## Neural Networks 1 - Multilayer neural networks 18NES1 - Lecture 8, Summer semester 2024/25

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## What We Covered Last Week

# Multilayer Neural Network (MLP) and the Backpropagation Algorithm

- Overview of Python libraries for deep learning, including code examples and instructions of local installation
- Interactive visualizations with TensorFlow Playground
- Brief analysis of the multi-layer neural network model with the backpropagation algorithm
- Step-by-step example using Keras on a sample task (binary classification). Setting hyperparameters and understanding their impact on the training process. Using TensorBoard.

## This Week

- Recall and finish the Keras example
- Ø More notes on hyperparameter setting
  - Learning algorithms for multilayer neural networks
- 3 Examples of various types of tasks:
  - Binary classification (already covered), multiclass classification, regression, time series prediction
  - Specifics of each task and data preprocessing
- Generalization in MLPs and techniques for preventing overfitting (with demonstrations and examples)

## Example from the last week

### keras\_simple\_example.ipynb

- A detailed example in Keras step-by-step learning procedure (on a binary classification task)
- Data preprocessing and analysis. Model creation and hyperparameter tuning. Training progress. Visualization. Evaluation.
- Hyperparameter tuning.
- Visualization using TensorBoard.

We will switch between the slides and the example notebook during the session.

Neural Networks 1 - Multilayer neural networks Setting Hyperparameters of an MLP Model

# Key Hyperparameters of an MLP Model

## Architecture

- **Model size:** Number of hidden layers and number of neurons per layer
- Activation functions in each layer: relu, sigmoid, tanh, softmax, ...

## Other key hyperparameters

- Loss function: MSE, binary crossentropy, ...
- Evaluation metrics: accuracy, MSE, precision, ...
- Optimization algorithm: SGD, Adam, RMSProp, ...
- Learning rate, and possibly other optimizer-specific parameters
- Batch size
- Number of epochs
- Weight initialization: Typically small random values
- Regularization: L2, Dropout, Early stopping, and the second

Neural Networks 1 - Multilayer neural networks Setting Hyperparameters of an MLP Model Learning Algorithm (Optimizer)

# Optimizers for Deep Neural Networks

- Based on gradient descent; often use adaptive and local learning rates
  - SGD (Stochastic Gradient Descent) basic optimizer, uses mini-batches; stable
  - Adam currently the most popular; adaptive learning rate; faster convergence
  - RMSprop suitable for sequential and online data
  - AdaGrad, Adadelta, AdaMax, NAdam, FTRL, ...
- Each optimizer has additional hyperparameters (e.g., SGD: learning\_rate, momentum, nesterov)

In most cases, the default settings work well.

https://keras.io/api/optimizers/

Neural Networks 1 - Multilayer neural networks Setting Hyperparameters of an MLP Model Learning Algorithm (Optimizer)

# TensorBoard

- A tool for visualizing training and evaluation of neural networks.
- Displays loss curves, metrics, model graph, weight distributions, and more.
- Enables real-time monitoring during training.
- Supports comparison of multiple model runs.

## Usage in Keras:

```
from keras.callbacks import TensorBoard
log_dir = "logs/fit/" + ...
tensorboard_callback = TensorBoard(log_dir=log_dir,...)
model.fit(..., callbacks=[tensorboard_callback,...])
```

### Run from terminal:

tensorboard --logdir=logs/fit Documentation: tensorflow.org/tensorboard Neural Networks 1 - Multilayer neural networks Setting Hyperparameters of an MLP Model Learning Algorithm (Optimizer)

# Example - Optional Homework from the last week

### keras\_simple\_example.ipynb

- Use this notebook to explore how different hyperparameter settings (architecture, learning rate, etc.) affect the training process and the final results.
- Suggestions for experiments are included directly in the notebook.
- Try working with TensorBoard (you can also run it locally on your own machine).
- Optionally, modify the code and try training an MLP on different datasets from the scikit-learn repository (e.g., iris, diabetes, wine).

Neural Networks 1 - Multilayer neural networks Learning Speed and Approximation Capabilities

# MLP Model Analysis Learning Speed and Approximation Capabilities

- Backpropagation is relatively slow.
- Poor hyperparameter choice can make it even slower.
- Nevertheless, it often outperforms many "fast algorithms", especially when:
  - The task has realistic complexity
  - The training set size exceeds a critical threshold

Neural Networks 1 - Multilayer neural networks Learning Speed and Approximation Capabilities

# MLP Model Analysis Learning Speed and Approximation Capabilities

# How to speed up learning while maintaining good approximation

- Proper initialization of weights and biases
- Preprocessing and normalization of input data
- Proper learning rate selection
- Use of fast learning algorithms
- Simultaneous adaptation of weights, biases, and network architecture

Neural Networks 1 - Multilayer neural networks Learning Speed and Approximation Capabilities

# Choosing a Suitable Learning Rate

- $\bullet\,$  The learning rate  $\alpha$  is a key parameter in training
- It controls how quickly the model learns

### How to choose the learning rate?

- Too small slow learning (tiny weight updates), risk of getting stuck in suboptimal local minima
- Too large large jumps, risk of oscillations and skipping over minima of the loss function

## What helps?

- Tuning the learning rate for a specific task
- Using momentum (momentum, nesterov)
- Adaptive learning rate methods (Adam, RMSprop,...)

# Backpropagation with Momentum

**Problem:** In narrow valleys of the error surface, following the gradient may cause large and frequent oscillations:

 $\bullet~$  The gradient fluctuates  $\rightarrow$  slows convergence

### Solution: Add a momentum term

- In addition to the current gradient, incorporate the previous weight updates
- Effect: Increased inertia helps maintain direction, reduces oscillations



https://www.andreaperlato.com/aipost/gradient-descent-with-momentum/

## Backpropagation with Momentum

### Updated weight update rule:

• Weight change from neuron i to neuron j at time t + 1:

$$\begin{aligned} \Delta w_{ij}(t+1) &= -\alpha \frac{\partial E_t}{\partial w_{ij}} + \alpha_m \Delta w_{ij}(t) \\ &= -\alpha \frac{\partial E}{\partial w_{ij}} + \alpha_m (w_{ij}(t) - w_{ij}(t-1)) \end{aligned}$$

- $\alpha$  ... learning rate
- $\alpha_m$  ... momentum coefficient

## Backpropagation with Momentum

### Momentum Term:

$$\Delta w_{ij}(t+1) = -\alpha \frac{\partial E_t}{\partial w_{ij}} + \alpha_m \Delta w_{ij}(t)$$

- Helps maintain direction in narrow valleys of the loss surface
- Reduces the risk of getting stuck in unstable states (local minima, saddle points)
- Speeds up convergence (longer stretches with consistent gradient direction)
- Too large  $\alpha_m$  excessive inertia, may overshoot the minimum

## Nesterov Momentum

### Improvement over classical momentum:

- "Looks ahead" computes gradient at the anticipated next position
- Provides better stability and faster convergence in practice

## Weight update steps:

Ompute the lookahead position:

$$ilde{w}_{ij}(t) = w_{ij}(t) + lpha_m \cdot \Delta w_{ij}(t-1)$$

Ompute gradient at this anticipated position:

$$\Delta w_{ij}(t) = -\alpha \cdot \frac{\partial E}{\partial w_{ij}} \bigg|_{w = \tilde{w}(t)} + \alpha_m \cdot \Delta w_{ij}(t-1)$$

Opdate the weight:

$$w_{ij}(t+1) = w_{ij}(t) + \Delta w_{ij}(t)$$

## Nesterov Momentum

### Weight Update Summary:

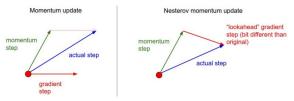
**Oracle Compute the lookahead position**:

$$\tilde{w}_{ij}(t) = w_{ij}(t) + \alpha_m \cdot \Delta w_{ij}(t-1)$$

e Evaluate the gradient at that position:

$$\Delta w_{ij}(t) = -\alpha \cdot \frac{\partial E}{\partial w_{ij}} \bigg|_{w = \tilde{w}(t)} + \alpha_m \cdot \Delta w_{ij}(t-1)$$

3 Update the weight:  $w_{ij}(t+1) = w_{ij}(t) + \Delta w_{ij}(t)$ 



 $https://github.com/cs231n/cs231n.github.io/blob/master/assets/\overline{n}n3/nestero\overline{v}.jpeg = - \mathfrak{O} \land \mathfrak{O} \circ \mathfrak{O} \land \mathfrak$ 

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# Momentum vs. Nesterov Momentum - Summary

## **Classical Momentum:**

- Reacts after the update
- Simpler to implement

### **Nesterov Momentum:**

- Looks ahead computes gradient before the update
- Better convergence in practice

In Keras: both variants available in SGD

optimizer = SGD(learning\_rate=0.01, momentum=0.9, nesterov=True)

https://keras.io/api/optimizers/sgd/

# Setting Learning Parameters

### • Learning rate $\alpha$

- $\bullet\,$  Small  $\alpha \to$  slow learning, risk of getting stuck in local minima
- $\bullet\,$  Large  $\alpha \to {\rm fast}$  learning, but risk of oscillations and instability

### • Momentum $\alpha_m$

- Helps overcome flat areas, stabilizes learning in steep regions
- $\bullet~$  Too large  $\rightarrow~$  may overshoot the minimum
- Typical values:  $0.8 \le \alpha_m \le 0.95$

## • Use Nesterov Momentum?

- Yes, when: the model is deep or the error surface is complex
- Useful when standard momentum leads to oscillations or slowdowns
- Often a good default choice in modern frameworks

Challenge: Proper parameter tuning is difficult and task-dependent Solution: Adaptive learning rate methods

# Adaptive Learning Rate Control

• Various strategies exist — from simple heuristics to sophisticated methods

## Primitive Heuristic (already discussed):

- The learning rate should decrease as the number of epochs increases
- Initial learning rate:  $0 \ll \alpha < 1$ 
  - Helps escape shallow local minima
  - Enables rapid early learning
- Final learning rate:  $\alpha \sim 0$ 
  - Prevents oscillations
  - Should not decrease too quickly; it is sufficient to ensure:  $\sum_{t=0}^{\infty} \alpha_t = \infty$ ,  $\sum_{t=0}^{\infty} \alpha_t^2 < \infty$

Adaptive Learning Rate

#### Local learning rate for each weight

• Weight update from neuron i to neuron j at time t + 1:

$$\Delta w_{ij}(t+1) = -\alpha_{ij,t+1} \frac{\partial E_t}{\partial w_{ij}} + \alpha_m \Delta w_{ij}(t)$$

# Resilient Propagation (Rprop) - Silva & Almeida

# Learning rule based on the sign change of the partial derivative:

- Initialize  $\alpha_{ij,0}$  with small random values
- Accelerate learning if the sign of  $\frac{\partial E}{\partial w_{ij}}$  remains the same for two consecutive iterations
- Slow down learning if the sign changes

## Variants:

- Basic Rprop (Silva & Almeida)
- Super SAB
- Rprop+

• ...

# Resilient Propagation (Rprop) - Silva & Almeida

### Learning rate adaptation at time (t + 1)

•  $\alpha_{ij,t+1} = u \cdot \alpha_{ij,t}$ , if  $\frac{\partial E_t}{\partial w_{ij}} \cdot \frac{\partial E_{t-1}}{\partial w_{ij}} > 0$ 

• 
$$\alpha_{ij,t+1} = d \cdot \alpha_{ij,t}$$
, if  $\frac{\partial E_t}{\partial w_{ij}} \cdot \frac{\partial E_{t-1}}{\partial w_{ij}} < 0$ 

• Constants: 
$$u > 1$$
,  $d < 1$ 

### Problems:

Learning rate grows or shrinks exponentially due to *u* and *d* → Issues may arise if many consecutive accelerations occur

# Resilient Propagation (Rprop) - Super SAB

## Algorithm:

- Initialize all  $\alpha_{ij}^0$  to a starting value  $\alpha_{\text{start}}$
- Perform step t of the backpropagation algorithm with momentum

• If 
$$\frac{\partial E_t}{\partial w_{ij}} \cdot \frac{\partial E_{t-1}}{\partial w_{ij}} > 0$$
:  $\alpha_{ij,t+1} = u \cdot \alpha_{ij,t}$ 

• If 
$$\frac{\partial E_t}{\partial w_{ij}} \cdot \frac{\partial E_{t-1}}{\partial w_{ij}} < 0$$
:

- Cancel previous weight update:  $w_{ij}(t+1) = w_{ij}(t) \Delta w_{ij}(t)$
- Decrease learning rate:  $\alpha_{ij,t+1} = d \cdot \alpha_{ij,t}$

## **Properties:**

- Orders of magnitude faster than standard backpropagation
- Relatively stable
- Robust to choice of initial parameters

# Resilient Propagation (Rprop+)

- Learning rate is adjusted based on changes in the error value, rather than the sign of the gradient
- Faster than Super SAB

## Algorithm:

- Initialize all  $\alpha_{ii}^0$  to a starting value  $\alpha_{\text{start}}$
- Perform step *t* of the backpropagation algorithm with momentum
- If  $E_t < E_{t-1}$ :
  - Increase learning rate:  $\alpha_{ij,t+1} = u \cdot \alpha_{ij,t}$
- If  $E_t > c \cdot E_{t-1}$ :
  - Cancel previous weight update:  $w_{ij}(t+1) = w_{ij}(t) \Delta w_{ij}(t)$
  - Decrease learning rate:  $\alpha_{ij,t+1} = \mathbf{d} \cdot \alpha_{ij,t}$
- Constants c > 1, u > 1, d < 1

# Modern Optimization Algorithms

## Foundation:

• SGD (Stochastic Gradient Descent) – the basic algorithm, improved using momentum (Momentum / Nesterov Momentum)

## Modern optimizers in libraries like Keras and PyTorch:

- RMSprop adaptive learning rate, suitable especially for recurrent models (RNNs)
- Adam (Adaptive Moment Estimation) currently the most widely used
- NAdam Adam combined with Nesterov momentum
- and many others (AdaGrad, Adadelta, AdaMax, FTRL, ...)
- Typical advantages of modern optimizers
  - faster convergence thanks to adaptive learning rates
  - lower sensitivity to hyperparameter settings

https://keras.io/api/optimizers/

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# RMSprop – Root Mean Square Propagation

## Key Idea:

- The error surface may have various steep and flat regions in different directions (flat vs steep vs bumpy surface)
- We don't want to use the same learning step in all directions
- RMSprop adjusts the step size for each weight individually, depending on how much the gradient varies in that direction
- It acts as an adaptive shock absorber for rough terrains

## How does it work?

• It tracks an exponential moving average of squared gradients for each weight:

$$v_{ij}(t) = \beta \cdot v_{ij}(t-1) + (1-\beta) \cdot \left(\frac{\partial E_t}{\partial w_{ij}}\right)^2$$

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# RMSprop – Root Mean Square Propagation

### How does it work?

• It tracks an exponential moving average of squared gradients:

$$m{v}_{ij}(t) = eta \cdot m{v}_{ij}(t-1) + (1-eta) \cdot \left(rac{\partial E_t}{\partial w_{ij}}
ight)^2$$

- If gradients are frequently large  $\rightarrow$  step size is reduced (slower learning)
- If gradients are small  $\rightarrow$  step size remains larger (faster learning)

Weight update:

$$\Delta w_{ij}(t) = -\frac{\alpha}{\sqrt{v_{ij}(t)} + \varepsilon} \cdot \frac{\partial E_t}{\partial w_{ij}}$$

$$w_{ij}(t+1) = w_{ij}(t) + \Delta w_{ij}(t)$$

# RMSprop – Root Mean Square Propagation

## Result:

- More stable learning, especially in networks with gradients of varying scale (e.g., RNNs)
- $\bullet\,$  Less dependent on manual tuning of the learning rate  $\alpha$

## Use Cases:

- Commonly used for recurrent neural networks (RNNs)
- Handles non-stationary gradients well

# Adam – Adaptive Moment Estimation

## Principle:

- Combines the benefits of momentum (1st moment) and RMSprop (2nd moment)
- Estimates the mean and variance of gradients using exponential moving averages
- Tracks:
  - $m_{ij}(t)$  moving average of gradients (1st moment estimate)
  - v<sub>ij</sub>(t) moving average of squared gradients (2nd moment estimate)
- Includes bias correction to account for initialization effects

## Adam – Adaptive Moment Estimation

### Weight update:

$$\Delta w_{ij}(t) = -lpha \cdot rac{\hat{m}_{ij}(t)}{\sqrt{\hat{v}_{ij}(t)} + arepsilon} \qquad w_{ij}(t+1) = w_{ij}(t) + \Delta w_{ij}(t)$$

#### Where:

$$g_{ij}(t) = \frac{\partial E_t}{\partial w_{ij}}$$

$$m_{ij}(t) = \beta_1 \cdot m_{ij}(t-1) + (1-\beta_1) \cdot g_{ij}(t)$$

$$v_{ij}(t) = \beta_2 \cdot v_{ij}(t-1) + (1-\beta_2) \cdot g_{ij}^2(t)$$

$$\hat{m}_{ij}(t) = \frac{m_{ij}(t)}{1-\beta_1^t}, \quad \hat{v}_{ij}(t) = \frac{v_{ij}(t)}{1-\beta_2^t}$$

Typical values:  $\alpha = 0.001$ ,  $\beta_1 = 0.9$ ,  $\beta_2 = 0.999$ ,  $\varepsilon = 10^{-7}$ 

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# Adam – Adaptive Moment Estimation

- General-purpose, reliable optimizer works well in most scenarios without much parameter tuning
- Combines the benefits of:
  - Momentum smoother, more stable weight updates
  - Adaptive step size like RMSprop
- Default choice in frameworks like Keras and PyTorch
- For some tasks (e.g., convex loss surfaces), it may lead to suboptimal solutions

 $\rightarrow$  in such cases, SGD or RMSprop may perform better

Keras:

optimizer = Adam( learning\_rate=0.001, beta\_1=0.9, beta\_2=0.999, epsilon=1e-7)

## Nadam – Nesterov-accelerated Adam

## Combines the benefits of:

- Adam (adaptive learning + momentum)
- Nesterov momentum (lookahead gradient evaluation)

## Effect:

- Faster and more stable convergence compared to standard Adam
- Suitable for deep networks and complex learning problems

# Summary of Modern Optimizers

Optimizer	Advantages	When to Use
SGD	simple, transparent	small models,
		manual tuning
SGD+Moment.	faster convergence	deeper networks
RMSprop	adaptive step size, stable	RNNs, sequential data
Adam	robust, minimal tuning	universal default
Nadam	even more stable	deep and complex
		models

Neural Networks 1 - Multilayer neural networks Learning Speed and Approximation Capabilities Other Tricks to Improve Learning

# Other Tricks to Improve Learning

### Run training multiple times

- Use different random weight initializations and select the best-performing model
- If the network fails to converge or converges very slowly
  - Try adding more neurons or layers
- Present important training examples more frequently
  - Helps reduce error for critical patterns

Neural Networks 1 - Multilayer neural networks Learning Speed and Approximation Capabilities Other Tricks to Improve Learning

## Other Tricks to Improve Learning

### "Network annealing" = injecting random noise

- Use when weights and biases settle but the error remains high
- Adapt weight from neuron *i* to *j*:

$$w_{ij}(t+1) = w_{ij}(t) + N(0,\epsilon)$$

- Choose  $\epsilon$  carefully:
  - $\bullet \ \ \mathsf{Too} \ \mathsf{small} \to \mathsf{ineffective}$
  - $\bullet\,$  Too large  $\to\,$  network may require full retraining

Neural Networks 1 - Multilayer neural networks Practical Examples of Different Task Types

## Practical Examples of Different Task Types

- Binary classification: Breast Cancer (already covered)
- Multiclass classification: MNIST
- Regression task: Wine Quality
- Time series prediction: Daily minimum temperatures in Melbourne

# Binary Classification Example: Breast Cancer

• Already covered last time

Model setup:

- Sigmoid activation in the output layer
- ReLU (or tanh) activation in hidden layers
- Loss function: **BinaryCrossentropy**; Metrics: **Accuracy**, **Precision**, **Recall**, ...

Neural Networks 1 - Multilayer neural networks Practical Examples of Different Task Types Multiclass Classification

# Multiclass Classification Example: MNIST

- 60,000 grayscale images of handwritten digits (28x28 pixels)
- Centered images, uniform digit size
- 10,000 test images written by different people
- Output label: digit 0–9 (10 classes)
- Data characteristics:
  - $\bullet\,$  All images have the same size  $\rightarrow\,$  no resizing needed
  - Input data is 3D  $\rightarrow$  needs to be flattened into vectors (vectorized)
  - Pixel values range from 0 to 255  $\rightarrow$  need to normalize to [0,1] or [-1,1]

Neural Networks 1 - Multilayer neural networks Practical Examples of Different Task Types Multiclass Classification

# Multiclass Classification Example: MNIST

#### Model setup:

- Softmax activation in the output layer
- ReLU (or tanh) activation in hidden layers
- Loss function: SparseCategoricalCrossentropy with SparseCategoricalAccuracy (if labels are integers)
- Or: CategoricalCrossentropy with CategoricalAccuracy (if labels are one-hot vectors)

#### **Observations:**

- $\bullet\,$  Test accuracy is typically around 85  $\%\,$
- $\bullet\,$  Similar training and validation errors  $\rightarrow$  model generalizes well
- Accuracy can be improved by increasing the learning rate, number of epochs, or changing the optimizer

# Regression Example: Wine Quality Data

- 11 numerical input features (e.g., acidity, alcohol content, sulfur dioxide, ...)
- 1 output feature wine quality (rating from 0–10, most values 3–8)

#### Data characteristics:

- Features have different value ranges  $\rightarrow$  normalization required (e.g., using StandardScaler)
- Sufficient number of samples ( 4900)
  - Allows training of larger models without immediate risk of overfitting
  - 2 Dataset can be split into training, validation, and test sets

### Regression Example: Wine Quality Data

#### Model setup for regression:

- ReLU (or tanh) activation in hidden layers
- Linear (identity) activation in the output layer
- Loss function: MeanSquaredError (MSE)
- Metrics: MeanAbsoluteError (MAE), RootMeanSquaredError (RMSE)

# Regression Example: Wine Quality Data

#### **Observations:**

- The model learns better for values in the center of the range than for the edges (due to data imbalance)  $\rightarrow$  possible solution: oversampling
- Without early stopping, overfitting may occur (especially with larger architectures)
- Performance is sensitive to normalization of input features

#### Summary:

- For regression tasks, use a linear output and MSE as the loss function.
- Normalize input features with varying ranges to improve model training.
- In addition to MSE, consider using MAE or RMSE for better interpretability.

### Alternative Approach: Wine Quality as Classification

**Same dataset, different perspective:** Predicting wine quality as a classification task instead of regression.

- Convert quality (0–10) into classes, e.g.:
  - 0–4: low quality
  - 5–6: medium quality
  - 7-10: high quality

**Question:** If we switch from a regression model to a classification model, what changes?

• Output layer, loss function, and evaluation metrics

# Alternative Approach: Wine Quality as Classification

#### Model setup for classification:

- Output layer: 3 neurons with softmax activation
- Loss function: categorical\_crossentropy or sparse\_categorical\_crossentropy (if using class indices)
- Metrics: accuracy, possibly precision, recall, F1-score

Note:

 $\bullet$  Class distribution is imbalanced  $\rightarrow$  track multiple metrics, not just accuracy

Classification vs. Regression – which makes more sense for this task?

• Consider the application and interpretability when choosing the approach

# Time Series Example: Daily Minimum Temperatures

- Dataset: Daily minimum temperatures in Melbourne, years 1981–1990
- Goal: predict the temperature of the next day based on previous values

#### Data characteristics:

- Single feature (temperature time series)
- Over 3600 records sufficient for training and testing
- Data points are not independent temporal dependencies must be captured

#### Using the Sliding Window Method:

- For each training sample, use e.g. the last 10 days to predict the next day
- This creates a tabular representation suitable even for MLP

# Daily Min. Temperatures - Model and Configuration

#### Input preparation:

- Create training, validation, and test sets using sliding windows (with separate time period for each set!)
- Normalize input values (e.g., MinMaxScaler)

#### Model configuration:

- Input layer: number of neurons = window size (e.g., 10)
- Hidden layers with ReLU or tanh activation
- Output layer with linear activation (1 value = temperature prediction)
- Loss function: MSE; Metrics: MSE / MAE / RMSE

#### **Observations:**

- The MLP needs tuning to outperform a baseline model
- The choice of window size significantly affects prediction quality
- The model can overfit if the architecture is too complex.

# Summary: Time Series and Sliding Window Method

- Time series do not consist of independent samples training, validation, and test sets must preserve temporal order.
- The sliding window method allows transformation of a time series into a training set for MLP.
- Window size (number of input values) is an important hyperparameter.
- **④** Use a linear output function, just like in regression.
- Although specialized architectures (RNNs, LSTMs) perform better on time series, an MLP with sliding window is a simple and intuitive starting point.

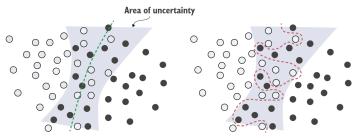
# Summary: Time Series and Sliding Window Method

#### Possible extensions:

- Model input can include not only past values of the target variable, but also other features (e.g., pressure, humidity, etc.)
- Instead of predicting just one future value, you can predict a longer time horizon or multiple future values

### Generalization of Neural Networks

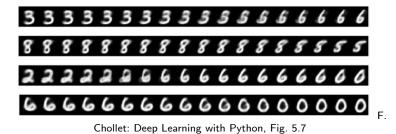
- The ability to produce correct outputs for inputs not seen during training
- Illustration: well-trained model vs. overfitted model



F. Chollet: Deep Learning with Python, Fig. 5.5

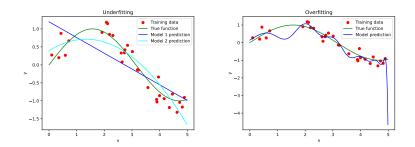
### Generalization of Neural Networks

• Class boundaries are often hard to define:



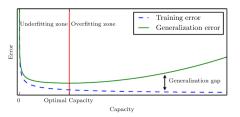
### Underfitting vs. Overfitting - Regression Example

• Typical illustration of underfitting and overfitting in regression tasks:



### Generalization and Model Capacity

- Generalization depends on the network's architecture and model capacity (i.e., number of parameters)
- Small model:
  - Potentially stable but inaccurate predictions
  - Risk of underfitting
- Large model:
  - Greater variability in performance
  - Risk of overfitting poor generalization



https://www.deeplearningbook.org/, Figure 5.3  $\rightarrow$  4  $\equiv$   $\rightarrow$  4 =  $\rightarrow$  1 =  $\rightarrow$  1 =

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### Model Capacity and Dataset Size

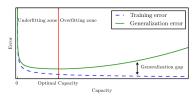
• The required training set size depends on model capacity

#### Small model:

- Stable but potentially underfit
- Needs fewer training samples to generalize well

#### Large model:

- Risk of overfitting
- Requires more training data to generalize properly



 $https://www.deeplearningbook.org/, \ Figure \ 5.3$ 

### Theoretical Insight: Generalization and Training Set Size

# Theorem: Relationship between model capacity and required number of training examples

 For a network with one hidden layer, w parameters, h hidden units, and generalization error ε, the minimum number of training samples N should satisfy:

$$\mathsf{N} \geq rac{\mathsf{w}}{\epsilon} \log_2(rac{h}{\epsilon})$$

 $\rightarrow$  If  $N < \frac{w}{\epsilon}$ , the model cannot generalize properly

• For target accuracy  $\geq$  90%, choose at least  $10 \cdot w$  training samples

### Generalization in Deep Networks

Estimated training set size for deeper architectures:

$$\mathsf{N} \ge O\left(rac{w \cdot \log w}{\epsilon}
ight)$$

- $\bullet~\mbox{More}$  layers  $\rightarrow~\mbox{more}$  parameters  $\rightarrow~\mbox{more}$  data needed
- Empirical rule: Often we need significantly more training samples than parameters
- To achieve good generalization:
  - Use a sufficiently large training set, or
  - Apply suitable regularization techniques