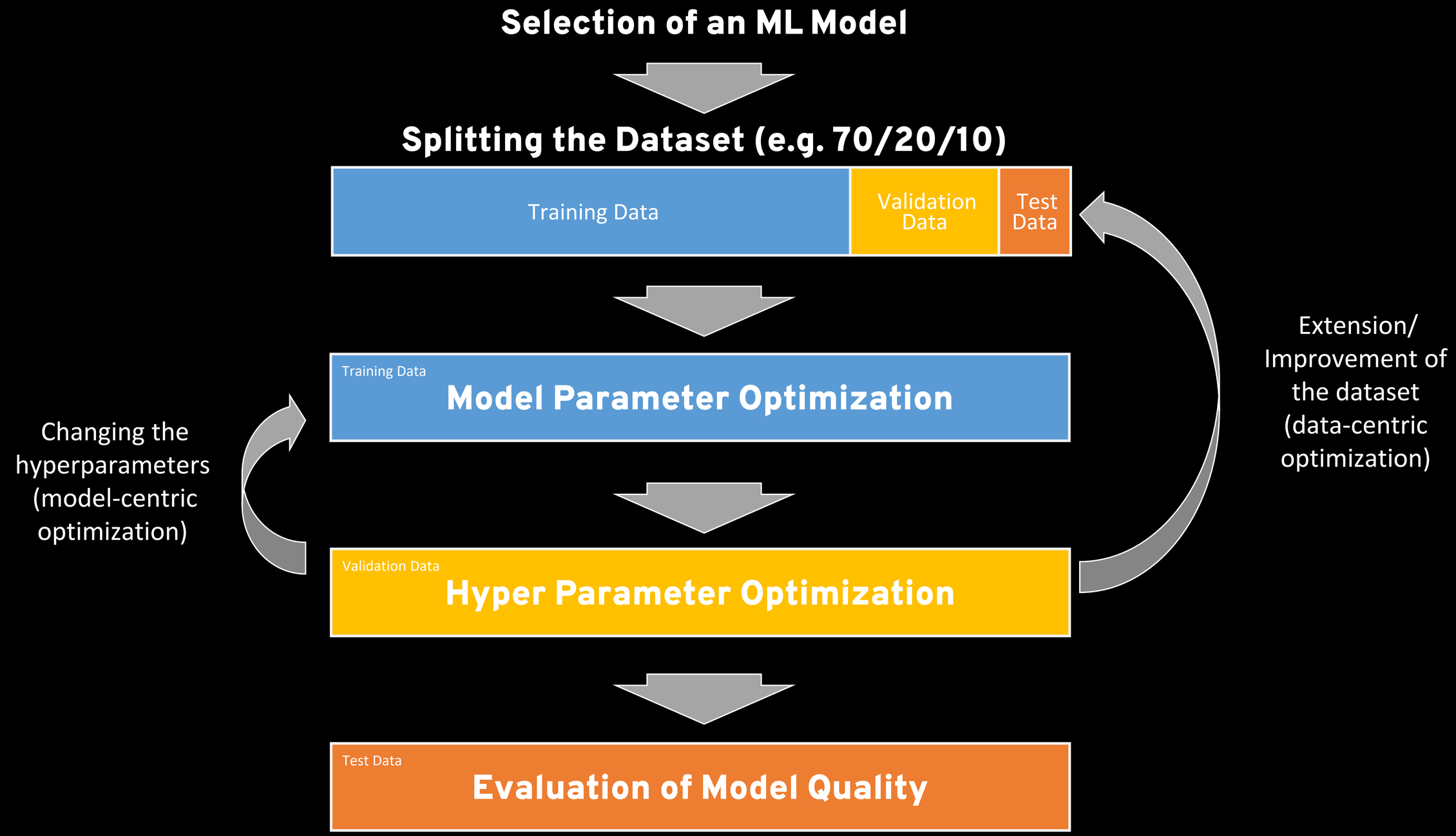
05.06.25

OPENCAMPUS.sh

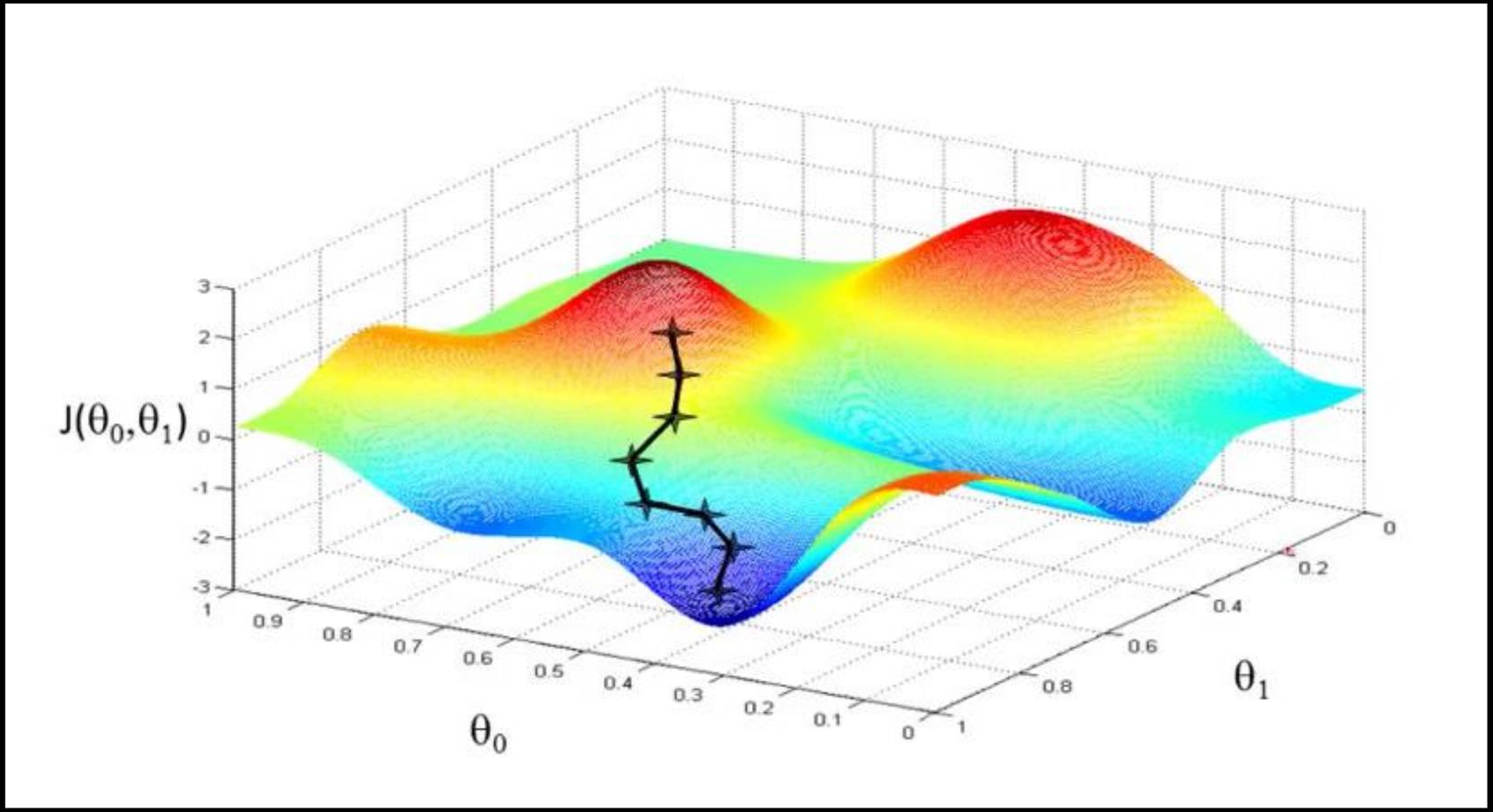
Introduction to Data Science and Machine Learning

OVERFITTING AND MODEL EVALUATION

- Review of Important Terms in Machine Learning
- Overfitting and Regularization
- Model Quality Criteria
- Introduction to Neural Networks


Selection of an ML Model
Splitting the Dataset (e.g. 70/20/10)
Training Data
Validation Data
Test Data
Training Data
Model Parameter Optimization
Validation Data
Hyper Parameter Optimization
Test Data
Evaluation of Model Quality
Changing the hyperparameters (model-centric optimization)
Extension/ Improvement of the dataset (data-centric optimization)

OPTIMIZATION FUNCTION (OPTIMIZER)



- **Iterative method (Gradient Descent) to find the minimum of the cost function.**
- **The learning rate ("learning parameter") describes the step size for approaching the minimum.**

Quelle: https://www.coursera.org/learn/machine-learning

OPTIMIZATION OF THE MODEL PARAMETERS

Forward Propagation

- **Computation of predictions for a dataset using the current model parameters (weights and biases)**
- **Computation of the total cost or loss based on the difference between predictions and actual values**

Backward Propagation

- **Calculation of the contribution of each model parameter to the total loss**
- **Computation of gradients (i.e., partial derivatives of the loss with respect to parameter) to determine how to update the parameters to reduce the loss**

Gradient Descent (Optimization Step)

- **Use the derivates to update ethe parameters**
- **Typical update rule:**

```
New Value = Old Value – Learning Rate × Partial Derivative
```

MODEL PARAMETERS VS. HYPER PARAMETERS

Model Parameters

- **Parameters that are optimized during training (the weights and biases).**

Hyper Parameters

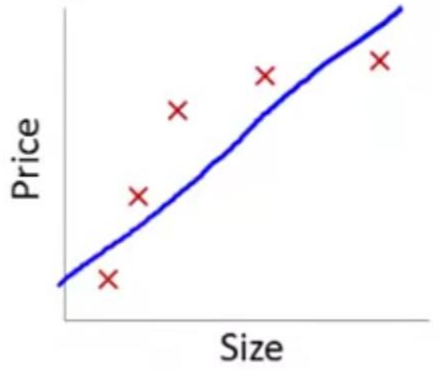
- **Parameters set before training (e.g., on how the parameters are optimized, how many are optimized, or how they relate to each other).**

FEATURES, LABELS, PARAMETER

Machine Learning	Statistics	Description
Feature, Input Variable	Independent Variable	Input data used for prediction
Label, Target Variable, Output	Dependent Variable	Observed outcomes used to train the model
Weights, (Modell) Parameter	Coefficients	Are optimized ("learned") during training

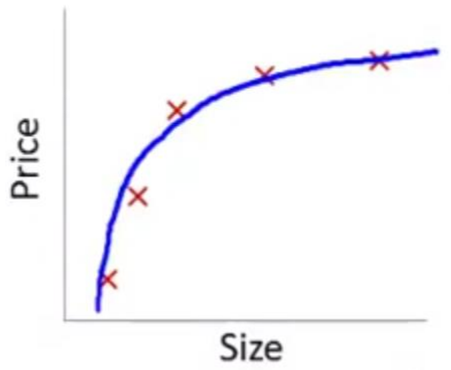
OVERFITTING

Example: Linear regression (housing prices)



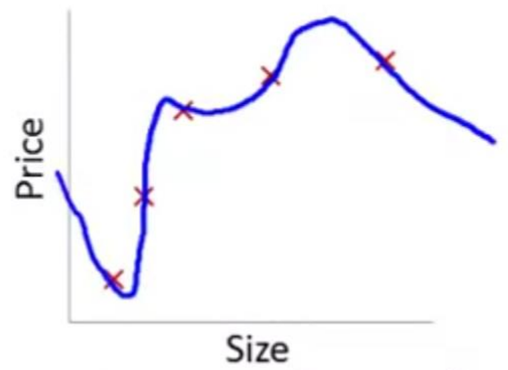
$\rightarrow \theta_0 + \theta_1 x$

"Underfit" "High bias"



$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2$

"Just right"



$\rightarrow \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$

"Overfit" "High variance"

Overfitting: If we have too many features, the learned hypothesis may fit the training set very well ($J(\theta) = \frac{1}{2m} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \approx 0$), but fail to generalize to new examples (predict prices on new examples).

Computer Science Engineering. (2017). *3.4.1 The Problem of Overfitting by Andrew Ng*. Abgerufen von https://www.youtube.com/watch?v=OSd30QGMl88

STRATEGIES TO AVOID OVERFITTING

Options:

1. Reduce number of features.
   - Manually select which features to keep.
   - Model selection algorithm

2. Regularization.
   - Keep all the features, but reduce magnitude/values of parameters θ_j.
   - Works well when we have a lot of features, each of which contributes a bit to predicting y.

Computer Science Engineering. (2017). *3.4.1 The Problem of Overfitting by Andrew Ng*. Abgerufen von https://www.youtube.com/watch?v=OSd30QGMI88

REGULARIZATION

"Penalizing" the Use of Variable Information within the Cost Function

Linear Model with Multiple Variables x_1, x_2 and possibly many others:

$$h_x(\theta_0, \theta_1, \theta_2, \dots) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots$$

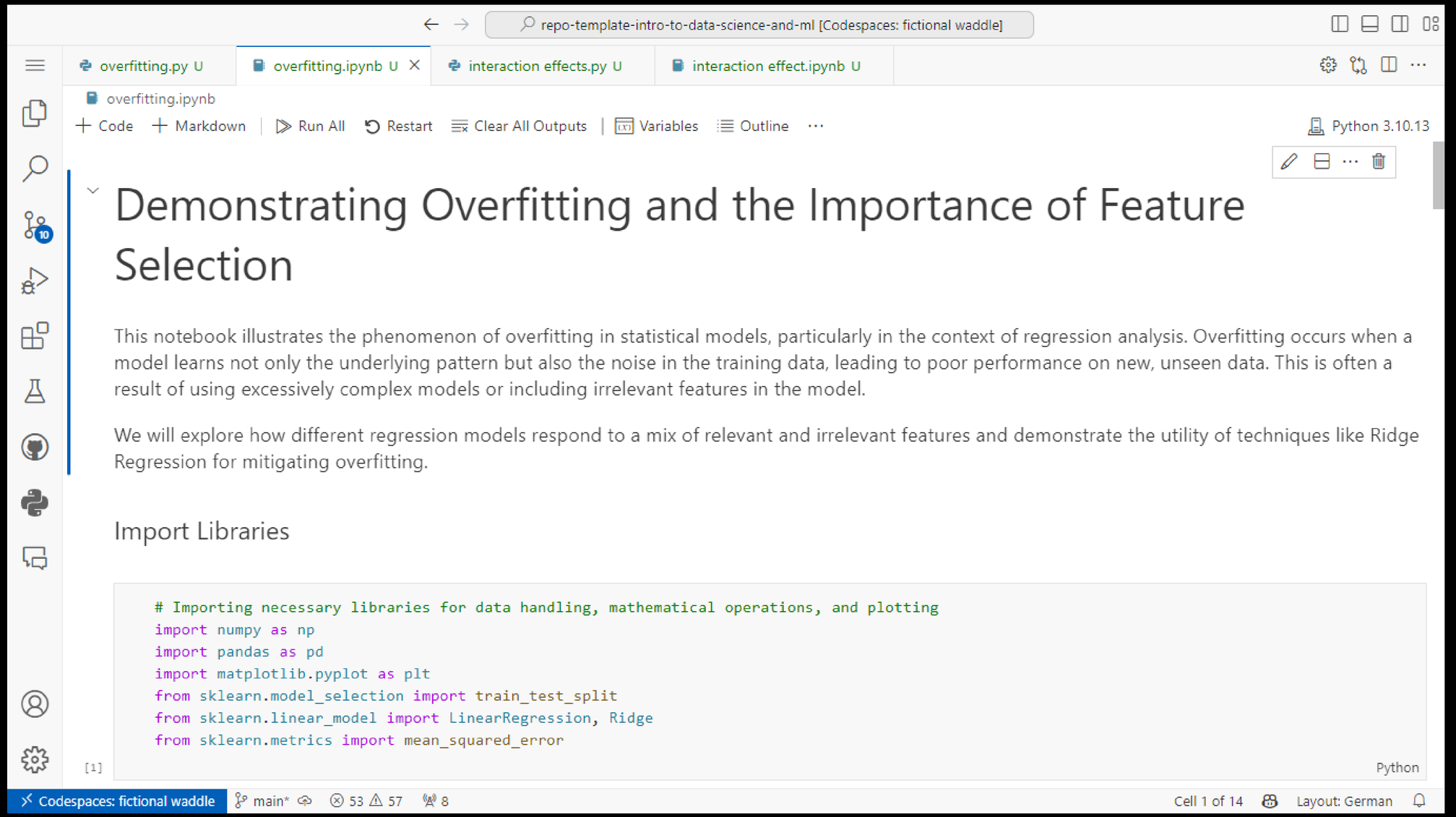
(with $\theta_0, \theta_1, \theta_2, \dots$ as the model parameters to be estimated)

Cost function with regularization:

$$J_x(\theta_0, \theta_1, \theta_2, \dots) = \frac{1}{m}\left[\sum_m (h_x(\theta_0, \theta_1, \theta_2, \dots) - y)^2 + \lambda(|\theta_0| + |\theta_1| + |\theta_2| + \cdots)\right]$$

(with λ as regularization parameter)

EXAMPLE NOTEBOOK



BATCHES, STEPS AND EPOCHS

Batch

- **The entire set of training data is divided into separate subgroups of equal size.**
- **The standard batch size in TensorFlow is 32.**

Step

- **A single iteration of gradient descent performed on one batch of data, during which all model weights are updated once.**

Epoche

- **Optimization of the model using the complete training data:**
  Number of Steps × Batch Size = Training Sample Size
- **Depending on the model, very few epochs may suffice, or several hundred or thousand may be needed for optimization.**

MODEL QUALITY CRITERIA FOR REGRESSION TASKS

errors:	forecast – actual	(also: residuals)
mae:	mean(abs(errors))	
mape:	mean(abs(errors/actual))	
mse:	mean(errors^2)	
rmse:	sqrt(mean(errors^2))	
rse:	sum(errors^2) / sum((actual-mean(actual))^2)	
r^2 =	1 – rse	

Video (3 minutes) with explanations of the criteria:

https://www.coursera.org/lecture/machine-learning-with-python/evaluation-metrics-in-regression-models-5SxtZ

MODEL QUALITY CRITERIA FOR CLASSIFICATION TASKS

$$\text{Accuracy} = \frac{\text{Number of Correct Predictions}}{\text{Total Number of Predictions}}$$

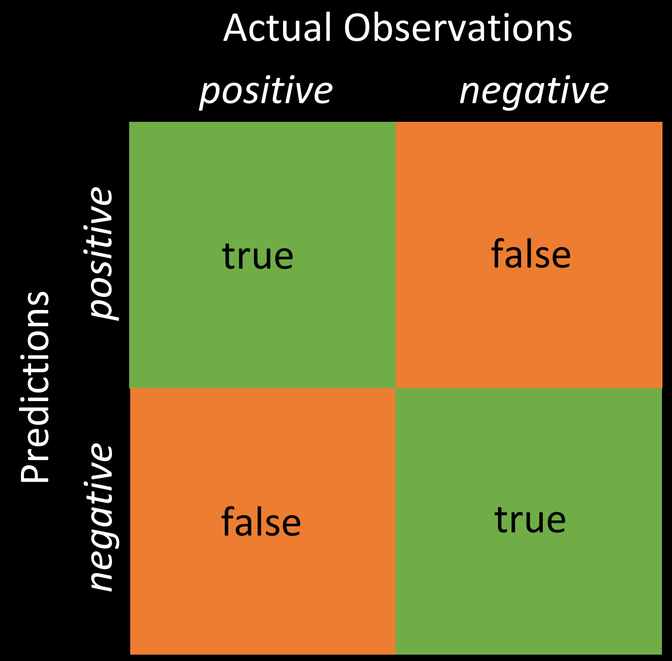
$$\text{Precision} = \frac{\text{Number of Correct Positive Predictions}}{\text{Total Number of Predictions}}$$

e.g., for spam detection

$$\text{Recall} = \frac{\text{Number of Correct Positive Predictions}}{\text{Number of Actual Positive Cases}}$$

e.g., credit card fraud detection

$$\text{F1}-\text{Score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$



Blog with more explanations on the above metrics:

https://towardsdatascience.com/performance-metrics-confusion-matrix-precision-recall-and-f1-score-a8fe076a2262/

BREAKOUT

Each team writes a post in Mattermost with answers to the following questions:

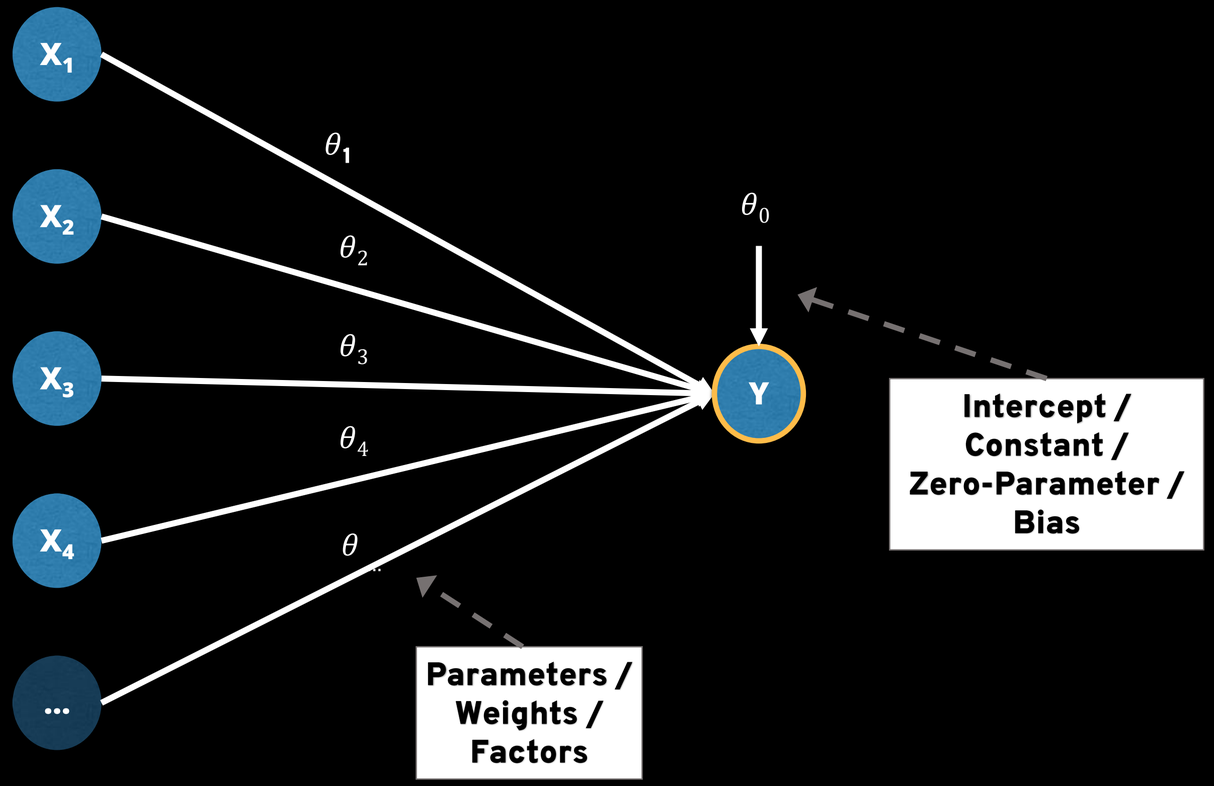
- **What is the r^2 of your currently best model?**

- **Have you tested a model on Kaggle?**
  ➔ If “No”: What problem are you currently facing?

LINEAR REGRESSION

Input Layer
represents the features of the data — each input node corresponds to one variable (feature or dimension).

Output Layer
Applies an activation function (in this case, a linear function) to aggregate the weighted inputs (parameters θ) from the previous layer.



NEURAL NETS

Input Layer

represents the features of the data

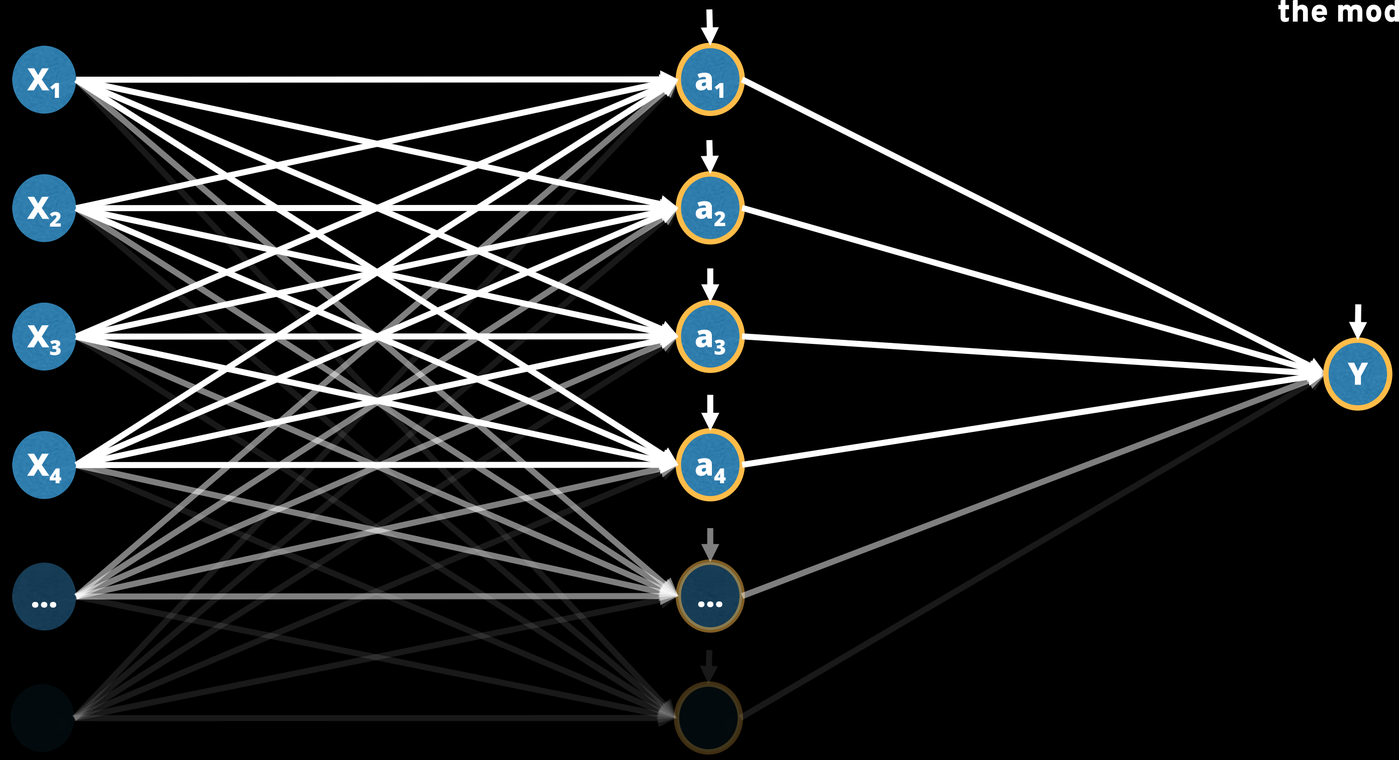
Hidden Layer

Computes weighted combinations of inputs and applies non-linear activation functions.

Output Layer

Aggregates the weighted outputs from the last hidden layer using an activation function.

Produces the final prediction of the model.



PROPERTIES OF THE LINEAR MODEL

- **Both with and without regularization, parameter optimization for the linear model is very easy and fast.**

  → For simple models, it is easy to obtain optimized parameters.

- **Models that are easier to optimize typically rely on stronger assumptions about the relationships between variables (in this case, linear relationships).**

  → Therefore, optimal selection and encoding of variables according to these assumptions becomes even more important.

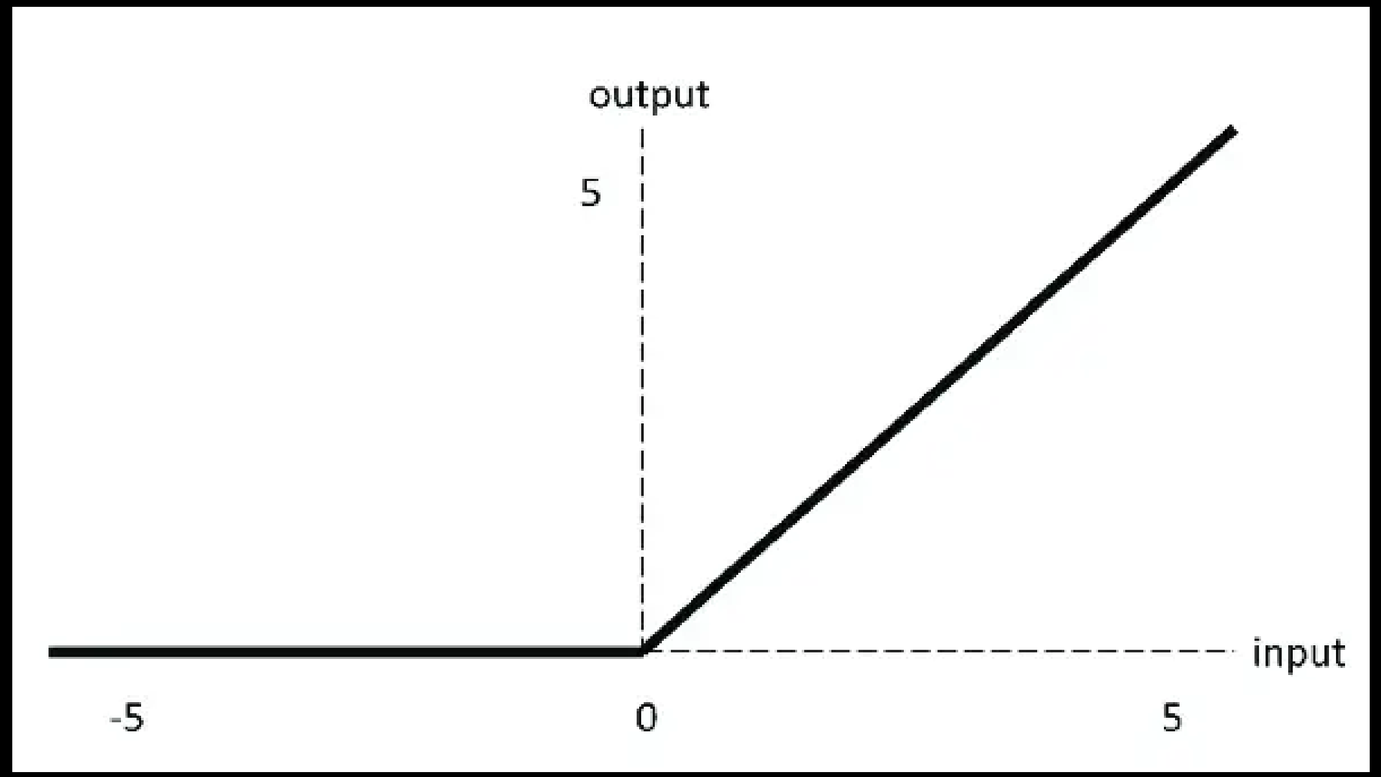
  → In some cases, the actual relationships may not be captured by the model.

PROPERTIES OF NEURAL NETS

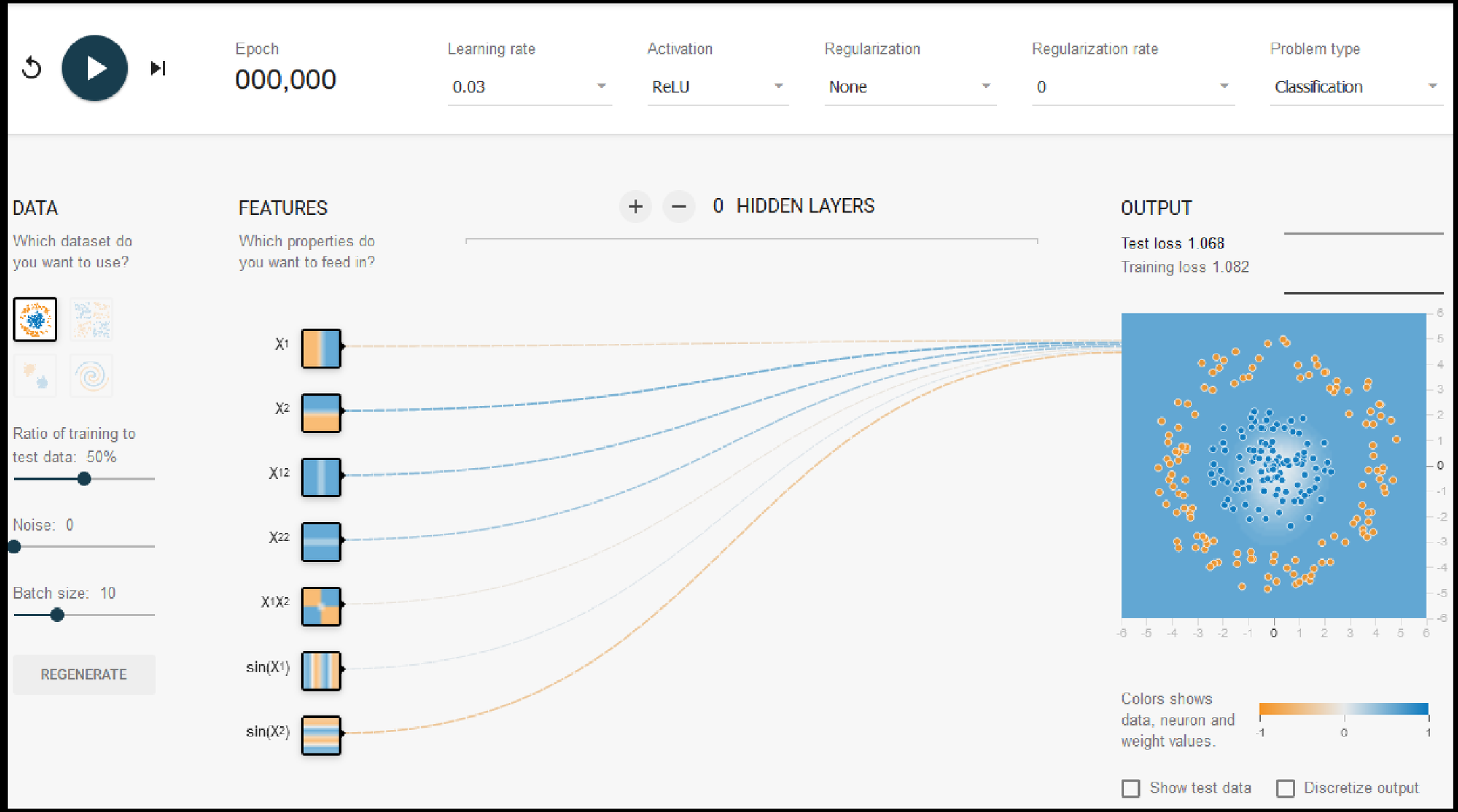
- Definition of additional "hidden layers" between input and output layer.
  → Statistics: Definition of latent variables, usually with unknown meaning
  → Allows implicit modelling of interaction effects

- Use of non-linear activation functions.
  → Allows modeling of non-linear effects

THE NON-LINEAR ACTIVATION FUNCTION RELU



$$f(x) = \max(0, x)$$


Epoch
000,000
Learning rate
0.03
Activation
ReLU
Regularization
None
Regularization rate
0
Problem type
Classification
DATA
Which dataset do you want to use?
Ratio of training to test data: 50%
Noise: 0
Batch size: 10
REGENERATE
FEATURES
Which properties do you want to feed in?
0 HIDDEN LAYERS
X1
X2
X12
X22
X1X2
sin(X1)
sin(X2)
OUTPUT
Test loss 1.068
Training loss 1.082
Colors shows data, neuron and weight values.
-1
0
1
Show test data
Discretize output

BREAKOUT

- Open the following tool: https://playground.tensorflow.org/

- Define two hidden layers and try changing the number of neurons so that you can predict the spiral-shaped dataset.

→ Have you found a systematic approach to arrive at a solution?
→ To what extent can you interpret the result in terms of the features used?

HYPERPARAMETERS

- Choice of model or model architecture
- Choice of activation functions
- Choice of loss function
  - MAE, MSE, …
- Choice of optimization function
  - Learning rate size
- Choice of batch size
- Depending on the model architecture and selected components, many more…

LEARNING RESOURCES

- Enroll into the Coursera course “Advanced Learning Algorthms” and watch the videos of the sections “Neural networks intuition” and “TensorFlow implementation”

Like this course? Become an expert by joining the Machine Learning Specialization.

Advanced Learning Algorithms

Limited access

Course Material

- Week 1
- Week 2
- Week 3
- Week 4

Grades

Notes

Messages

Course Info

Neural Networks

1h of videos left · 2 min of readings left · 5 graded assessments left

This week, you'll learn about neural networks and how to use them for classification tasks. You'll use the TensorFlow framework to build a neural network with just a few lines of code. Then, dive deeper by learning how to code up your own neural...

Show Learning Objectives

- Neural networks intuition
- Practice quiz: Neural networks intuition — 1 graded assessment left
- Neural network model
- Practice quiz: Neural network model — 1 graded assessment left
- TensorFlow implementation
- Practice quiz: TensorFlow implementation — 1 graded assessment left

TASKS

- **Further extend the dataset with additional variables that could be relevant for estimating revenue.**
- **Test your model's predictive performance on Kaggle!**