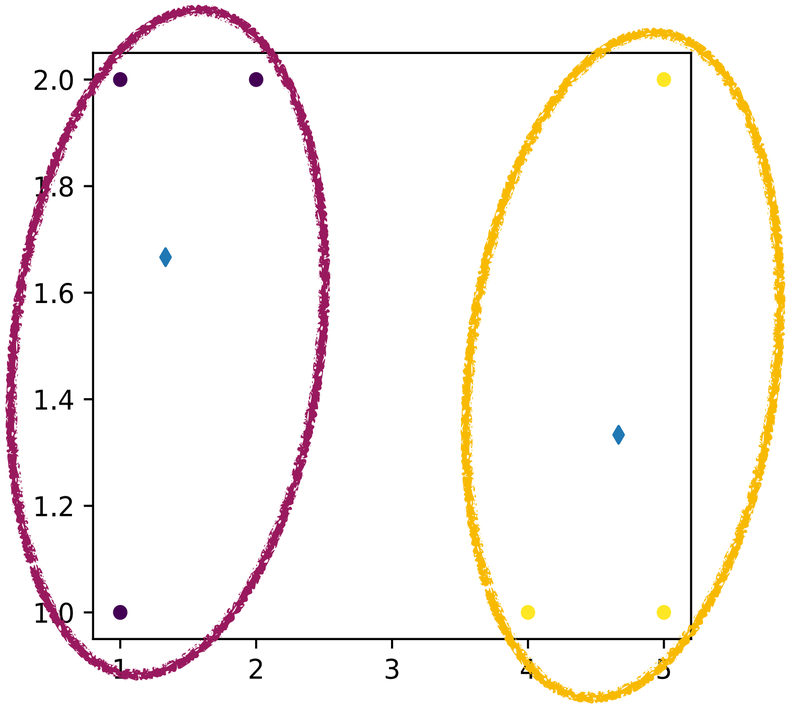
```

```
[0]
```



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```

```
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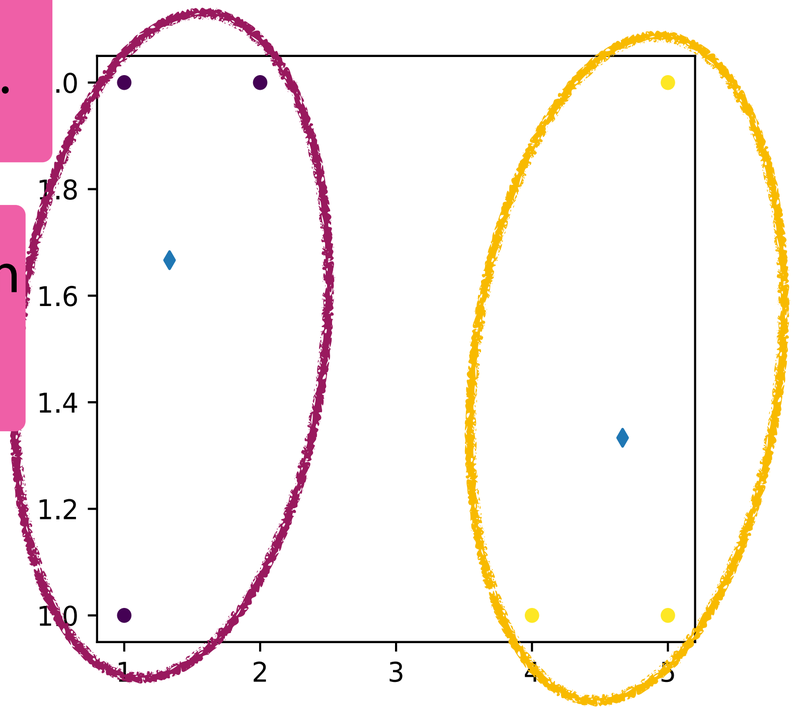
```

```
[0]
```



Klasse mit gewählten Hyperparametern erzeugen.

Modell mittels *k*-Means auf den Daten *X* trainieren.

Einige Werte können direkt den Attributen der Klasse entnommen werden.

Datenpunkte und Plot mittels Matplotlib.

Vorhersage für neues Datum bestimmen.

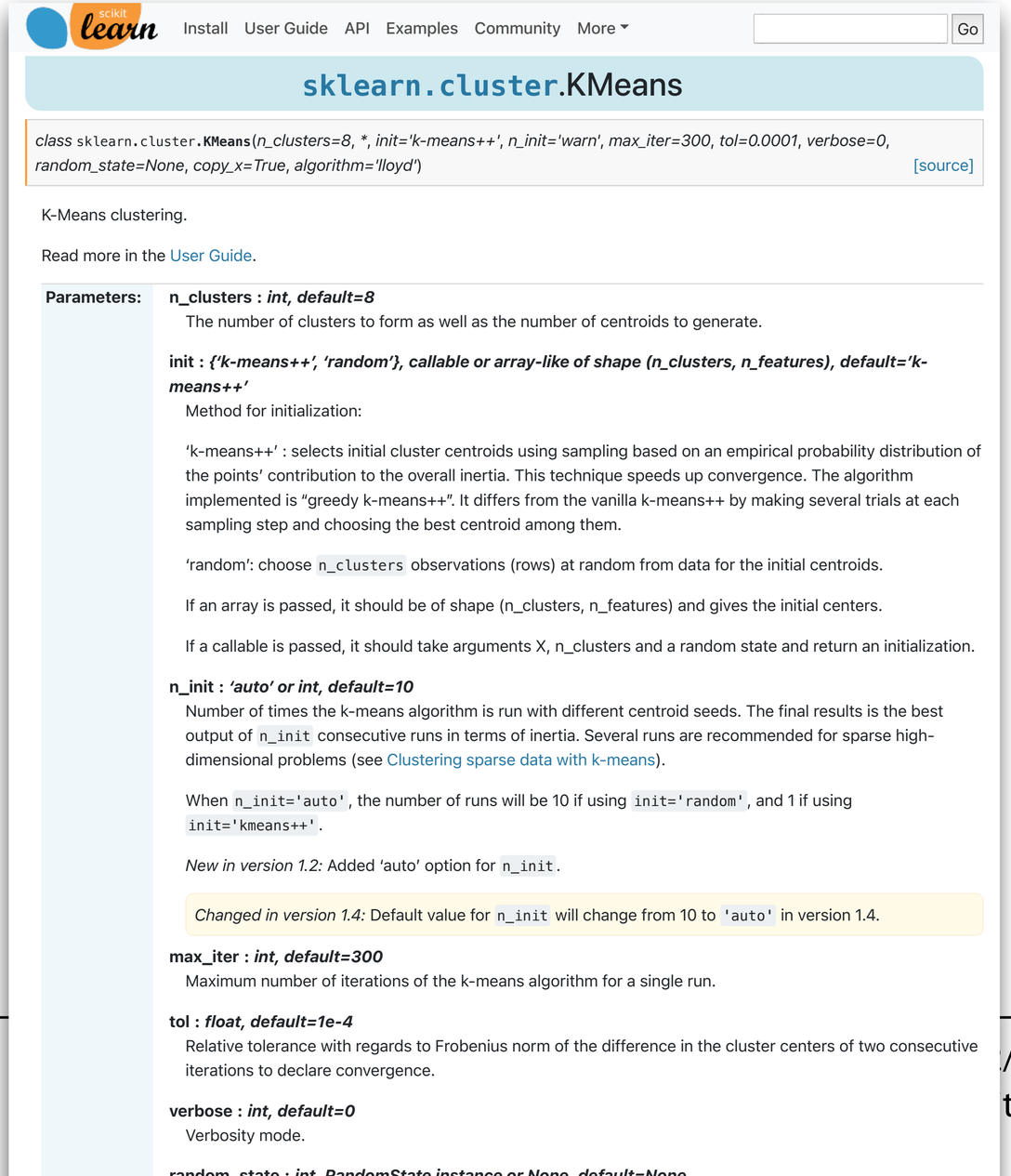
Methodenstruktur SKLearn

```
km = sklearn.cluster.KMeans(
  n_clusters=8, init='k-means++', n_init='warn',
  max_iter=300, tol=0.0001, verbose=0,
  random_state=None, copy_x=True,
  algorithm='lloyd'
)

# Attributes
km.cluster_centers_
km.labels_
km.n_iter_

# Methods
fit(X[, y, sample_weight])
fit_predict(X[, y, sample_weight])
fit_transform(X[, y, sample_weight])
get_feature_names_out([input_features])
predict(X[, sample_weight])
transform(X)
```

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html



scikit learn Install User Guide API Examples Community More Go

sklearn.cluster.KMeans

class sklearn.cluster.**KMeans**(*n_clusters=8, *, init='k-means++', n_init='warn', max_iter=300, tol=0.0001, verbose=0, random_state=None, copy_x=True, algorithm='lloyd'*) [source]

K-Means clustering.

Read more in the User Guide.

Parameters:

n_clusters : *int, default=8*
The number of clusters to form as well as the number of centroids to generate.

init : *{'k-means++', 'random'}, callable or array-like of shape (n_clusters, n_features), default='k-means++'*
Method for initialization:

'k-means++' : selects initial cluster centroids using sampling based on an empirical probability distribution of the points' contribution to the overall inertia. This technique speeds up convergence. The algorithm implemented is "greedy k-means++". It differs from the vanilla k-means++ by making several trials at each sampling step and choosing the best centroid among them.

'random': choose `n_clusters` observations (rows) at random from data for the initial centroids.

If an array is passed, it should be of shape (n_clusters, n_features) and gives the initial centers.

If a callable is passed, it should take arguments X, n_clusters and a random state and return an initialization.

n_init : *'auto' or int, default=10*
Number of times the k-means algorithm is run with different centroid seeds. The final results is the best output of `n_init` consecutive runs in terms of inertia. Several runs are recommended for sparse high-dimensional problems (see Clustering sparse data with k-means).

When `n_init='auto'`, the number of runs will be 10 if using `init='random'`, and 1 if using `init='kmeans++'`.

New in version 1.2: Added 'auto' option for `n_init`.

Changed in version 1.4: Default value for `n_init` will change from 10 to `'auto'` in version 1.4.

max_iter : *int, default=300*
Maximum number of iterations of the k-means algorithm for a single run.

tol : *float, default=1e-4*
Relative tolerance with regards to Frobenius norm of the difference in the cluster centers of two consecutive iterations to declare convergence.

verbose : *int, default=0*
Verbosity mode.

random_state : *int, RandomState instance or None, default=None*

Methodenstrukt

```
km = sklearn.cluster.KMeans(
  n_clusters=8, init='k-means++', n_init='warn',
  max_iter=300, tol=0.0001, verbose=0,
  random_state=None, copy_x=True,
  algorithm='lloyd'
)

# Attributes
km.cluster_centers_
km.labels_
km.n_iter_

# Methods
fit(X[, y, sample_weight])
fit_predict(X[, y, sample_weight])
fit_transform(X[, y, sample_weight])
get_feature_names_out([input_features])
predict(X[, sample_weight])
transform(X)
```

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html

"lloyd".

Changed in version 0.18: Added Elkan algorithm

Changed in version 1.1: Renamed "full" to "lloyd", and deprecated "auto" and "full". Changed "auto" to use "lloyd" instead of "elkan".

Attributes:

cluster_centers_ : *ndarray of shape (n_clusters, n_features)*
Coordinates of cluster centers. If the algorithm stops before fully converging (see `tol` and `max_iter`), these will not be consistent with `labels_`.

labels_ : *ndarray of shape (n_samples,)*
Labels of each point

inertia_ : *float*
Sum of squared distances of samples to their closest cluster center, weighted by the sample weights if provided.

n_iter_ : *int*
Number of iterations run.

n_features_in_ : *int*
Number of features seen during fit.

New in version 0.24.

feature_names_in_ : *ndarray of shape (`n_features_in_`,)*
Names of features seen during fit. Defined only when `X` has feature names that are all strings.

New in version 1.0.

See also:

`MiniBatchKMeans`
Alternative online implementation that does incremental updates of the centers positions using mini-batches. For large scale learning (say n_samples > 10k) MiniBatchKMeans is probably much faster than the default batch implementation.

Notes

The k-means problem is solved using either Lloyd's or Elkan's algorithm.

The average complexity is given by O(k n T), where n is the number of samples and T is the number of iteration.

The worst case complexity is given by O(n^(k+2/p)) with n = n_samples, p = n_features. Refer to "How slow is the k-means method?" D. Arthur and S. Vassilvitskii - SoCG2006. for more details.

In practice, the k-means algorithm is very fast (one of the fastest clustering algorithms available), but it falls in local minima. That's why it can be useful to restart it several times.

If the algorithm stops before fully converging (because of `tol` or `max_iter`), `labels_` and `cluster_centers_` will not be consistent, i.e. the `cluster_centers_` will not be the means of the points in each cluster. Also, the estimator will reassign `labels_` after the last iteration to make `labels_` consistent with `predict` on the training set.

Examples

```
>>> from sklearn.cluster import KMeans
>>> import numpy as np
>>> X = np.array([[1, 2], [1, 4], [1, 0],
...               [10, 2], [10, 4], [10, 0]])
>>> kmeans = KMeans(n_clusters=2, random_state=0, n_init="auto").fit(X)
```

Methodenstruk

```
km = sklearn.cluster.KMeans(
  n_clusters=8, init='k-means++', n_init='warn',
  max_iter=300, tol=0.0001, verbose=0,
  random_state=None, copy_x=True,
  algorithm='lloyd'
)

# Attributes
km.cluster_centers_
km.labels_
km.n_iter_

# Methods
fit(X[, y, sample_weight])
fit_predict(X[, y, sample_weight])
fit_transform(X[, y, sample_weight])
get_feature_names_out([input_features])
predict(X[, sample_weight])
transform(X)
```

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html

`get_params`([deep])	Get parameters for this estimator.
`predict`(X[, sample_weight])	Predict the closest cluster each sample in X belongs to.
`score`(X[, y, sample_weight])	Opposite of the value of X on the K-means objective.
`set_output`(*[, transform])	Set output container.
`set_params`(**params)	Set the parameters of this estimator.
`transform`(X)	Transform X to a cluster-distance space.

`fit`(*X*, *y=None*, *sample_weight=None*) [source]

Compute k-means clustering.

Parameters:

X : *{array-like, sparse matrix} of shape (n_samples, n_features)*
Training instances to cluster. It must be noted that the data will be converted to C ordering, which will cause a memory copy if the given data is not C-contiguous. If a sparse matrix is passed, a copy will be made if it's not in CSR format.

y : *Ignored*
Not used, present here for API consistency by convention.

sample_weight : *array-like of shape (n_samples,), default=None*
The weights for each observation in X. If None, all observations are assigned equal weight.

New in version 0.20.

Returns:

self : *object*
Fitted estimator.

`fit_predict`(*X*, *y=None*, *sample_weight=None*) [source]

Compute cluster centers and predict cluster index for each sample.

Convenience method; equivalent to calling fit(X) followed by predict(X).

Parameters:

X : *{array-like, sparse matrix} of shape (n_samples, n_features)*
New data to transform.

y : *Ignored*
Not used, present here for API consistency by convention.

sample_weight : *array-like of shape (n_samples,), default=None*
The weights for each observation in X. If None, all observations are assigned equal weight.

Returns:

labels : *ndarray of shape (n_samples,)*
Index of the cluster each sample belongs to.

`fit_transform`(*X*, *y=None*, *sample_weight=None*) [source]

Compute clustering and transform X to cluster-distance space.

Equivalent to fit(X).transform(X), but more efficiently implemented.

Parameters:

X : *{array-like, sparse matrix} of shape (n_samples, n_features)*
New data to transform.

y : *Ignored*
Not used, present here for API consistency by convention.

sample_weight : *array-like of shape (n_samples,), default=None*
The weights for each observation in X. If None, all observations are assigned equal weight.

Methodenstruk

```
km = sklearn.cluster.KMeans(
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# Attributes
km.cluster_centers_
km.labels_
km.n_iter_

# Methods
fit(X[, y, sample_weight])
fit_predict(X[, y, sample_weight])
fit_transform(X[, y, sample_weight])
get_feature_names_out([input_features])
predict(X[, sample_weight])
transform(X)
```

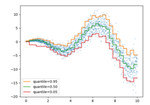
`transform`(*X*) [source]

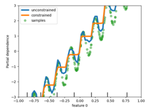
Transform X to a cluster-distance space.

In the new space, each dimension is the distance to the cluster centers. Note that even if X is sparse, the array returned by `transform` will typically be dense.

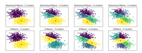
Parameters:	**X : *{array-like, sparse matrix} of shape (n_samples, n_features)*** New data to transform.
Returns:	**X_new : *ndarray of shape (n_samples, n_clusters)*** X transformed in the new space.

Examples using `sklearn.cluster.KMeans`


Release Highlights for scikit-learn 1.1

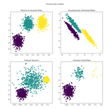

Release Highlights for scikit-learn 0.23

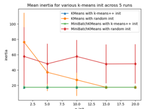

A demo of K-Means clustering on the handwritten digits data

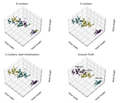

Bisecting K-Means and Regular K-Means Performance Comparison

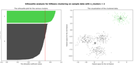

Color Quantization using K-Means

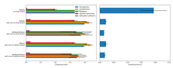

Comparison of the K-Means and MiniBatchKMeans clustering algorithms


Demonstration of k-means assumptions


Empirical evaluation of the impact of k-means initialization


K-means Clustering


Selecting the number of clusters with silhouette analysis on KMeans clustering


Clustering text documents using k-means

Toggle Menu

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html

Methodenstruk

```
km = sklearn.cluster.KMeans(
  n_clusters=8, init='k-means++', n_init='warn',
  max_iter=300, tol=0.0001, verbose=0,
  random_state=None, copy_x=True,
  algorithm='lloyd
)

# Attributes
km.cluster_centers_
km.labels_
km.n_iter_

# Methods
fit(X[, y, sample_weight])
fit_predict(X[, y, sample_weight])
fit_transform(X[, y, sample_weight])
get_feature_names_out([input_features])
predict(X[, sample_weight])
transform(X)
```

Ausführliche Dokumentation für jede Klasse, mit ähnlichem Aufbau und ähnlichen Methoden, z.B. `fit()`, …

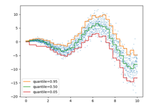
`transform(X)` [source]

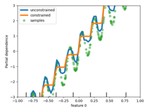
Transform X to a cluster-distance space.

In the new space, each dimension is the distance to the cluster centers. Note that even if X is sparse, the array returned by `transform` will typically be dense.

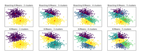
Parameters:	**X : *{array-like, sparse matrix} of shape (n_samples, n_features)*** New data to transform.
Returns:	**X_new : *ndarray of shape (n_samples, n_clusters)*** X transformed in the new space.

Examples using `sklearn.cluster.KMeans`


Release Highlights for scikit-learn 1.1

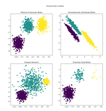

Release Highlights for scikit-learn 0.23

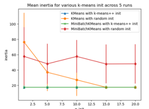

A demo of K-Means clustering on the handwritten digits data


Bisecting K-Means and Regular K-Means Performance Comparison


Color Quantization using K-Means


Comparison of the K-Means and MiniBatchKMeans clustering algorithms


Demonstration of k-means assumptions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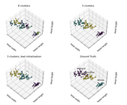
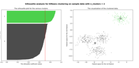

K-means Clustering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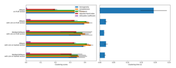
Clustering text documents using k-means

Toggle Menu

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html

Beispiel

```
from sklearn.cluster import KMeans
from sklearn.datasets import make_blobs
import matplotlib.pyplot as plt
import numpy as np

X_a, y_a = make_blobs(n_samples=1500, random_state=170)
X_b, y_b = np.dot(X_a, [[0.60834549,… ]]), y_a
X_c, y_c = make_blobs(n_samples=1500, cluster_std=[1.0, 2.5, 0.5], random_state=170)
X_d, y_d = np.vstack(…), … * 10

# Plot Data

km_a = KMeans(n_clusters=2, random_state=170).fit(X_a)
km_b = KMeans(n_clusters=3, random_state=170).fit(X_b)
km_c = KMeans(n_clusters=3, random_state=170).fit(X_c)
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# Plot Cluster
```

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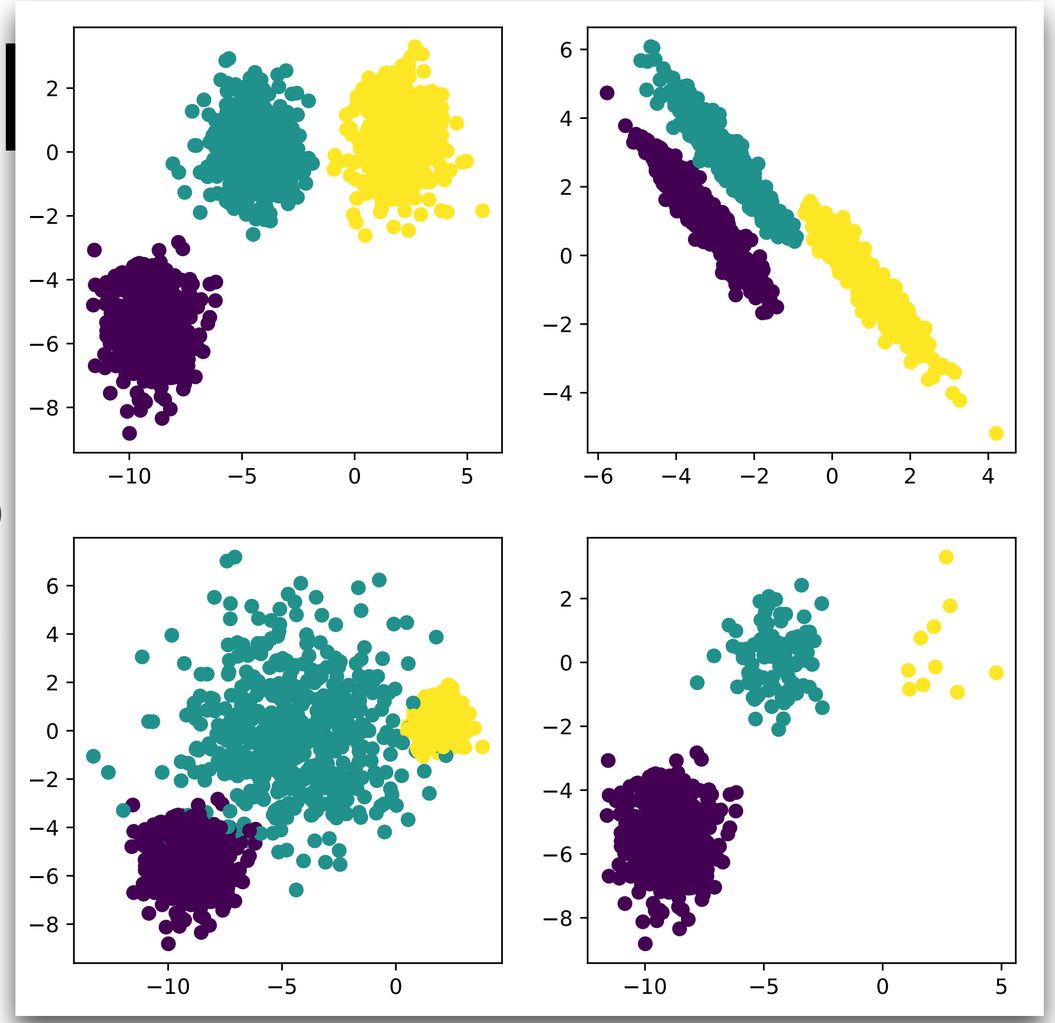

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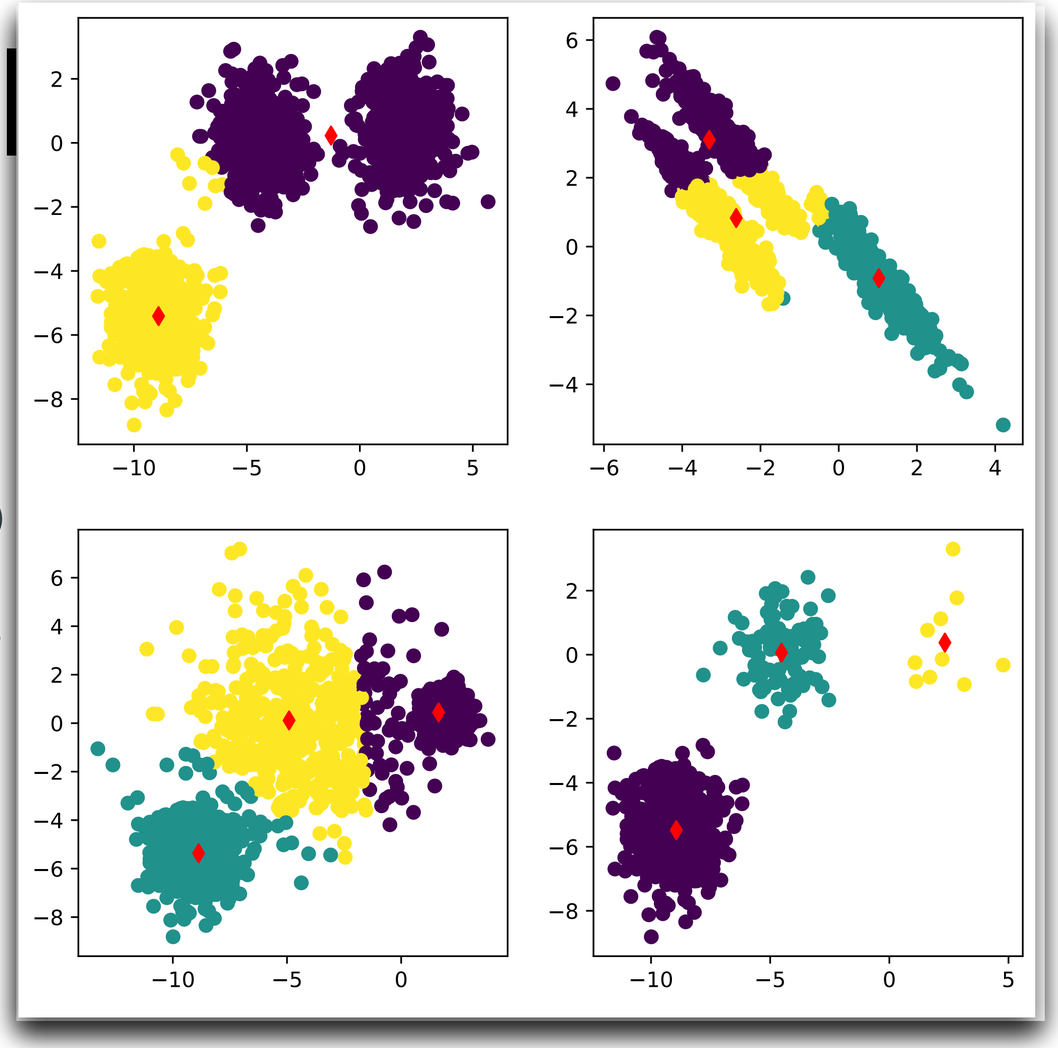

Beispiel

Beispieldaten erzeugen und in verschiede „spannende" Instanzen transformieren.

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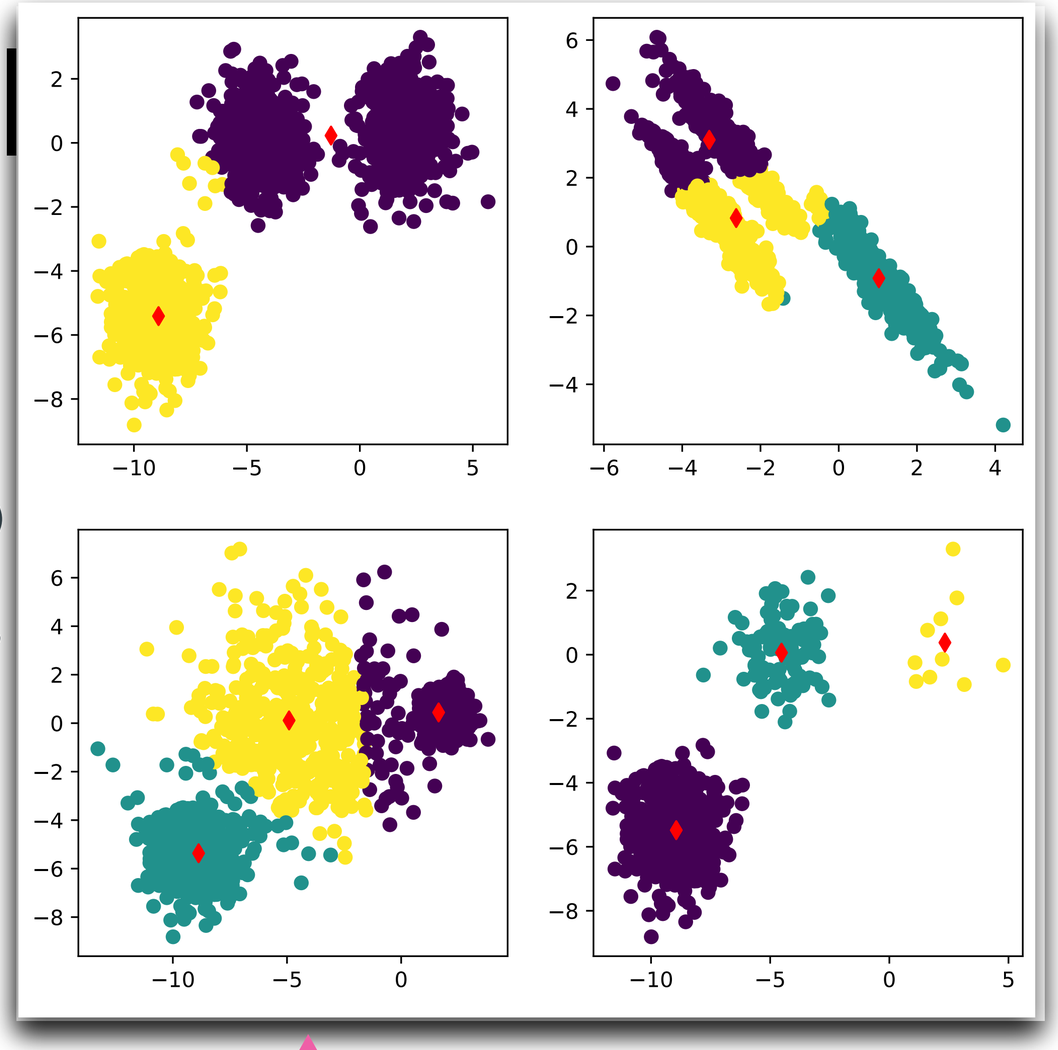

Jeweils ein Modell mittels k-Means berechnen.

Rote Rauten sind die Zentroiden, man sieht, dass das Ergebnis teilweise suboptimal ist.

https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_assumptions.html

Diskussion *k*-Means

- Meist relativ wenige Schritte notwendig
  - Findet aber ggf. nur lokales Optimum
- Nur anwendbar, wenn Mittel definiert

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Ergebnis

Wunsch

Zusammenfassung

I. Projektaufgabe 4

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Nächste Woche gucken wir uns weitere Beispiele für ML Verfahren an.

Inhaltsübersicht

1. Programmiersprache Python
   a) *Einführung, Erste Schritte*
   b) *Grundlagen*
   c) *Fortgeschritten*
2. Auszeichnungssprachen
   a) *LaTeX, Markdown*
3. Benutzeroberflächen und Entwicklungsumgebungen
   a) *Jupyter Notebooks lokal und in der Cloud (Google Colab)*
4. Versionsverwaltung
   a) *Git, GitHub*
5. Wissenschaftliches Rechnen
   a) *NumPy, SciPy*
6. Datenverarbeitung und -visualisierung
   a) *Pandas, matplotlib, NLTK*
7. Machine Learning (scikit-learn)
   a) *Grundlegende Ansätze (Datensätze, Auswertung)*
   b) Einfache Verfahren (Clustering, …)
8. DeepLearning
   a) TensorFlow, PyTorch, HuggingFace Transformers