INTRODUCTION TO MACHINE LEARNING

Deep Learning for Climate Scientists

ML Workshop @ DKRZ

<Name>
Deutsches Klimarechenzentrum (DKRZ)

Course Expectations

- What is your name?
- What do you expect to learn in this course?
- Name one thing that you associate with ML. Prior experiences with it?
- How do you think your work can benefit from ML approaches?

Workshop Outline – Day 1

Day 1
Sitzung

10:30–12:30 Uhr	**Introduction to Machine Learning**	**Sprecher** Alexander Fischer
12:30–14:00 Uhr	**Lunch Break**	
14:00–15:45 Uhr	**Architectures and Applications**	**Sprecher** Paul Keil
15:45–16:00 Uhr	**Coffee break**	
16:00–17:30 Uhr	**Introduction to PyTorch: Core Concepts**	**Sprecher** Etienne Plésiat

Workshop Outline – Day 2

Day 2
Sitzung

09:00–10:45 Uhr **Introduction to PyTorch: Application to climate data**

Sprecher
Etienne Plésiat

10:45–11:00 Uhr **Coffee Break**

11:00–11:30 Uhr **Introduction to PyTorch: Application to climate data**

Sprecher
Etienne Plésiat

11:30–12:30 Uhr **Introduction to Pytorch Lightning**

Sprecher
Caroline Arnold

12:30–14:00 Uhr **Lunch break**

14:00–15:30 Uhr
Advanced Deep Learning use-case: Reconstructing missing climate data

Sprecher
Johannes Meuer

15:30–15:45 Uhr **Coffee break**

15:45–16:45 Uhr
Advanced Deep Learning use-case: Reconstructing missing climate data

Sprecher
Johannes Meuer

16:45–17:30 Uhr **Snackchat**

Sprecher
Alexander Fischer, Caroline Arnold, Etienne Plésiat, Johannes Meuer, Paul Keil

Workshop Outline – Day 3

Day 3
Sitzung

09:00–10:45 Uhr **Beyond CNNs: Advanced Deep Learning Methods for Climate Data**

Sprecher
Alexander Fischer, Johannes Meuer, Maximilian Witte

10:45–11:00 Uhr **Coffee break**

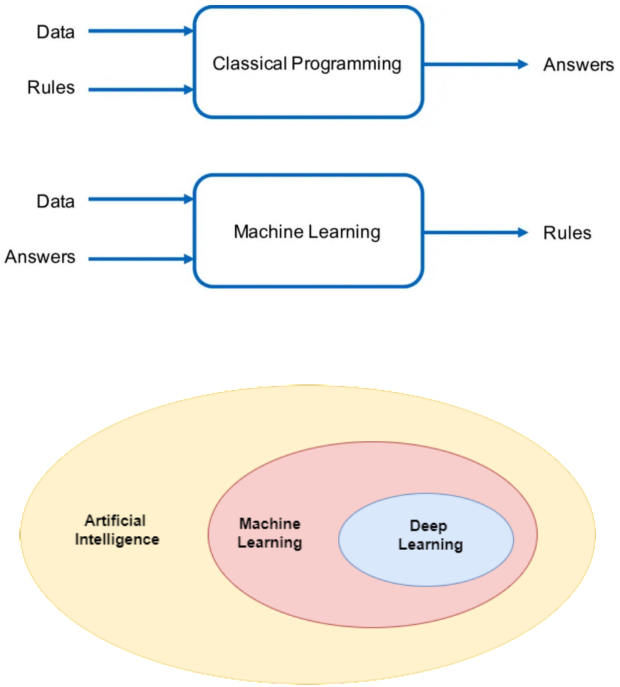
11:00–12:00 Uhr **Advanced Deep Learning Use Case: AI Weather Prediction**

Sprecher
Caroline Arnold, Paul Keil

12:00–12:30 Uhr **Closing remarks**

Sprecher
Paul Keil

What exactly is Machine Learning?



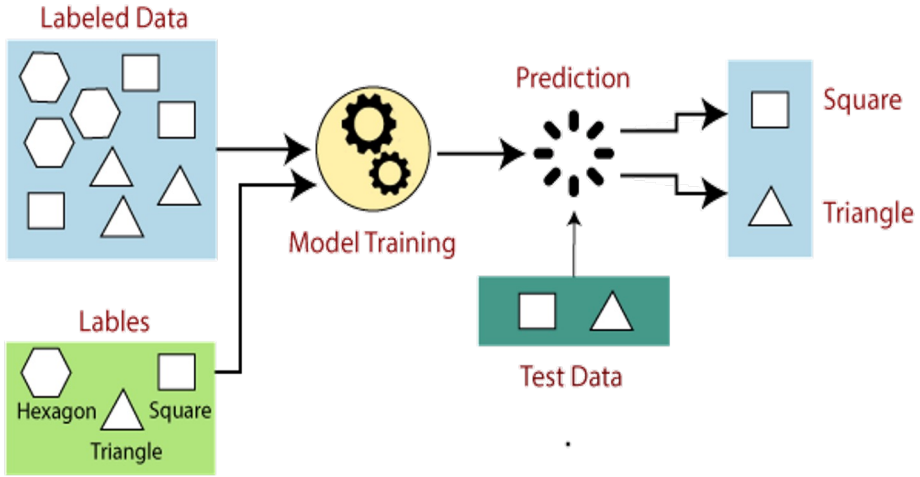
- **Classical Programming:** Humans define *deterministic rules (code)* to process input data → well-defined, predictable outputs
- **Machine Learning (ML):** Rules/patterns are purely *learned* from input data (features) and output labels
- **Deep Learning (DL):** Uses multi-layered neural networks to *automatically* learn complex, high-level features

Machine Learning – A Short Timeline…

- **1990s**: Support Vector Machines
- **2010s**: Deep Learning Resurgence: CNNs
- **2014**: Generative Adversarial Networks
- **2015**: AlphaGo: Reinforcement Learning
- **2018**: Transformer (BERT)
- **2020**: AlphaFold, Diffusion Models
- **2022**: LLMs (GPT-3)

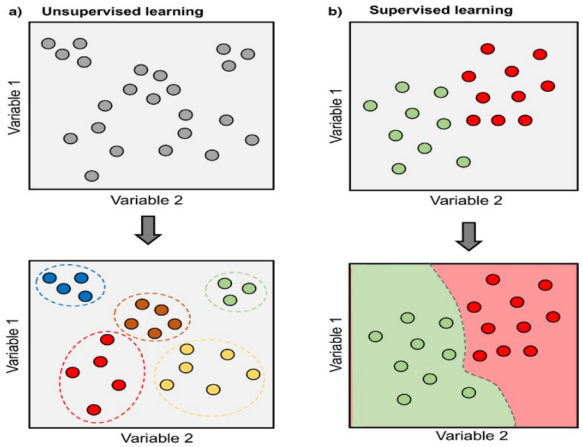
Types of Machine Learning – Supervised ML

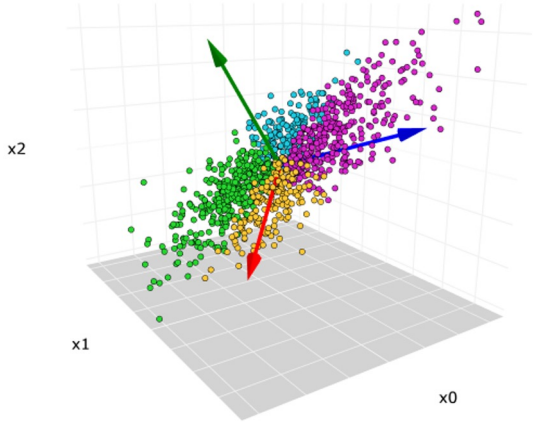
- The algorithm is trained on a *labeled* dataset
- Input data is paired with corresponding target labels
- Examples: Classification, Regression



Types of Machine Learning – Unsupervised ML

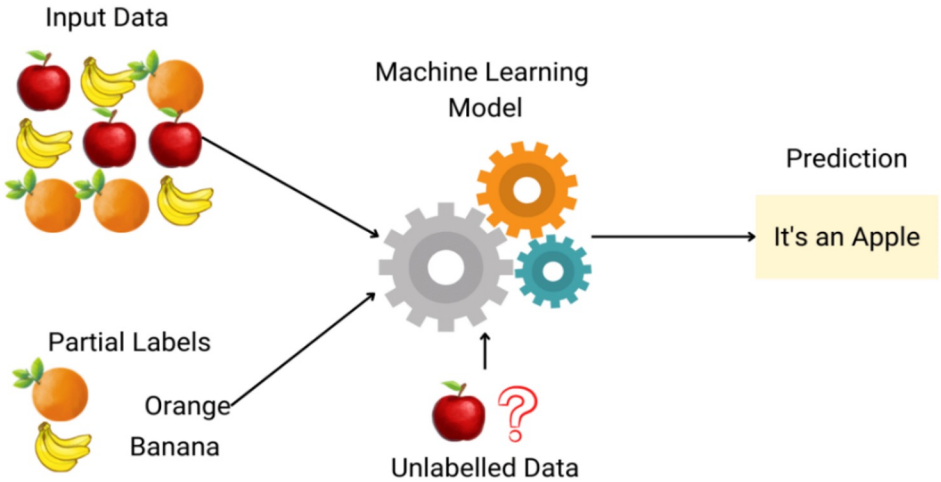
- The algorithm is trained on an *unlabeled* dataset
- Discover hidden patterns, relationships, or coherent structures within the data
- Examples: Clustering, Dimensionality Reduction, PCA





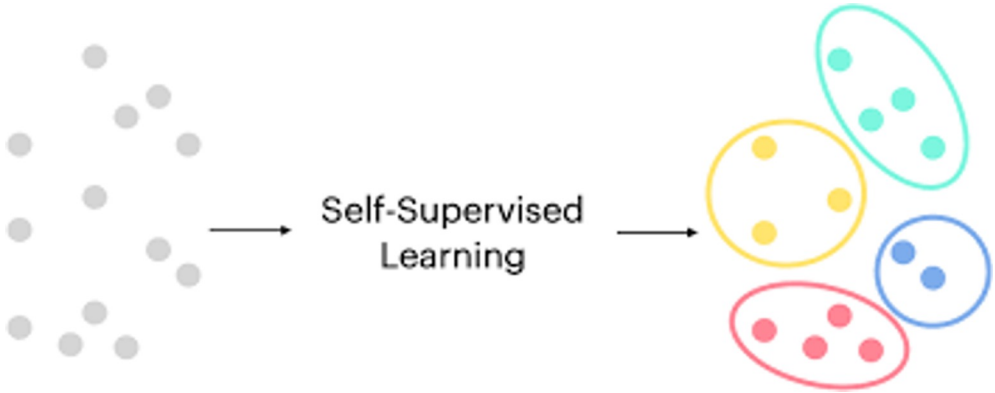
Types of Machine Learning – Semi-Supervised ML

- The algorithm is trained on a labeled *and* an unlabeled dataset
- Leveraging on labelled and unlabeled data to improve performance



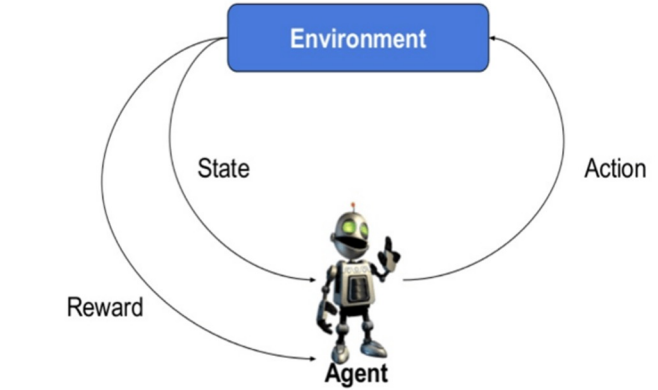
Types of Machine Learning – Self-Supervised ML

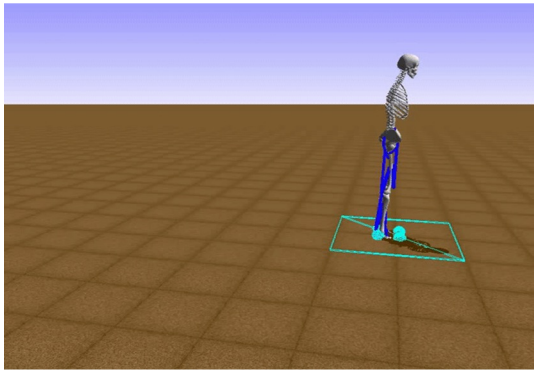
- The algorithm generates *its own labels* for training from input dataset
  → does not require external / manual labels
- Examples: Auto-encoders, Contrastive learning, Masked Language Modeling



Types of Machine Learning – Reinforcement Learning

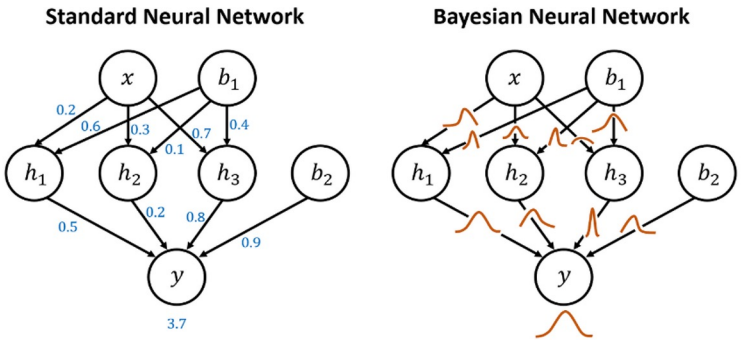
- An agent interacting with an environment → model learns based on feedback
- Learn a policy that maximizes the cumulative reward
- Examples: Humanoid robots, Games, autonomous systems

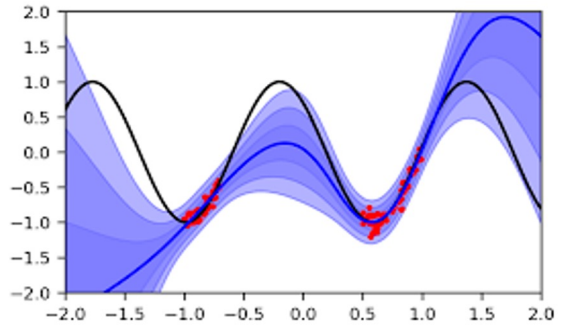




Types of Machine Learning – Probabilistic ML

- Data and Model include *uncertainties (aleatoric, epistemic)*
- Capture uncertainties for more reliable predictions
- Probability distributions are maintained over weights
- Example: Mean-Variance Estimation, Bayesian Neural Networks (BNN)

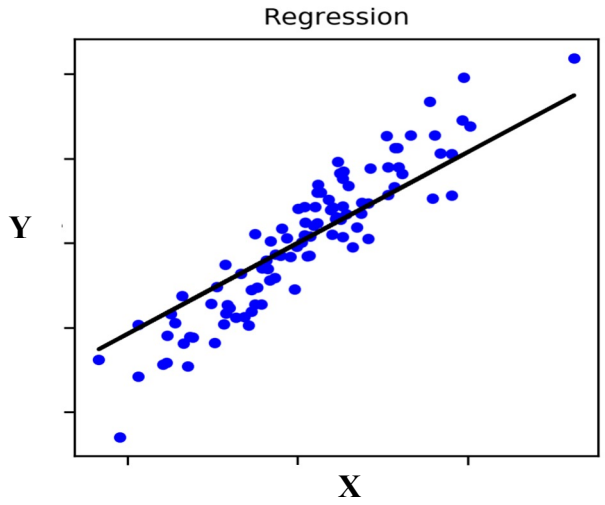




Questions?

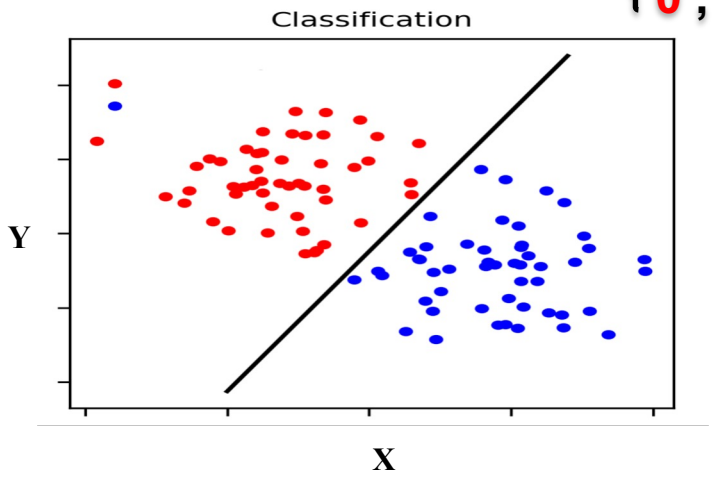
Regression and Classification in Machine Learning

- **Regression**: Predicting a *continuous* outcome
- In- & outputs are continuous values



- **Classification**: Assigning *discrete* instances to classes
- The outputs are seen as class *probabilities*

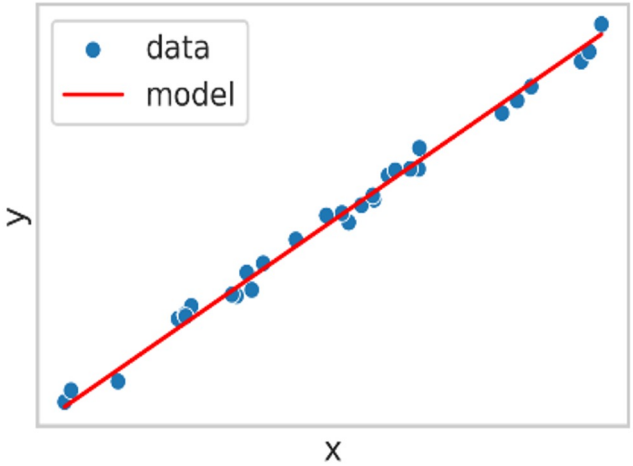
{ 0 , 1 }



Typical Machine Learning Procedure (Linear Regression)

- Data set: $D = \{x, y\}$
- 1D Model:
  - Defined as $\hat{y} = wx + b$
  - Trainable parameters: w, b
- Loss function:
  - $L(\hat{y}, y; w, b) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$
- Training objective:
  - Minimize loss function
    → yields optimal parameters w^*, b^*

Is this data labeled or not?

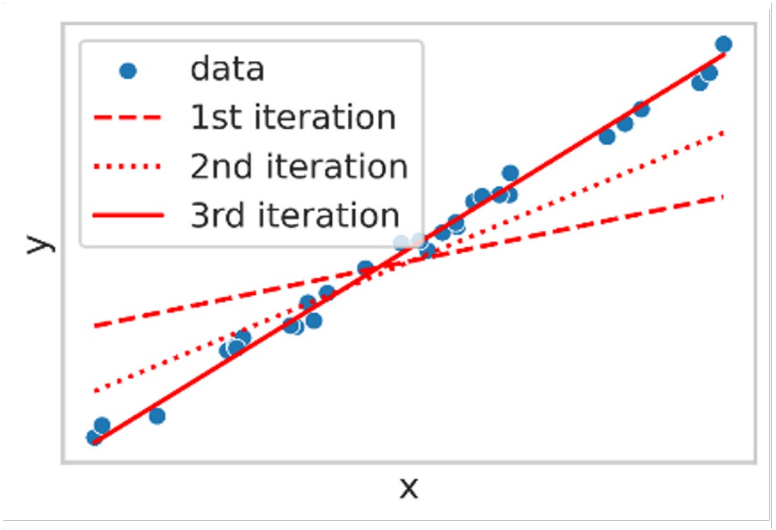


Optimization with Gradient Descent

- Start with a random guess for the trainable parameters
- Compute the output, then the loss function value
- Parameter update in the direction of the *negative gradient*

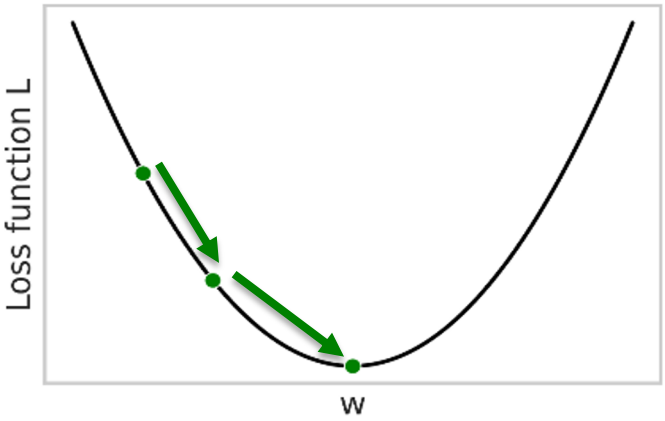
$$w_{i+1} = w_i - \alpha \nabla_{w_i} L(w_i)$$

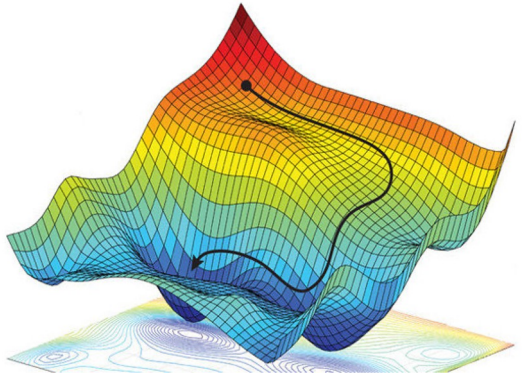
- Learning Rate $\alpha \in [0.0001, 0.1]$



Optimization with Gradient Descent

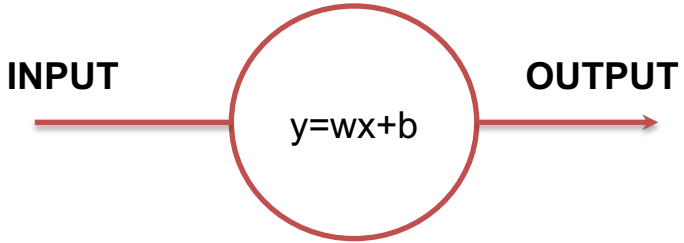
- Loss functions measure the *disparity* between predicted and actual values (scalar value)
- Learning objective: minimize the loss *w.r.t.* the model's parameters
- Step-wise optimization helps to find the *most suitable path*
  - Stochastic Gradient Descent (SGD)
  - Adaptive Momentum (Adam)
  - Adaptive Gradient (Adagrad)



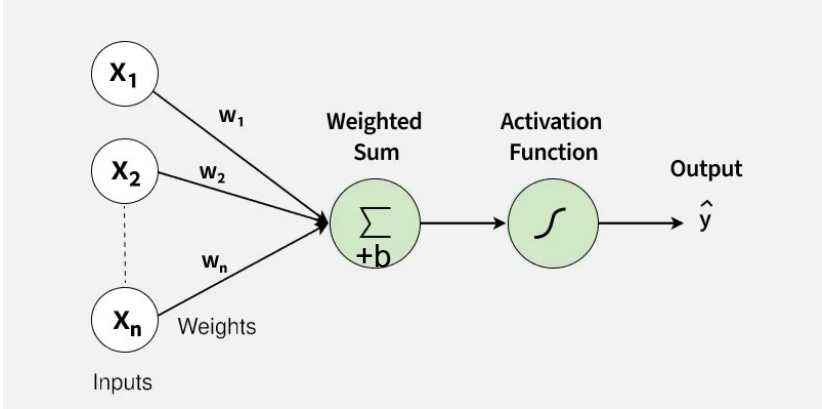


From Linear Regression to Neural Networks

- Linear regression: building block for complex models
- Simplest form:
  perceptron = neuron

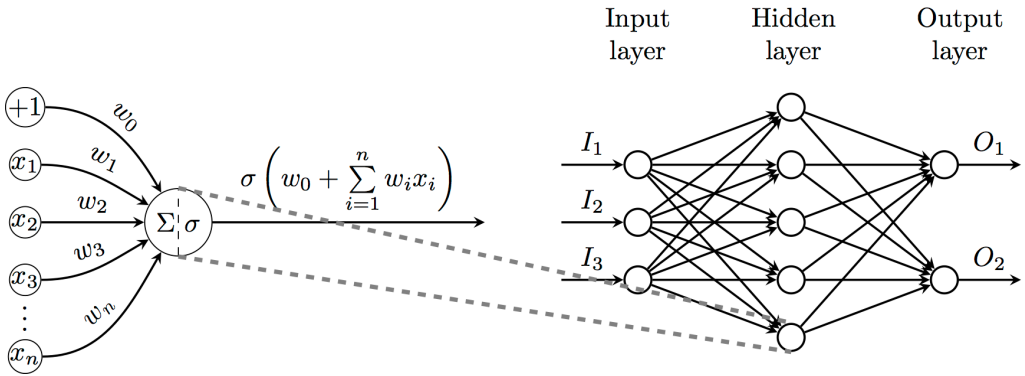


- Neural network: stack neurons and add nonlinear activation function
  $O = \sum_{i=1}^{n} w_i x_i + b; \hat{y} = \sigma(O)$



From Linear Regression to Neural Networks

- **Universal approximation theorem**:
  NN can approximate any “well-behaved” non-linear function
- Combine and stack several neurons per layer
  → different processing variants of the same input
- Add hidden layer(s) for more *representative capacity*



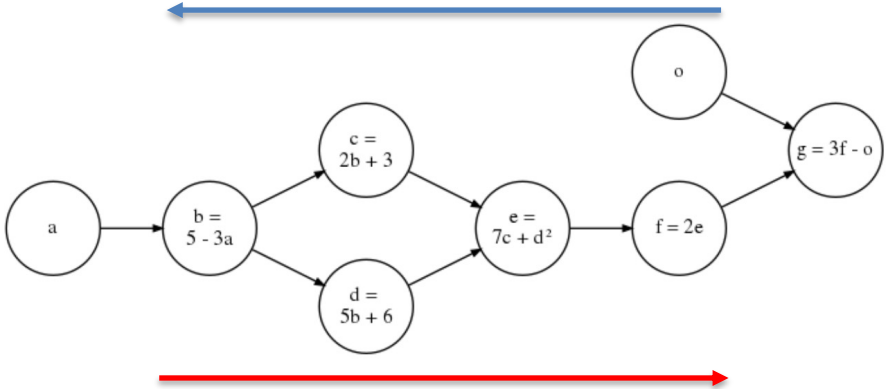
Matrix-Vector notation

$$\boldsymbol{O}_1 = \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b},\ \boldsymbol{a}_1 = \sigma(\boldsymbol{O}_1)$$
$$\boldsymbol{O}_{l+1} = \boldsymbol{W}_{l+1}\boldsymbol{a}_l + \boldsymbol{b}_{l+1}$$
$$\hat{\boldsymbol{y}} = \sigma(\boldsymbol{a}_l) = f_1 \circ f_2 \circ \cdots \circ f_L$$

Forward & Backward Pass – How do models infer & learn?

- Outputs generated by *passing* the inputs through the *parametrized* model
  → forward pass $y = f(x; \boldsymbol{w})$, where f can be any complex, nested function with a set of learnable parameters $\boldsymbol{\theta} = \{\boldsymbol{w}, \boldsymbol{b}\}$

- Training: Compute the gradients of weights to iteratively update them
  → we need *partial derivatives* of loss w.r.t. all learnable params $\frac{\partial L}{\partial w_i}; \frac{\partial L}{\partial b_i}$
  → use *chain rule* to recursively *propagate back* the loss through the model



Loss Function Types

- Regression:
  Mean Squared Error (MSE)
  Mean Absolute Error (MAE)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

$$\mathbf{MAE} = \frac{\sum_{i=1}^{n}|\boldsymbol{y_i} - \boldsymbol{x_i}|}{\boldsymbol{n}}$$

- Classification: Cross-Entropy Loss (Log-likelihood)

$$\text{Cross Entropy Loss}_b = -\frac{1}{n}\sum_{i=1}^{n}[y_i \log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i)]$$

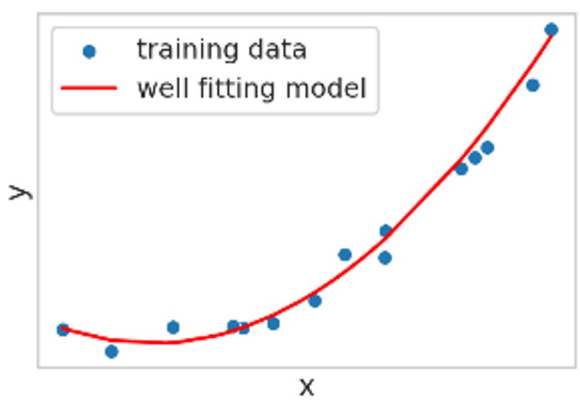
$$\text{Cross Entropy Loss}_m = -\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{m} y_{ij}\log(\hat{y}_{ij})$$

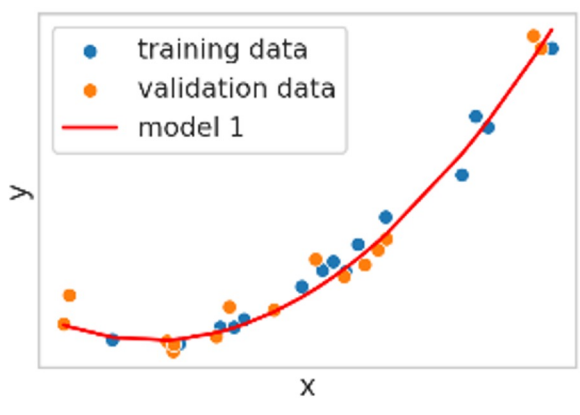
- Domain-informed loss function
  - Coherence with physical principles, e.g. based on governing equations
  - Example: PINN (Physics Informed Neural Network)

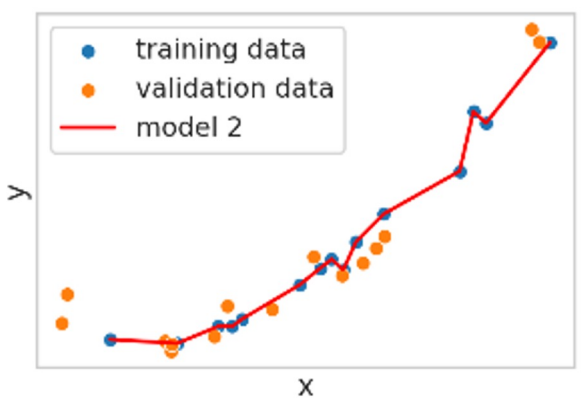
Questions?

Evaluating Machine Learning Algorithms

What do you think: Which model performs better overall?



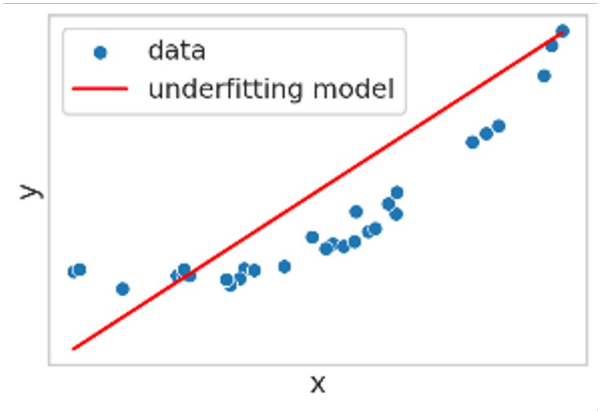


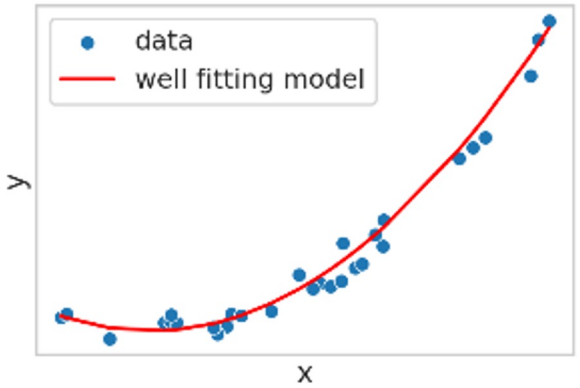


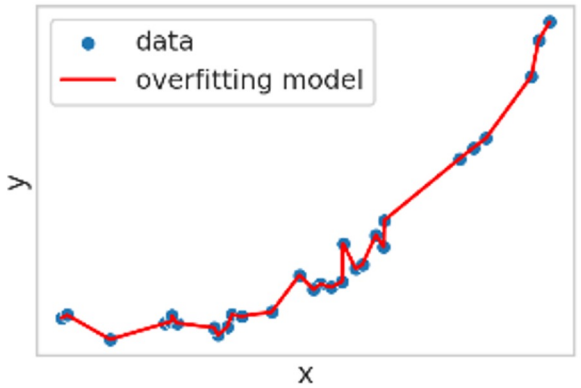
Evaluating Machine Learning Algorithms

Identifying Overfitting

- Neural network eventually learns to reproduce training data exactly → inefficient + does *not* generalize well to unseen data
- *Bias-variance tradeoff*

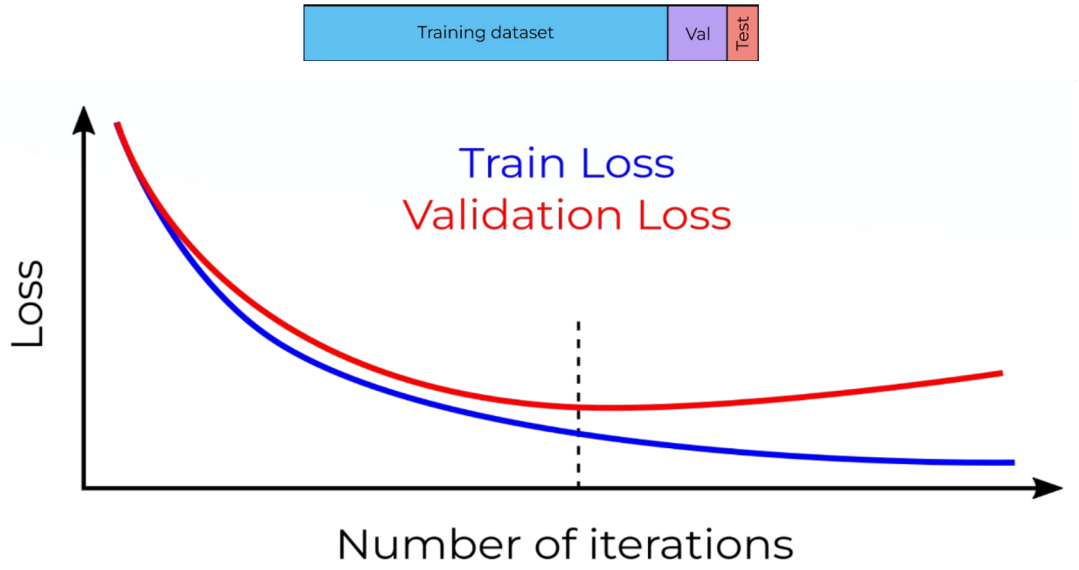






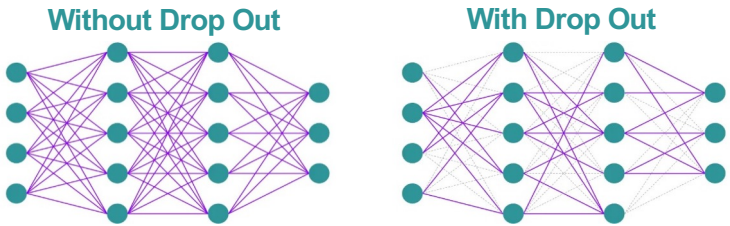
Solution I – Training-Validation-Test Split

- Separate validation data (typically 10-20%)
- After each training step, calculate the loss function using *only* the validation set

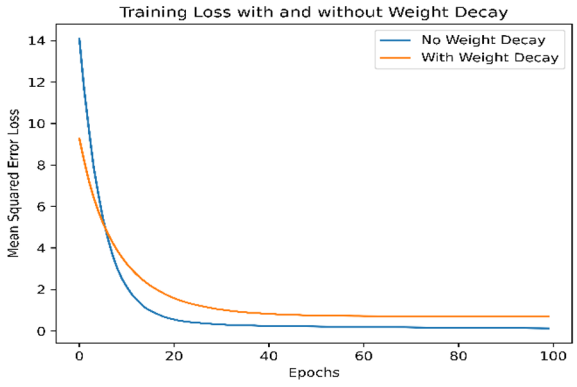


Solution II – Regularization Techniques

- Dropout
  - Neurons are randomly dropped during training
  - It prevents over-dependencies on particular neurons

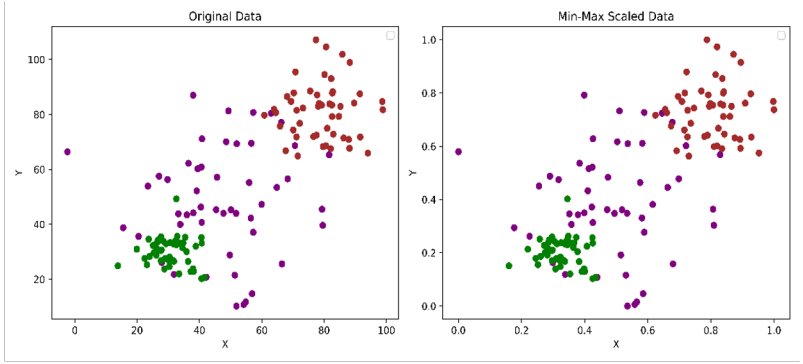


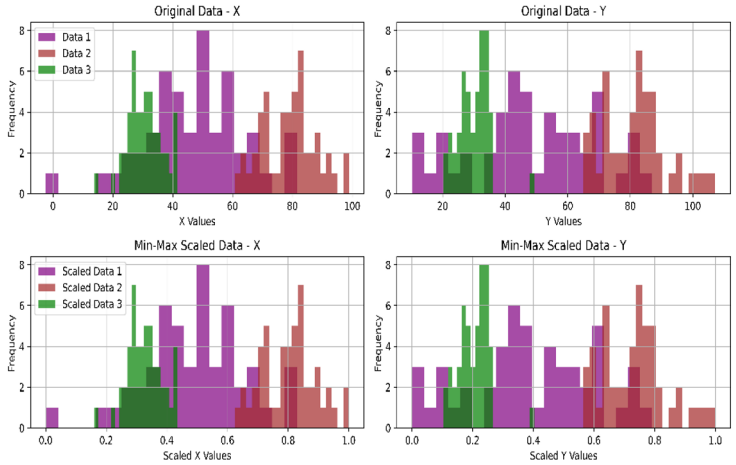
- Weight Decay
  - Penalize large weight values
  - Promote sparsity in weight matrices



Improve Model Training – Normalization

- General Idea
  - Ensure features of similar scale
  - Helps in convergence of model
  - Indirectly prevents over-fitting
- Common Normalization Methods
  - Mix-Max Scaler
  - Z-score Normalization
  - Log Transform
  - Robust Scaler

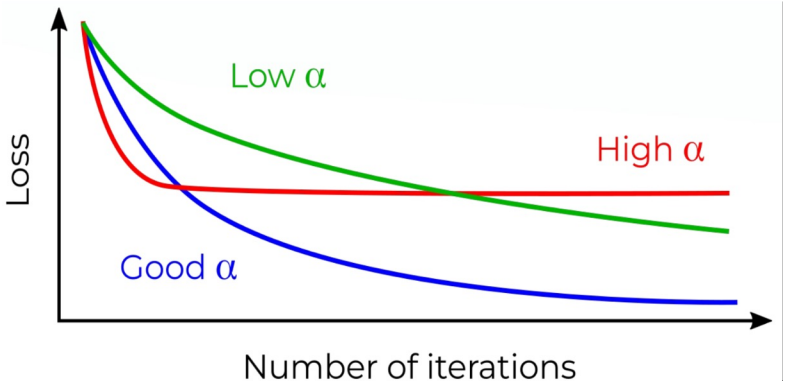




Improve Model Training – Hyper-parameter Optimization

Common Hyper-parameters

- Learning rate α
- Batch size *B*
- Epoch size
- Activation function
- # of neurons & layers
- Dropout rate

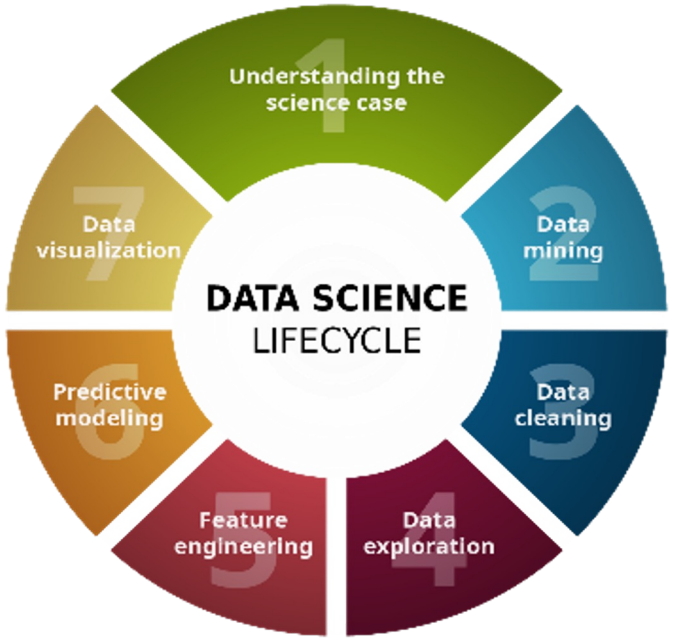


General aspects to consider

- Batching strategy → stochastic, full vs. mini batch
- Choice of model, loss function & optimizer

Typical machine learning project cycle

- Common thinking: I will spend a lot of time in model development
- Reality: 90% of time is spent in data science parts
- Always set your code up for an iterative process
- Always follow best practices



What is Needed for Successful Machine Learning Projects?

- Data that holds the necessary information and of good quality
  - „Garbage in, garbage out“
  - Think in advance: How much data do you have? Can you obtain more?
- Model: find the right model for your task (we will cover some in the course)
  → what *data structures / properties* should be “covered”?
  → what can the *model represent*?
- Computational resources: Machine learning relies on GPUs
- Storage & data through-put

Python Libraries for Data Science & ML/DL

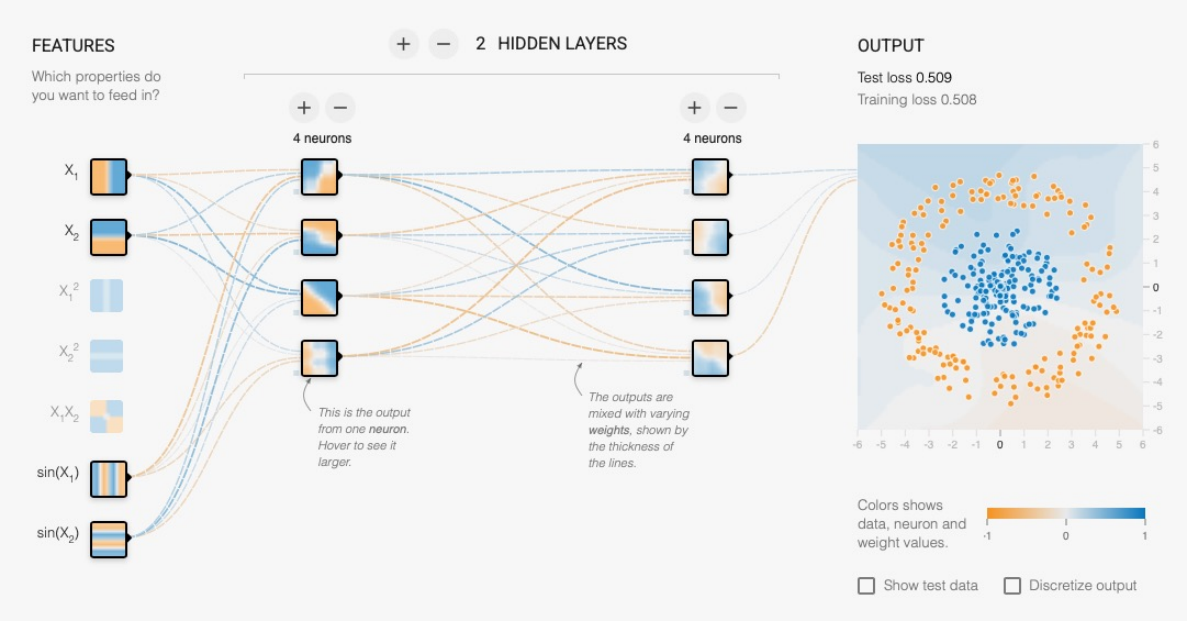
- Foundational data science
  - **NumPy**, **Pandas**, **SciPy** → exploratory data evaluation, sorting & filtering, feature engineering
  - **Visualization** → Matplotlib, Seaborn
- Machine Learning
  - Scikit-learn, **XGBoost** → classical machine learning algorithms
- Deep Learning
  - PyTorch **(Tensorflow)** → highly flexibel, fast, abstract API
  - JAX → modern, fucntional, very fast DL overlay on NumPy
  - Hugging Face Transformers → NLP, open-source models

Thank you for your attention!

Questions?
Thoughts?

Bonus

Tensorflow ML Playground



Lunch Options

- Geomatikum Mensa
- Veggie Mensa
- Rucola e Parma, Italian
- Quan19, Vietnamese
- Dulfs Burger
- Hindukusch, Afghan
- Many more…

- We are here (DKRZ)