Seminar: Deep Learning for Molecular Biology

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Helmholtz Center for Infection Research & TU Braunschweig
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Seminar overview

Max. number of participants: 10

Language: English

Requirements:

- Student pairs with both practical (implementation in Python) and theoretical presentations
- At least one meeting with the assistants
- >5 page summary of the topic, with scientific report template, for example with literature references (to be sent two weeks before seminar date)
- approx . 15 minutes of presentation per person, plus 10 discussion (to be set via doodle)

Designated for Bachelor and Master students of Computer Science

Course Takeaways

Basic Knowledge of Machine Learning: Understanding of fundamental concepts in machine learning.

- Machine Learning:
  a. A hot topic in both scientific research and industry applications.
  b. Wide-ranging impact across various domains, from healthcare to finance.

Basic Knowledge of Deep Learning: Familiarity with the principles of deep learning.

- Deep Learning:
  - Specialized models built upon neural network architectures.
  - Remarkable success in tackling complex and challenging problems across domains.

Basic Knowledge of Bioinformatics:

- Understanding of bioinformatics principles and applications.
- Awareness of how machine learning and deep learning are applied in bioinformatics research.

Experience in Problem Solving:

- Practical experience in applying machine learning and deep learning techniques to bioinformatics problems.

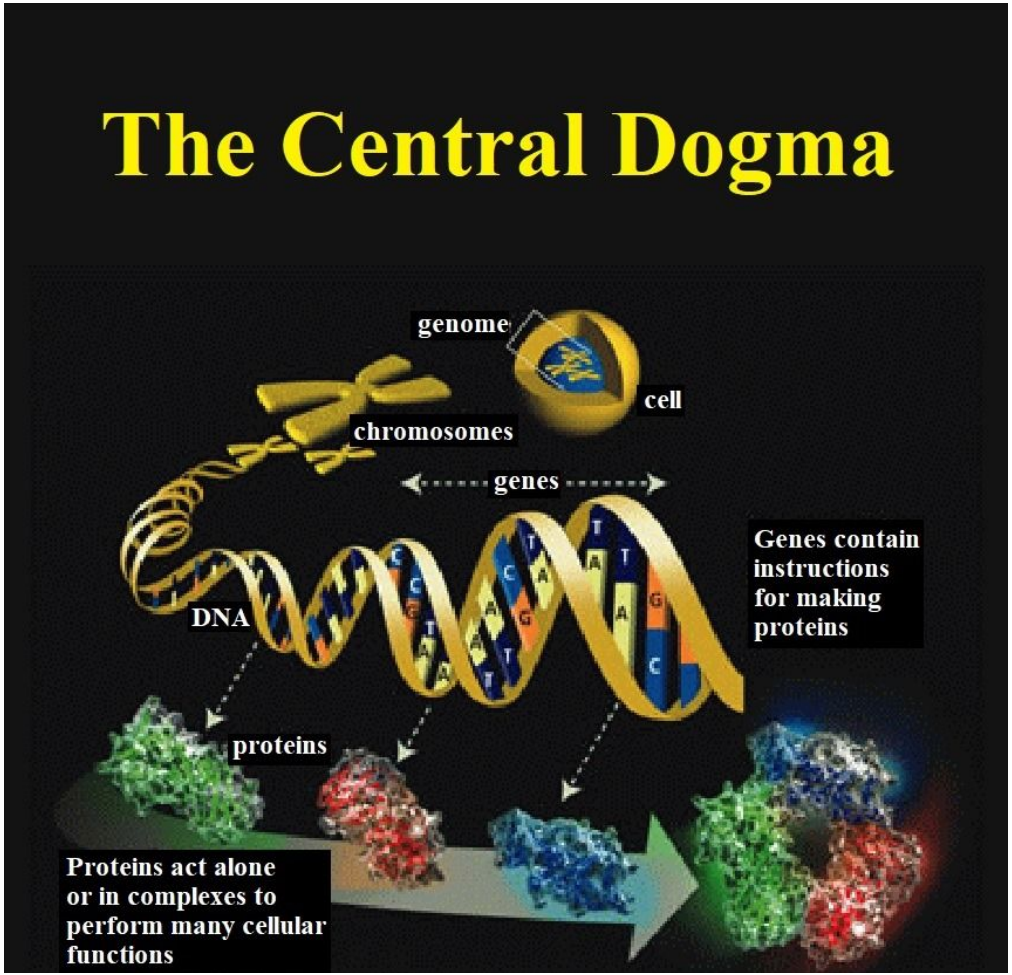
Introduction to Bioinformatics, Machine Learning, and Deep Learning

What is bioinformatics

(Current) Biology =

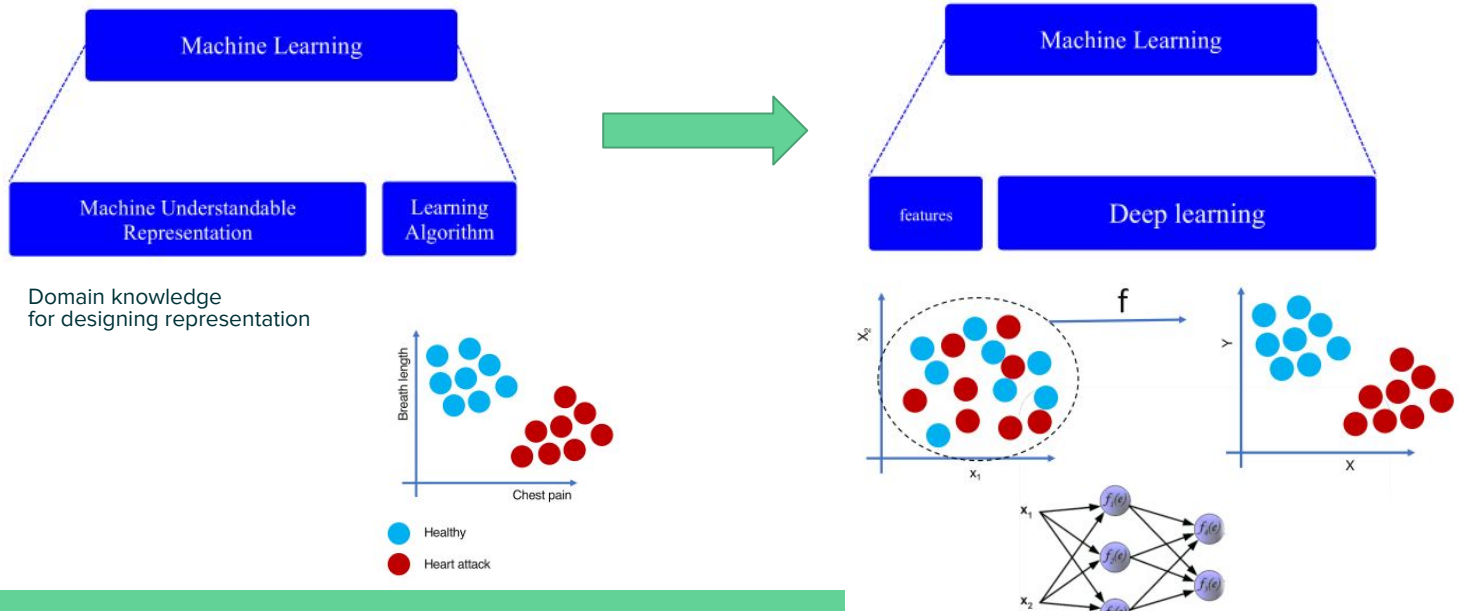
- DNA + RNA + Protein + Interactions

Bioinformatics: Computational analysis of the biological data



What is machine learning

- We alter data appearance to be interpretable by the audience.
  - Machine as the audience? Numerical values, vectors, matrices
- Finding a proper representation has been critical in machine learning



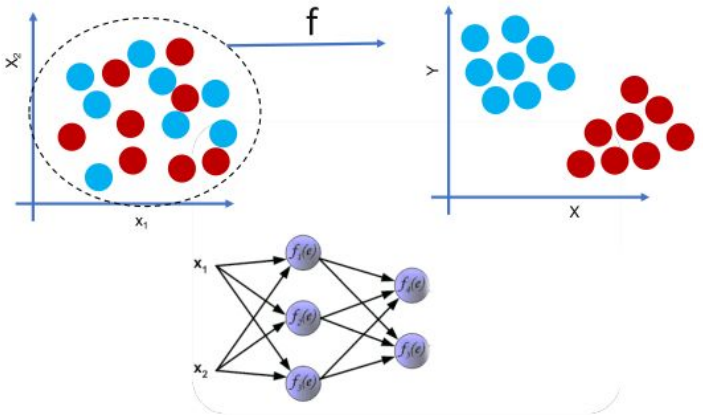
Machine Learning

Given an observed sample set, finding inherent structure of the data, in order to

- Understand what is happening there
- Predict some unknown features

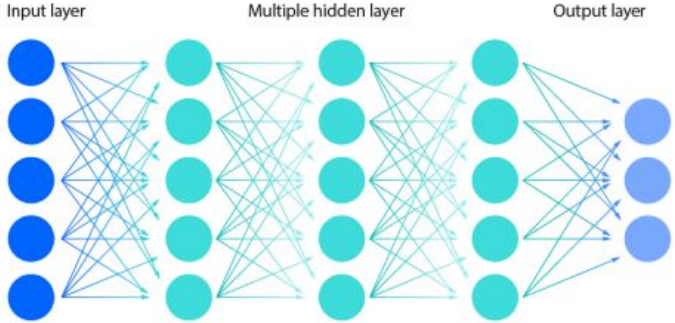
Representation learning:

- Data, could be represented as points in n-dimensional space (of features)
- Finding a transformation separating different data samples?
    - Then, we can solve several problems, e.g. classification.

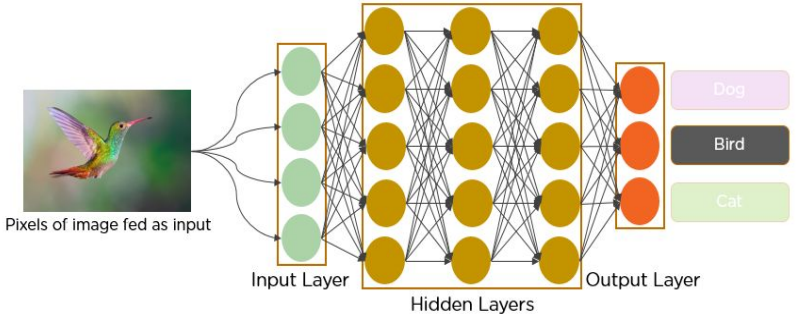


Specific ML models: NN, RNN, CNN

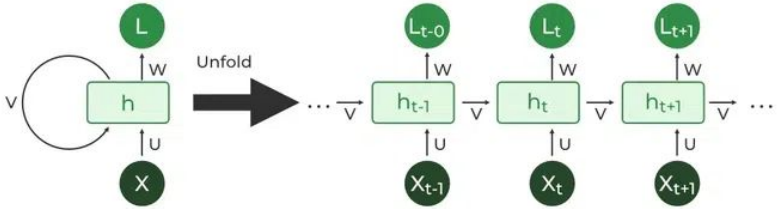
Neural network (NN): Inspired by brain



Convolutional Neural Network (CNN): NN with fewer (redundant) parameters



Recurrent Neural Network (RNN): Dealing with sequential information



What is a transformer?

- An architecture with breakthrough performances
- Encoder/Decoder architecture
- Used in a wide range of applications
- Effective
- Highly parallelizable
- Ideal for transfer learning

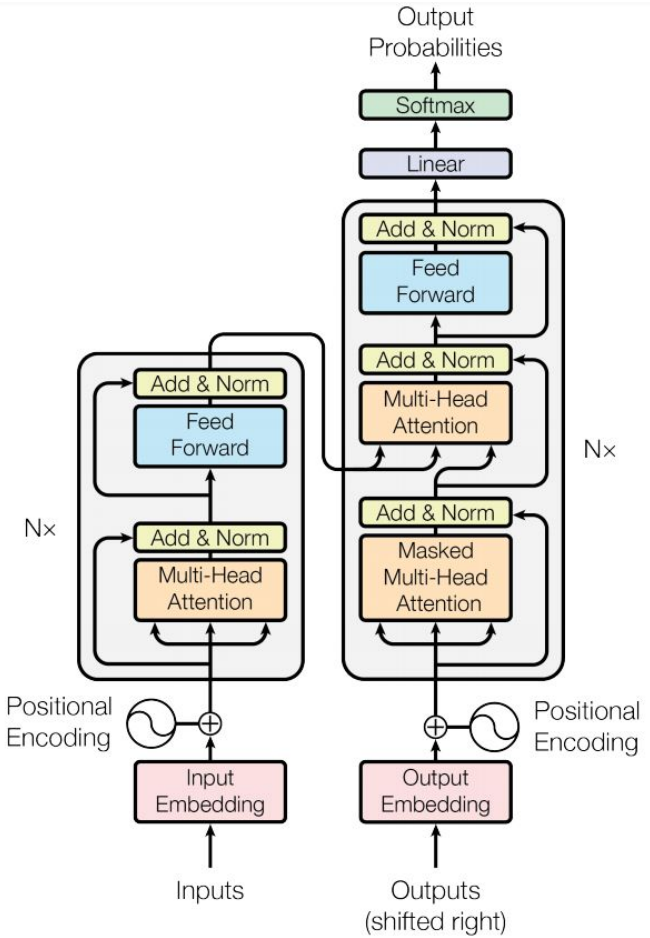
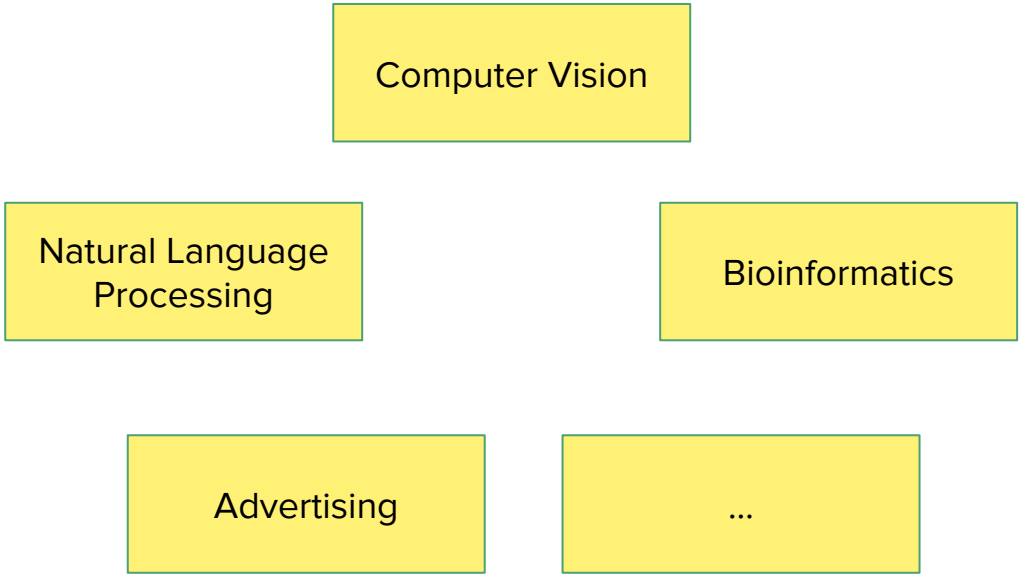


Figure 9. Transformers model architecture.

Vaswani et al, Attention is all you need. (NIPS 2017)

Applications of deep learning



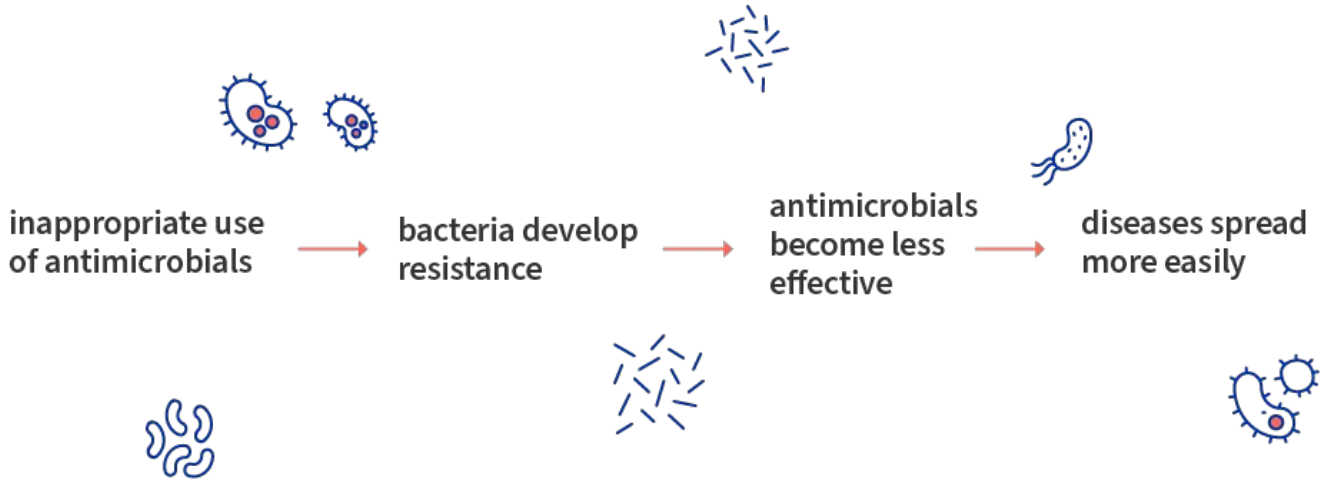
Your task

- Make groups
- Chooses a topic (from the following list)
- Study the topic
  - Useful material is provided
  - Meeting and consultation with the lecturers (at least once)
  - Implement and test your topic with the dataset (if applicable)
  - Evaluate (Metrics, precision/recall, TP, TN, ...)
- Create a written report
  - It is allowed to use AI tools; report them in acknowledgements!
- Present your topic in the presentation day

Implementation Tasks

Antimicrobial Resistance of pathogens (AMR)

> “AMR occurs when bacteria, viruses, fungi and parasites change over time and no longer respond to medicines making infections harder to treat and increasing the risk of disease spread, severe illness and death.” WHO



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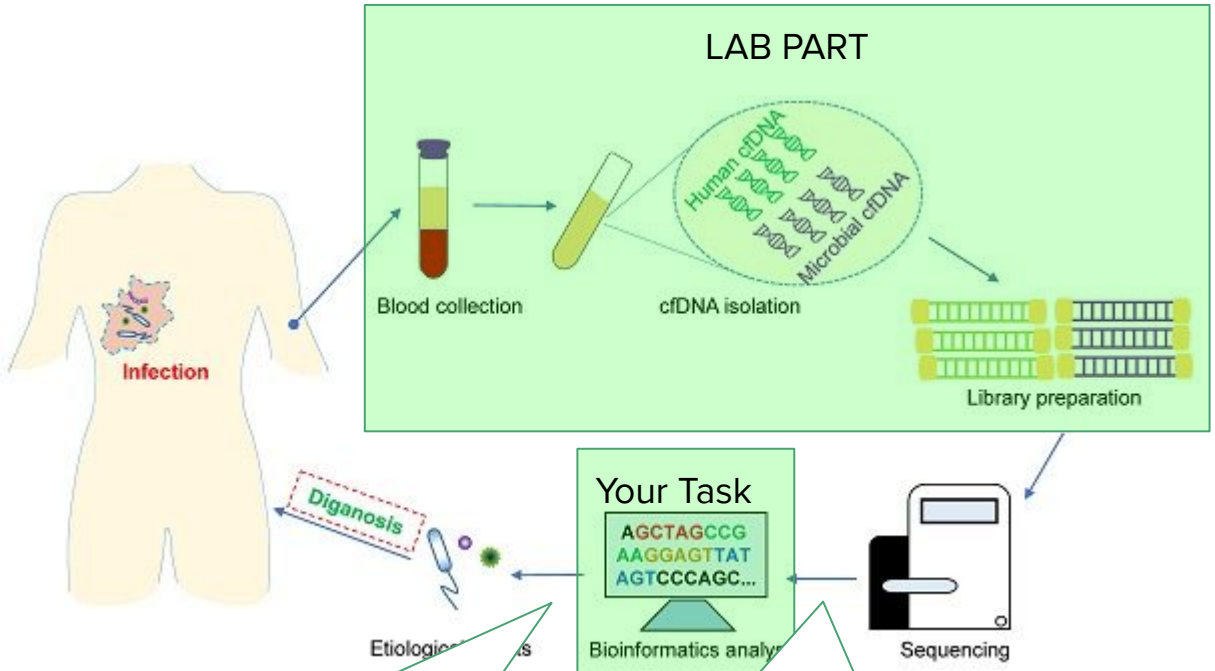

Source: https://www.thno.org/v10p5501.htm

Dataset description

- Git repository: https://github.com/hzi-bifo/seminar-dlmb-2024-winter-public
- 150 genomes
  - Training set (135 samples) and test set (15 samples)
- Labels: 0 (non-resistant), 1 (resistant)
- Primary implementation task:
  - Predict AMR for a pathogen (Staphylococcus aureus) against an antibiotics (Cefoxitin) given the genomic sequence of one of its genes (gene pbp4) as input
- Extended implementation task:
  - Pathogen: Klebsiella pneumoniae, antibiotics: Aztreonam, gene: all genes

Topics

Topics

- Feed-forward Neural Networks and back propagation [2 students]
- Convolutional Neural Networks (CNN) [2 students]
- Recurrent Neural Networks and LSTMs [2 students]
- Transformers - Encoders [2 students]
- Transformers - Decoders, Encoder-Decoders [2 students]

Feed-forward Neural Networks and back propagation [2 students]

Goals: Getting familiar with the basics of neural networks

- Introduction to linear classification, multilayer perceptron (MLP), and back propagation algorithm
- Implementation in python using MLP

Suggested references

- Linear prediction: Lec. 1,2 at (https://bit.ly/1DIpc51) and (Chapter 4: https://stanford.io/2voWjra)
- G. Hinton's lecture 2, 3: https://bit.ly/3TNBPqw
- Lecture from U of Waterloo: https://bit.ly/2A2mzgN
- Stanford Tutorial: https://stanford.io/1FRrkZw
- Practicals: In Keras (keras.io) or Pytorch (pytorch.org)

Convolutional Neural Networks (CNN) [2 students]

Goals: Getting familiar with the convolutional neural network

- CNN
- Implementation in python using only CNN

Suggested references

- MIT notes: https://tinyurl.com/3c8fk4mz
- G. Hinton's lecture: https://bit.ly/3TNBP qw
- Stanford Tutorial: https://stanford.io/1FRrkZw
- A more advanced reference: deeplearningbook.org
- Practicals: In Keras (keras.io) or Pytorch (pytorch.org), e.g. https://tinyurl.com/yfy56ay5

Recurrent Neural Networks [2 students]

Goals: Getting familiar with the RNNs and in particular LSTM

- Understanding “Vanilla” RNN
- Understanding the LSTM architecture (in particular read: https://bit.ly/1S6gmjZ)
- Implementation in python using only RNNs and LSTM

Suggested references

- Lecture from U of Waterloo: https://bit.ly/2RCNEhn
- Understanding LSTMs: https://bit.ly/1S6gmjZ
- MIT notes: https://tinyurl.com/2x4z77fz
- G. Hinton’s lecture: https://bit.ly/3TNBPqw
- A more advanced reference: deeplearningbook.org
- Practicals: In Keras (keras.io) or Pytorch (pytorch.org)

Transformers - Encoders only models [2 students]

Goals: Getting familiar with the concept of transformers architecture

- Encoder part of a transformer model (e.g. Bert)
- Implementation in python using encoders-based transformers models

Suggested references

- Representation learning: https://arxiv.org/pdf/1206.5538.pdf
- Transformer paper: https://arxiv.org/abs/1706.03762
- Simple explanation of transformers: https://jalammar.github.io/illustrated-transformer/
- Simple explanation of the details: https://serrano.academy/
- Practicals: In Keras (keras.io) or Pytorch (pytorch.org)
- Practicals: https://huggingface.co/docs/transformers/notebooks

Transformers - Decoder-only and Encoder - Decoders [2 students]

Goals: Getting familiar with the concept of representation learning

- Decoder-only models (GPT)
- Encoder-decoder models
- Their applications on bioinformatics

Suggested references

- Representation learning: https://arxiv.org/pdf/1206.5538.pdf
- Transformer paper: https://arxiv.org/abs/1706.03762
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Further steps:

Send an email (to both of us):
- From one member
- CC all other members
- Send three preferred topics in the order of preference
- Until 22nd of October
- If you have problem forming a team, send an email with and let us know!

Up to you how to split the tasks: collaborate!

Meeting and consultation with the lecturers (at least once)

Final seminar date:
- tbd 9:00 - 13:00 at BRICS.

Any question? Contact us:
- mohammad-hadi.foroughmand-araabi@helmholtz-hzi.de
- georgios.kallergis@helmholtz-hzi.de

The End

References

- AMR image https://www.consilium.europa.eu/en/infographics/antimicrobial-resistance/
- Deep learning in Life Science Youtube series