InterKIWWU - An interdisciplinary teaching initiative on artificial intelligence

Physics, mathematics and computer science, chemistry, medicine, sports science and psychology in cooperation with ZfN, ZfW, REACH Euroregio, IVV NWZ

Coordination

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Dr. O. Kamps
Dr. K. Schmietendorf

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Goals of the Center for Nonlinear Science (CeNoS)

- Understanding of the phenomena and self-organized structures that can be observed in nonlinear complex systems in nature, technology and society.
- Inherently interdisciplinary undertaking with a current focus on the mathematical and scientific disciplines.
- Methods for modeling and analyzing complex systems
- Aim: Improvement of scientific exchange and cooperation

Physics, mathematics and computer science, chemistry, medicine, sports science and psychology

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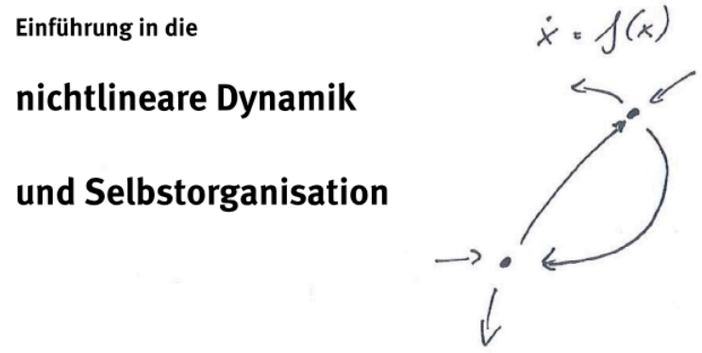

The need for interdisciplinary teaching

- Knowledge is the basis for interdisciplinary cooperation
- Expansion of AI teaching at universities

Our approach

- The teaching is supplemented by interdisciplinary courses in which the basic knowledge of the analysis and modeling of complex systems is conveyed

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Introduction to Bayesian statistics

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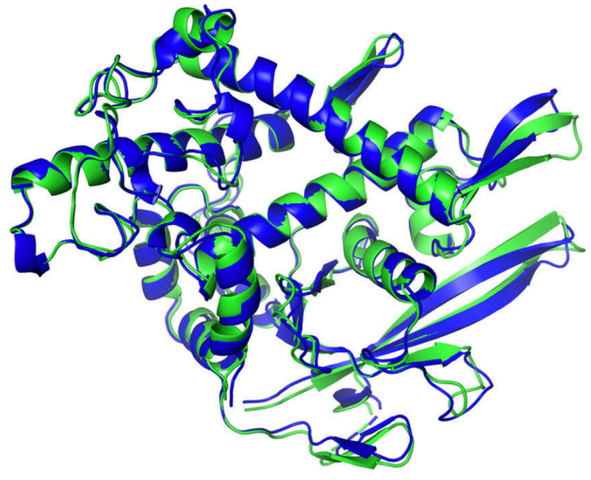
AI/ML and Science

- Availability of data and computing power enables the use of ML/AI in many new areas of application

- Increasingly important in science / also in the area of complex systems

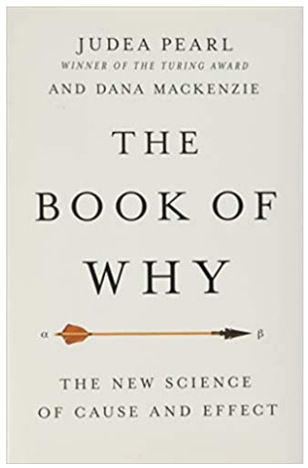


Structures of a protein that were predicted by artificial intelligence (blue) and experimentally determined (green) match almost perfectly. DEEPMIND

‘The game has changed.’ AI triumphs at solving protein structures

Comment

- “All the impressive achievements of deep learning amount to just curve fitting” (Judea Pearl)



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The Need for Interdisciplinary Teaching — Machine Learning (ML)/ Artificial Intelligence (AI)

- Basic knowledge in AI and ML is becoming increasingly important for science
- AI and ML are suitable for interdisciplinary teaching

Our contribution

- Interdisciplinary block course on AI and ML since summer semester 2019

Einführung in das Maschinelle Lernen

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Federal-state initiative to promote artificial intelligence in higher education

GEFÖRDERT VOM

Bundesministerium
für Bildung
und Forschung

The BMBF initiative to promote AI

- AI professionals for science and business
- Expansion of AI teaching at universities

The project InterKIWWU

- Funding for four years (12.2021 - 11.2025) - 2Mio€
- 1 Postdoc, 8 PhD, 4 SHBs
- (CeNoS) Physics, mathematics and computer science, chemistry, medicine, sports science and psychology
- Cooperation with ZfN, ZfW, REACH Euroregio, IVV NWZ
- Two Phases: 1 Creating the material and the courses / 2 „clean up“

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Our goal

- Students from different disciplines should learn AI skills in order to be able to assess and apply them in their subjects or in professional life outside of the university
- Largest possible long-term effect for the WWU
- Interconnection between teaching and research

Our way

- Development of a university-wide, multi-level, coordinated interdisciplinary teaching program on AI
- The departments that are members in CeNoS and some centers are involved
- **However, the program is fundamentally open to others**

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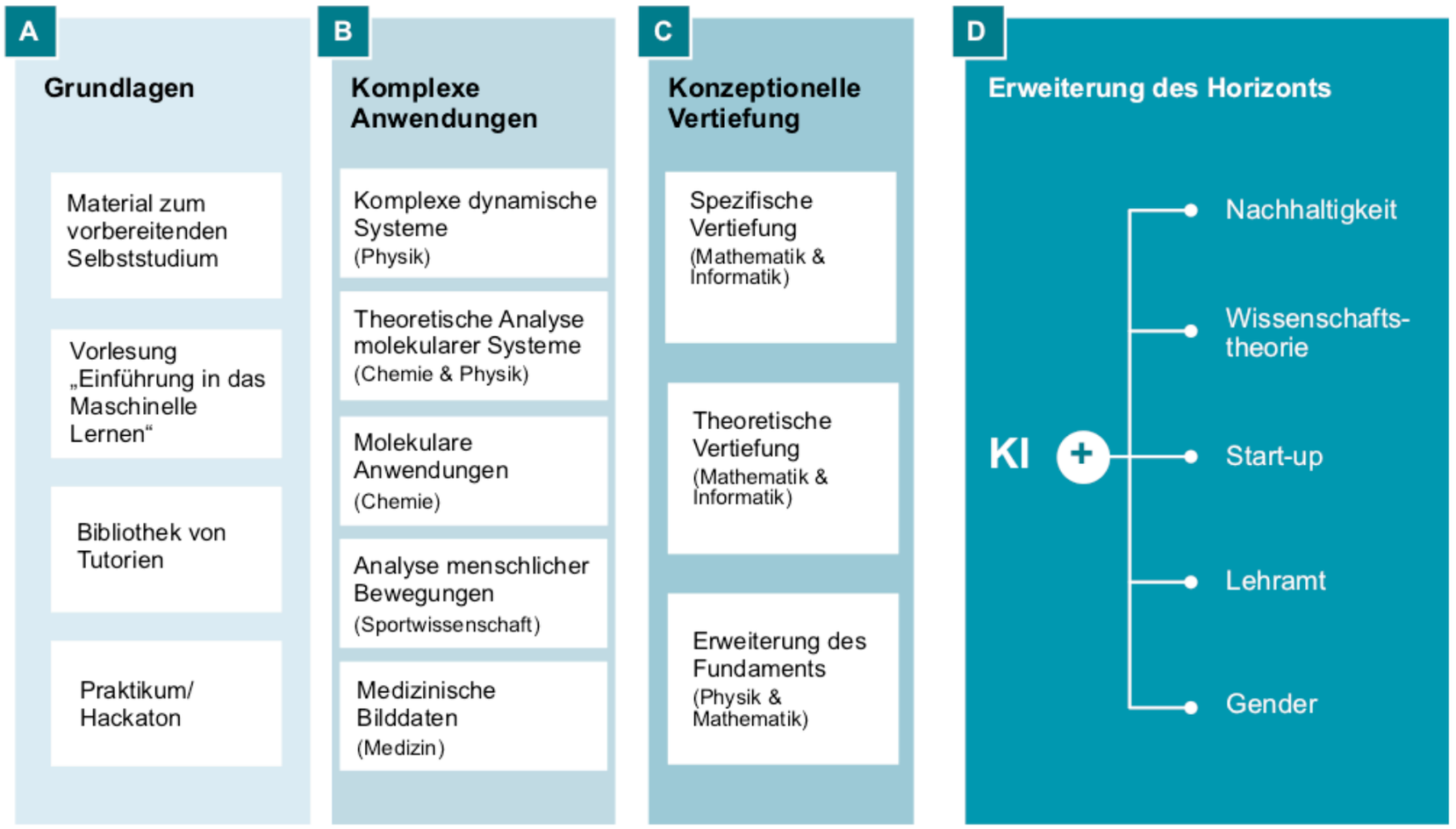
Conceptual structure of the multi-level teaching program



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Module A: Basic understanding of AI

- Students from different disciplines with correspondingly heterogeneous previous knowledge systematically acquire basic knowledge of AI

Contents

- self-study courses [M. Korth (IVV NWZ), O. Kamps (CeNoS)]
- PhotonAI - User-friendly interface [T. Hahn (Medicine)]
- Lecture „Introduction to machine learning“ [O. Kamps (CeNoS), B. Risse (Computer Science)]
- Library of tutorials in the form of Jupyter Notebooks [O. Kamps (CeNoS)]
- Hackaton [O. Kamps (CeNoS)]

Module B: Complex applications

- Acquiring the ability to independently work on complex applications from research, development and application with AI methods.

Inhalt

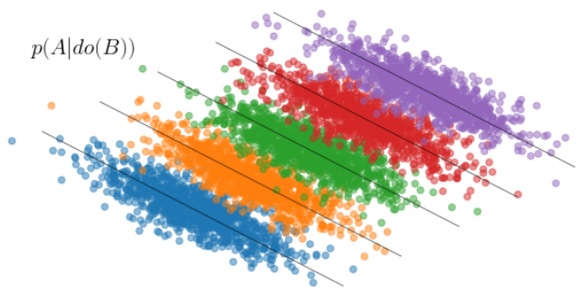
- AI for complex dynamical systems [S. Gurevich (Physics), U. Thiele (CeNoS)]
- ML in the theoretical analysis of molecular systems [J. Neugebauer, A. Heuer (Chemistry, Physik), N. Doltsinis (Physics): Center für Multiscale Theory & Computation]
- ML for molecular applications [F. Glorius (Chemistry), O. Koch (Pharmacy)]
- ML for the analysis of human movement [H. Wagner (psychology and sports science)]
- ML for medical imaging [T. Hahn (Medicine)]

Module C: Conceptual deepening

- Acquisition of in-depth AI knowledge to work on the development of new AI-based methods.

Inhalt

- Specific AI topics [B. Risse, X. Jiang (Mathematics and Computer Science)]
- Theoretical AI topics [B. Risse, X. Jiang, C. Engwer (Mathematics and Computer Science)]
- Enlarging the fundamental knowledge [O. Kamps, U. Thiele (CeNoS)]



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Modul D: KI im gesellschaftlichen Kontext

- Questions about ethics, sustainability and other social issues that are related to AI are in the focus of this module

Contents

- AI and sustainability (Zentrum f. interdisziplinäre Nachhaltigkeitsforschung, D. Fuchs)
- AI and theory of science (Zentrum f. Wissenschaftstheorie, R. M. Erdbeer, M. Klasen)
- AI for StartUps (REACH Euroregio Start-up Center, T. Wiesel, D. Bendig)
- AI and teacher education [Didactics of Physics, S. Heusler, S. Gurevich]
- AI and gender [S. Gurevich, O. Kamps]

Implementation — period of four years

Jahr	1	2	3	4
A (i)	Mitarbeit Aufbau Selbstlernkurse (WHK 10h)			
A (ii)	Weiterentwicklung der Softwareschnittstelle (WMA 75%)			
A (iii)	Mitarbeit bei der Weiterentwicklung der Einführungsvorlesung (WHK 10h)			
A (iv)	Aufbau der Notebook Bibliothek / zentraler Webauftritt / Koordination (WMA 100%)			
A (v)	Entwicklung von Projekten für den Hackaton / Begleitung des Hackatons (siehe oben)			
B (i)	Entwicklung des Materials für Untermodul B (i) (WMA 75%)			
B (ii)		Entwicklung des Materials für Untermodul B (ii) (WMA 75%)		
B (iii)	Entwicklung des Materials für Untermodul B (iii) (WMA 75%)			
B (iv)	Entwicklung des Materials für Untermodul B (iv) (WMA 75%)			
B (v)	Entwicklung des Materials für Untermodul B (v) (WMA 75%)			
C (i)	Entwicklung des Materials für Untermodul C (i) (WMA 75%)			
C (ii)	Entwicklung des Materials für Untermodul C (ii) (WMA 75%)			
C (iii)	Entwicklung von Material für die Verknüpfung zu anderen Vorlesungen (WHK 10h)			
D (i)	Entwicklung des Materials für Untermodul D (i) (WMA 50%)			
D (ii)	Entwicklung INCUB.AI.TOR (WMA 50%)			
D (iii)	Entwicklung Material für D (iii) (WMA 50%) [nur Monate 6-30]			
D (iv)	Notebooks für das Lehramt (WHK 10h)			
D (v)			Gestaltung des Gender Moduls WHK 10h)	

What can the further events be based on?

Module A: Basic understanding of AI

- Students from different disciplines with correspondingly heterogeneous previous knowledge systematically acquire basic knowledge of AI
- Self-study courses - Mathematical basics, software installation, etc.
- Interface photonAI (https://www.photon-ai.com)
- **The basic lecture**
- **The library of tutorials in the form of Jupyter Notebooks**

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Inhalt der Einführungsvorlesung - Gesamtüberblick über ML

- **Supervised learning: Learning from labeled data.**

  Labeled data. A teacher giving us the right answers to example problems and we have to apply this to an unknown example.

  – Classification –categorial data
  – Regression – continuous data

- **Unsupervised Learning: Finding patterns / structures in unlabeled data**

  Data, but no labels. Are there structures in the data?

- **Reinforcement learning: An agent learns by interacting with its environment**

  Imagine a robot trying to find its way from A to B in a rough landscape.

Inhalt der Einführungsvorlesung — Grundlegendes Verständnis von ML

Input data **Mapping / function (unknown)** **Output**

Pictures

Sensor data

$$x \longrightarrow f(x, \Theta) \longrightarrow y$$

Label

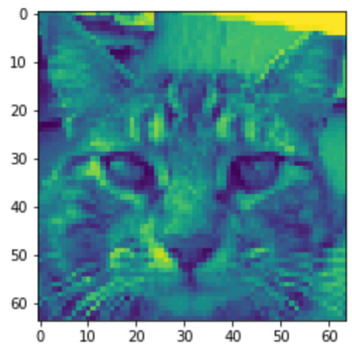
Action

Observations

Number of Clusters

Make an ansatz (polynom, neural network, ….) for f and estimate Θ

Use this model to make predictions for y given new x



dog!

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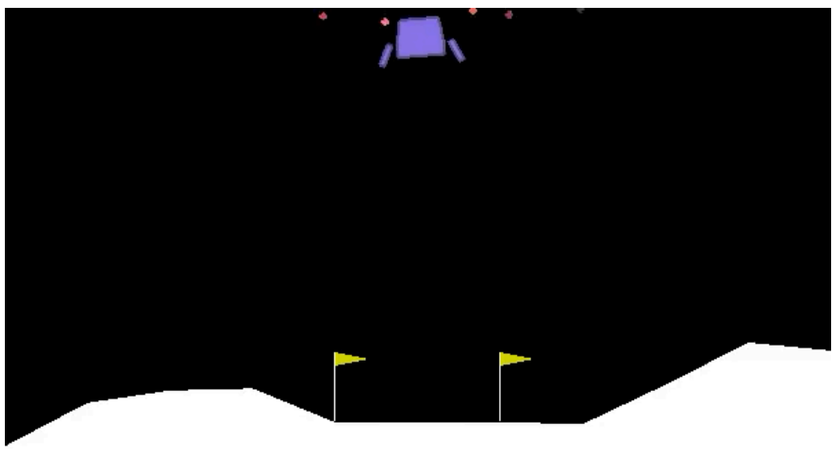
Content of the introductory lecture — Transfer to various fields of knowledge

Basic concept

- Explanation of deep learning based on the classification of dogs and cats

Examples

- Detection of phases in the Ising model
- Classification of diseases from patient data



Reinforcement learning example - lunar lander

Central building block — library of tutorials in the form of Jupyter notebooks

- Examples and solutions from all possible scientific and application areas
- Implementation of the information provided in one's own actions
- Connected to central gitlab
- **Open for use by anyone interested in AI/ML at Münster University**
- **Ideas for interesting example applications are welcome!**

1 k-armed bandit: ε-greedy and ε-decay strategies

This tutorial will focus on the multi-armed (k-armed) bandit problem and two solution strategies, namely ε-greedy and ε-decay strategies.

1.1 Problem setup

The multi-armed bandit problem can be imagined as playing a game of slot-machines, where there are multiple arms to pull (either because one bandit has mutliple arms or because there are multiple bandits). The goal of the game is then to maximize the rewards obtained by pulling on any of the k arms, without knowing how likely you are to receive a reward pulling each individual arm. Assuming you only have finite money to play with one episode of the game ends after finitely many pulls (say a thousand) and you want to maximize your reward during playtime. We will call

$$q_*(a) = E\left[R_t | A_t = a\right] \tag{1}$$

the expectation value of reward R_t at time t given the action a. This expectation value can be estimated in via the following:

$$Q_t(a) = \frac{\text{sum of rewards when } a \text{ was taken prior to } t}{\text{number of times } a \text{ was taken prior to } t}. \tag{2}$$

That action which maximizes the estimated reward is called the *greedy* action and we write it as follows:

1.2 Implementation

We now implement a `Bandit` class which represents a k-armed bandit and is able to perform ε as well as ε-decay strategies. We start by importing the `numpy` package for array manipulation and seeding our random number generator:

[1]:
```
import numpy as np
seed = 1773
np.random.seed(seed)
```

Now follows the actual bandit class. During initialization we want to tell the bandit how many arms `k` it has and also if the ε-decay strategy is used or not. If it is not used we also pass the probability value ε. Here we draw each of the rewards from individual normal distributions as provided by `numpy`, so we also set the way the mean values are to be set for each of the `k` arms. Other attributes of the bandit are used as commented.

[2]:
```
class Bandit:
    def __init__(self, k, decay = False, epsilon=None, mu="random"):
        assert decay is not False or epsilon is not None, "A bandit needs to be␣
↪initialized while specifying"\
                                                          " either decay or␣
↪epsilon."
        # number of arms
        self.k = k
```

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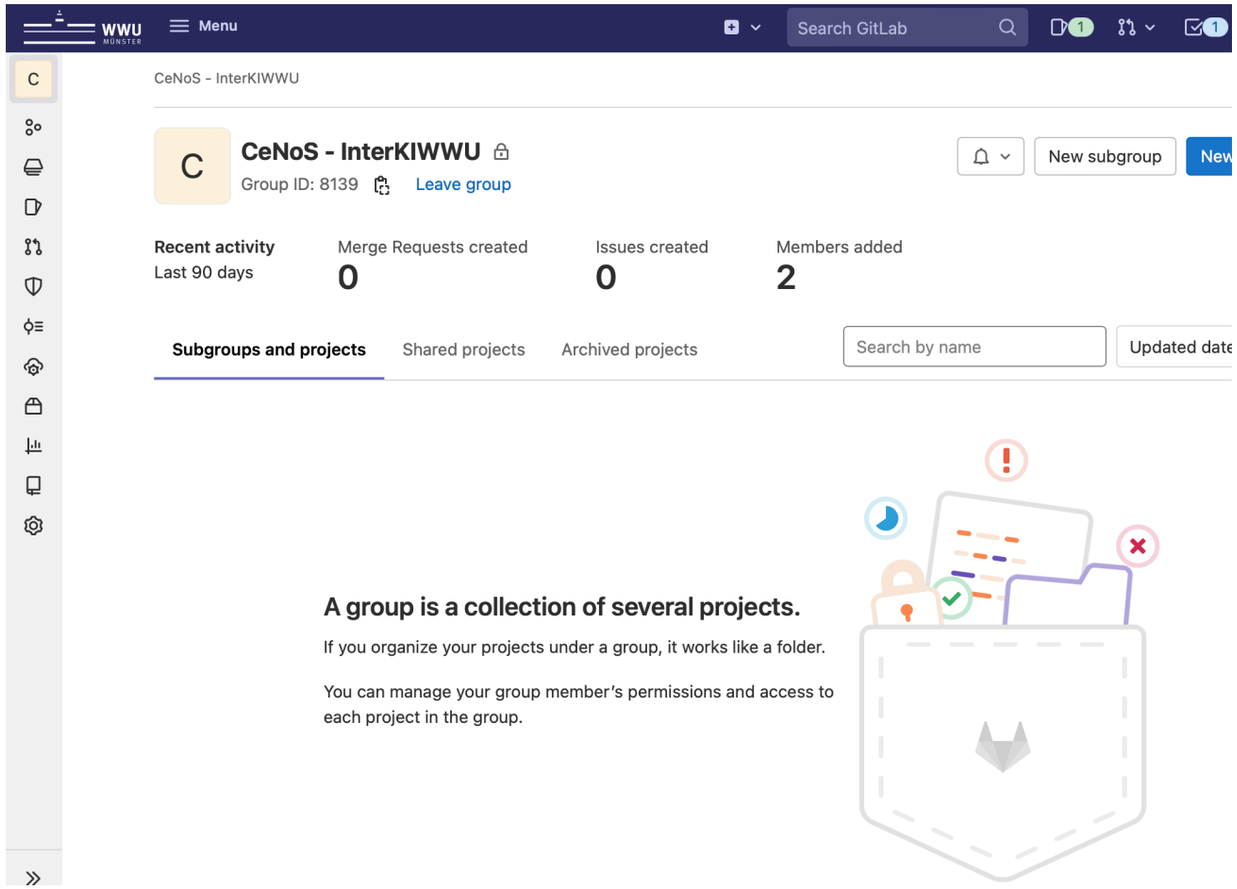
Zusammenarbeit

- Coordination by K. Schmietendorf und O. Kamps
- One workshop pro semester
- Mattermost channel
- Common gitlab



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What should be at the end?

- The teaching program is mainly developed over three years and finalized in the last year of funding
- A complete interdisciplinary teaching program (courses and materials) that can be used by the departments involved to train students in AI
- The resulting pool is prepared in such a way that the material can be used to set up events in other departments that have not previously been involved in the project
- **The project is open to the participation of anyone interested in AI/ML at Münster University**
- **The project is intended to serve as a nucleus for collaboration in the application of and research on ML/AI**

https://www.uni-muenster.de/CeNoS/InterKIWWU

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