

Deep Learning on Supercomputers

An introduction

Fahad Khalid [f.khalid@fz-juelich.de]. Simulation Laboratory Neuroscience, Jülich Supercomputing Centre

November 29, 2019 | Introduction to the Programming and Usage of Supercomputing resources at Jülich

Agenda

1. Concepts: Fundamentals
 - i. Supervised learning
 - ii. Artificial Neural Networks
 - iii. Error backpropagation
2. Code examples: Training with one GPU
 - i. Handwritten digit recognition
 - ii. The MNIST dataset
 - iii. Implementation with `tf.keras`
3. Concepts: Distributed training
 - i. Why use distributed training?
 - ii. Model parallelism
 - iii. Data parallelism
 - iv. Gradient aggregation
4. Pit stop: Parallel computing
 - i. Shared memory vs. Distributed memory
 - ii. The hpc4neuro Python library
5. Back to distributed training: Examples
 - i. MNIST classification: Epoch distributed
 - ii. Handling custom data
 - iii. Distributing training data
6. The “Deep Learning on Supercomputers” tutorial
 - i. Introduction
 - ii. Running code samples on JUWELS
 - iii. Job configuration
7. Conclusion

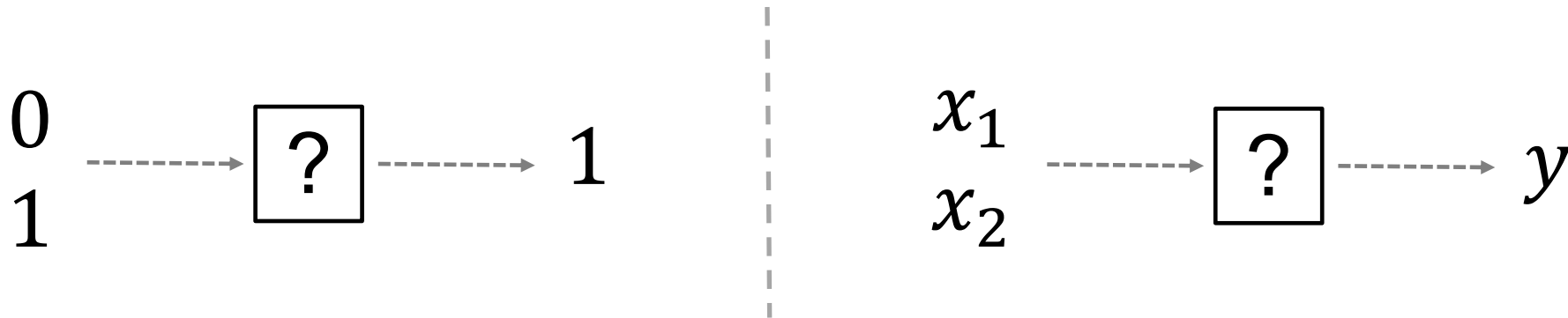
Agenda

1. Concepts: Fundamentals
 - i. Supervised learning
 - ii. Artificial Neural Networks
 - iii. Error backpropagation
2. Code examples: Training with one GPU
 - i. Handwritten digit recognition
 - ii. The MNIST dataset
 - iii. Implementation with `tf.keras`
3. Concepts: Distributed training
 - i. Why use distributed training?
 - ii. Model parallelism
 - iii. Data parallelism
 - iv. Gradient aggregation
4. Pit stop: Parallel computing
 - i. Shared memory vs. Distributed memory
 - ii. The hpc4neuro Python library
5. Back to distributed training: Examples
 - i. MNIST classification: Epoch distributed
 - ii. Handling custom data
 - iii. Distributing training data
6. The “Deep Learning on Supercomputers” tutorial
 - i. Introduction
 - ii. Running code samples on JUWELS
 - iii. Job configuration
7. Conclusion

Concepts

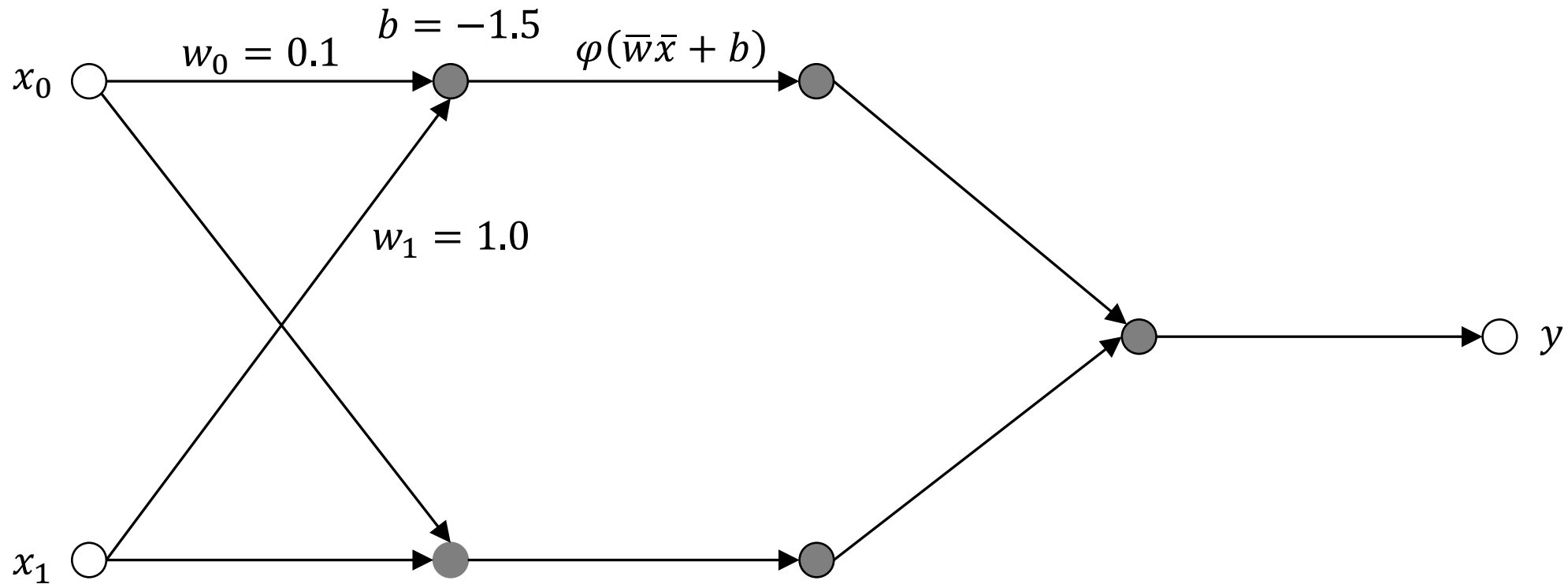
Supervised learning (1)

x_1	x_2	y
0	0	0
0	1	1
1	0	1
1	1	0



Concepts

Artificial Neural Networks

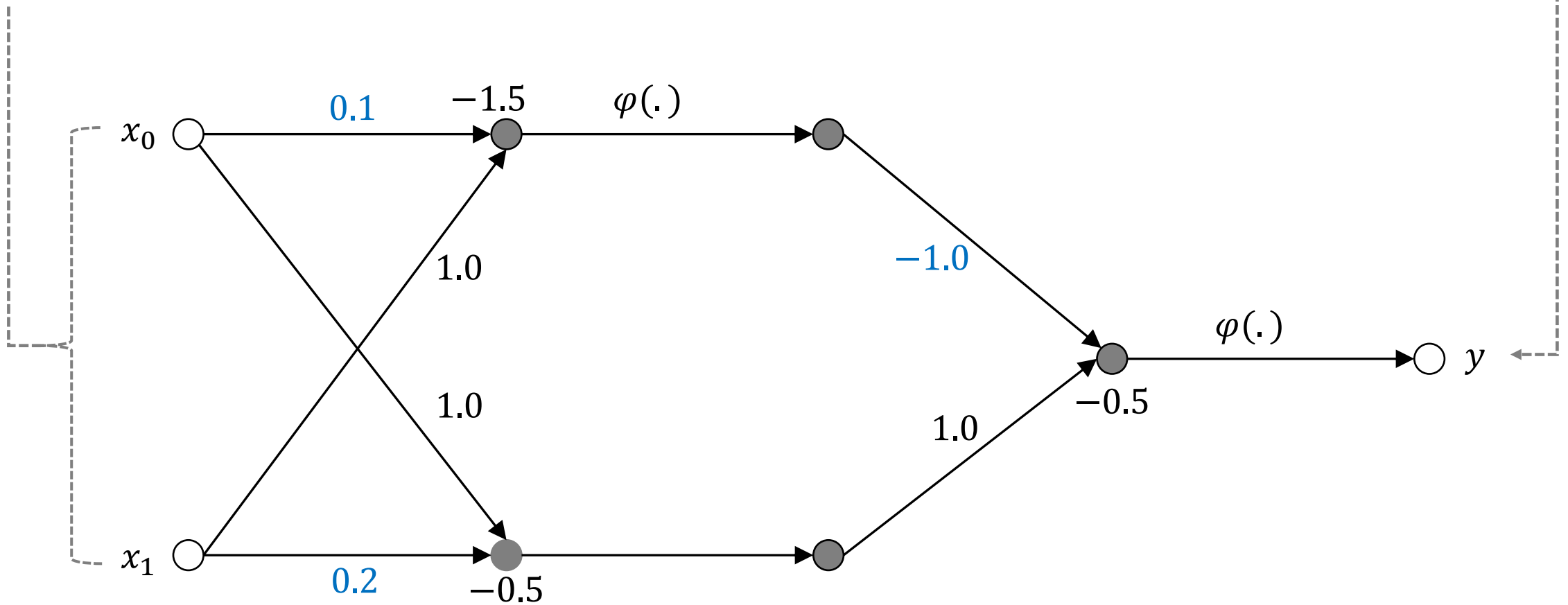


Concepts

Instance
 $\{(x_0, x_1), \hat{y}\}$

Error backpropagation (1)

Error
 $\hat{y} - y$

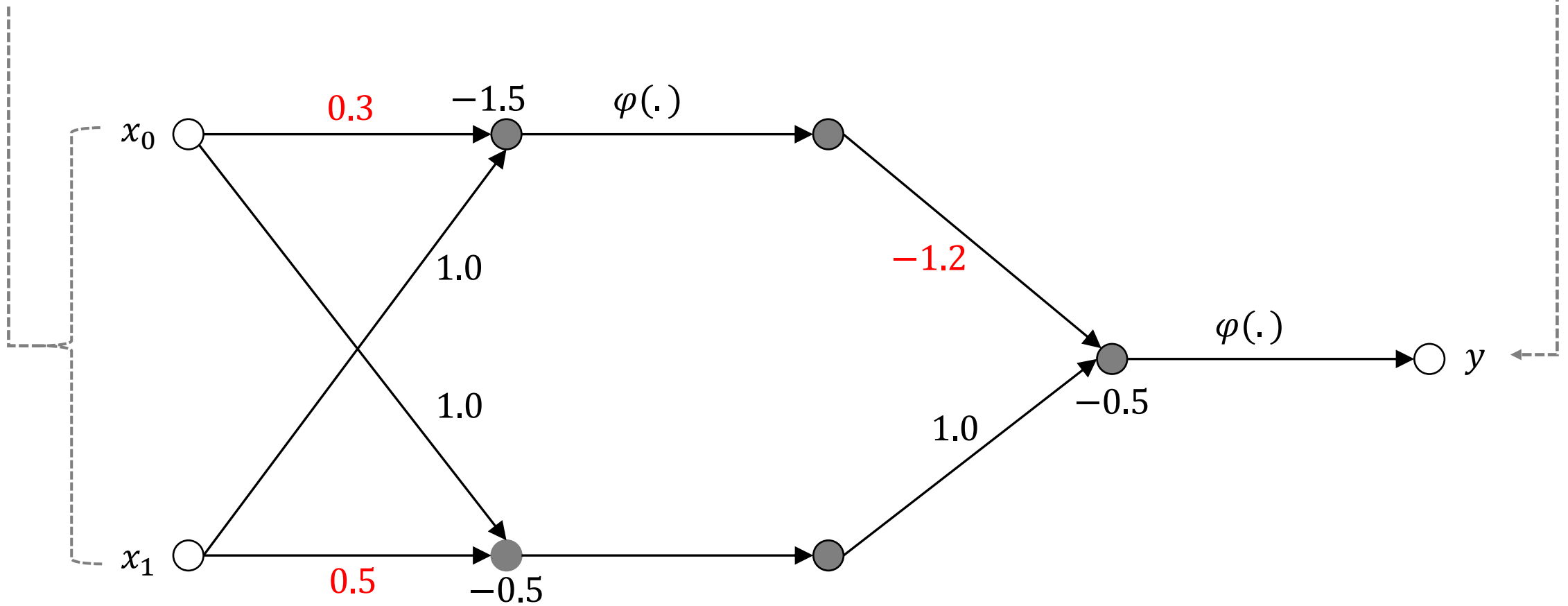


Concepts

Instance
 $\{(x_0, x_1), \hat{y}\}$

Error backpropagation (2)

Error
 $\hat{y} - y$

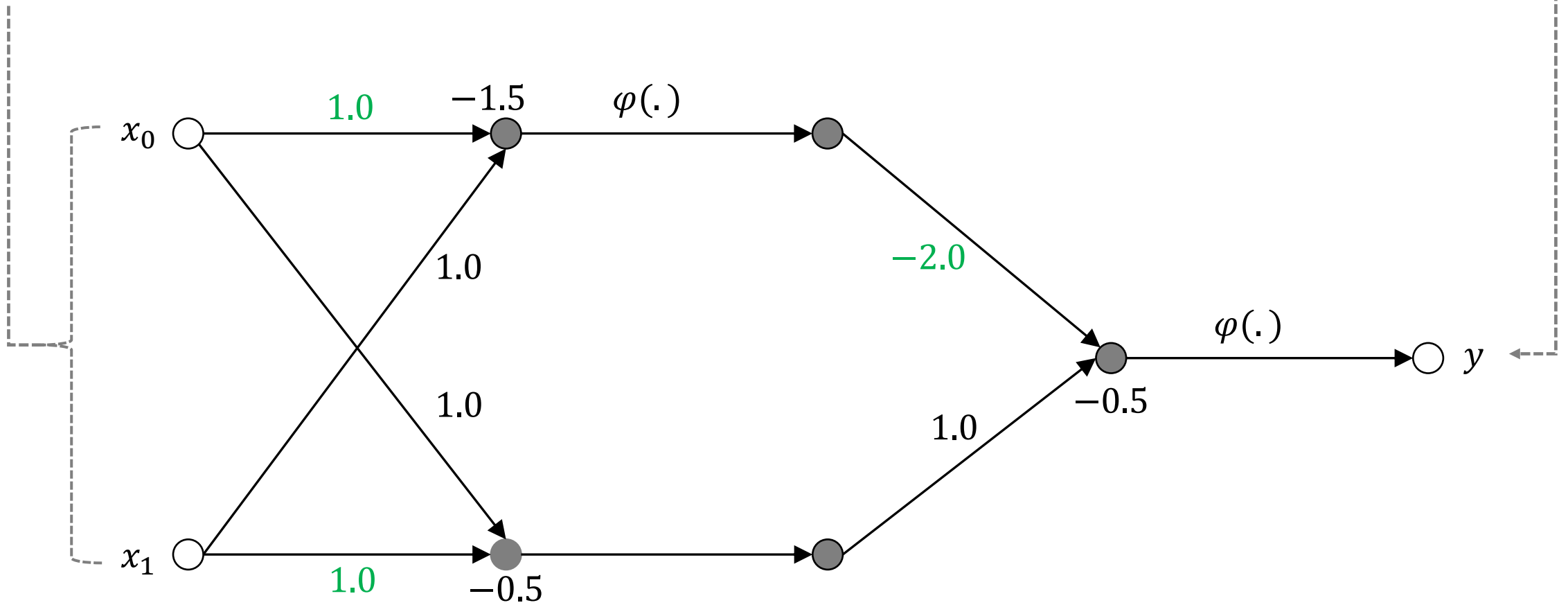


Concepts

Instance
 $\{(x_0, x_1), y\}$

Error backpropagation (3)

Error
 $\hat{y} - y$

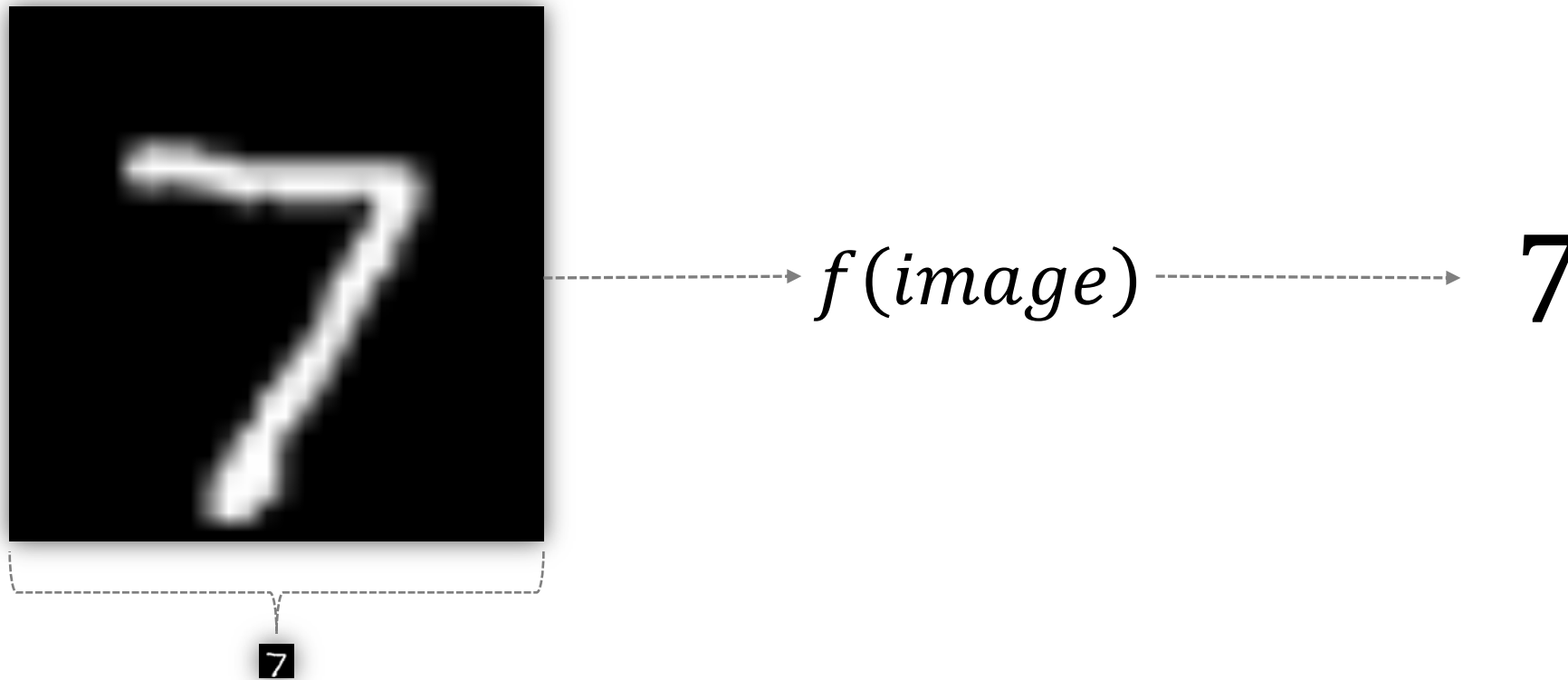


Agenda

1. Concepts: Fundamentals
 - i. Supervised learning
 - ii. Artificial Neural Networks
 - iii. Error backpropagation
2. Code examples: Training with one GPU
 - i. Handwritten digit recognition
 - ii. The MNIST dataset
 - iii. Implementation with `tf.keras`
3. Concepts: Distributed training
 - i. Why use distributed training?
 - ii. Model parallelism
 - iii. Data parallelism
 - iv. Gradient aggregation
4. Pit stop: Parallel computing
 - i. Shared memory vs. Distributed memory
 - ii. The hpc4neuro Python library
5. Back to distributed training: Examples
 - i. MNIST classification: Epoch distributed
 - ii. Handling custom data
 - iii. Distributing training data
6. The “Deep Learning on Supercomputers” tutorial
 - i. Introduction
 - ii. Running code samples on JUWELS
 - iii. Job configuration
7. Conclusion

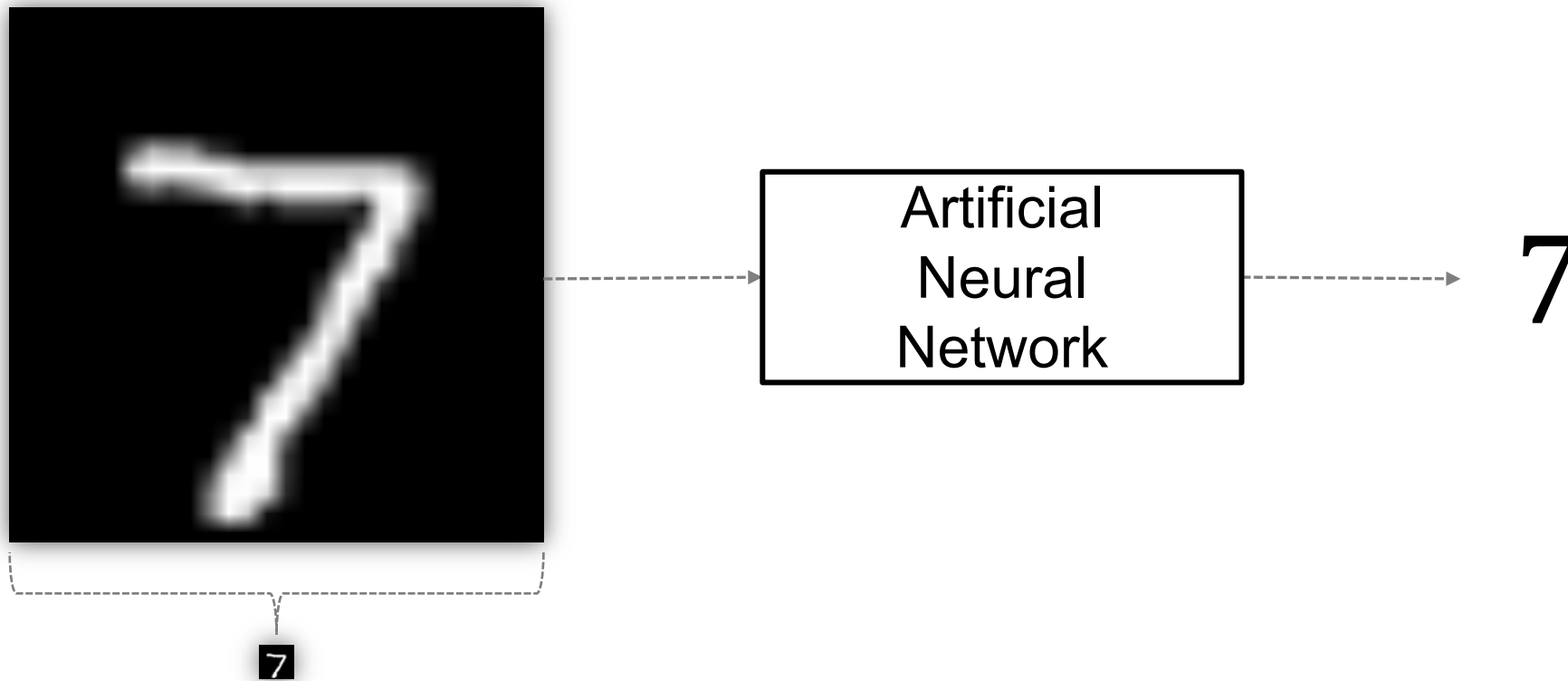
Examples

Handwritten digit recognition



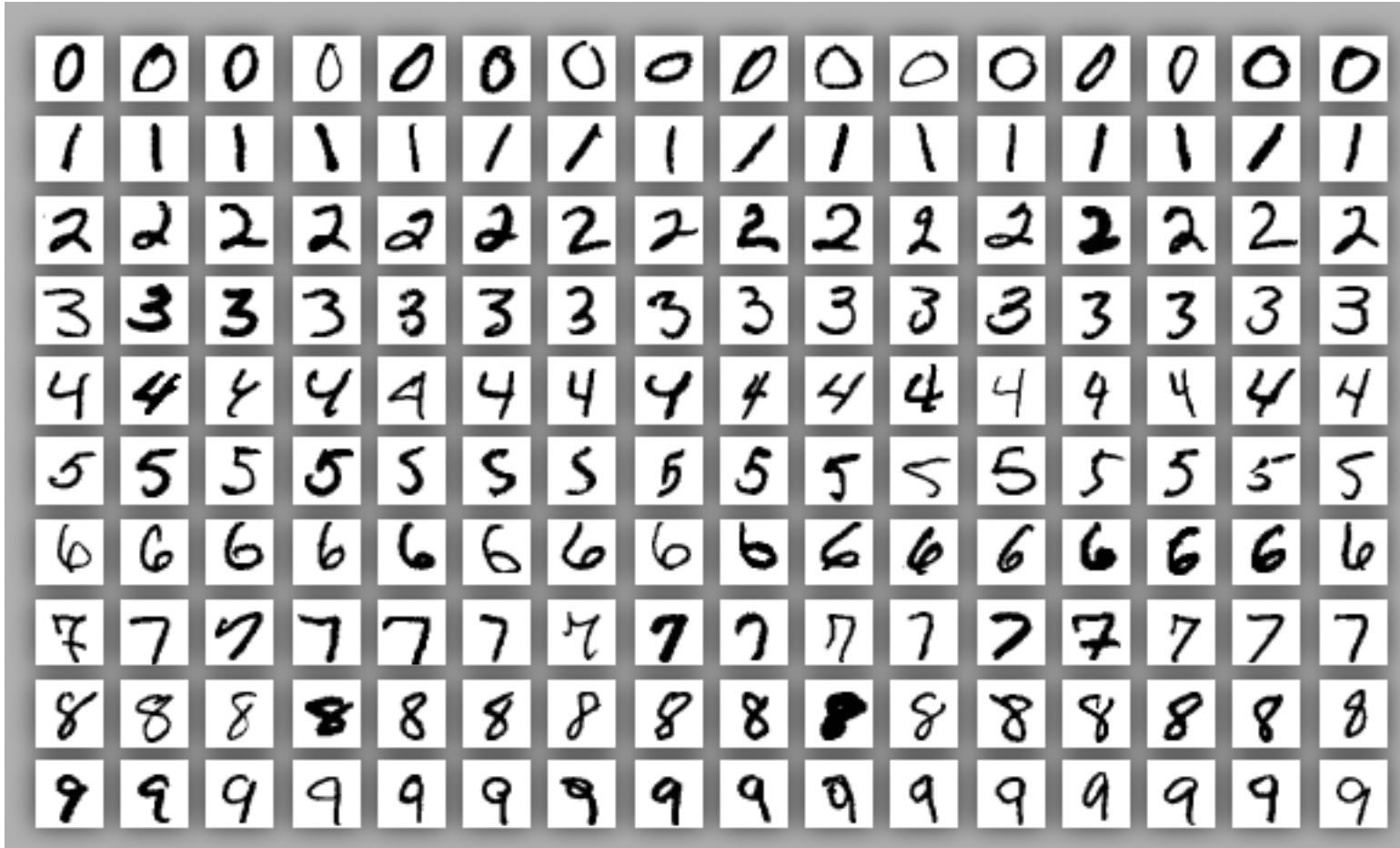
Examples

Handwritten digit recognition



Examples

Modified National Institute of Standards and Technology (MNIST) database

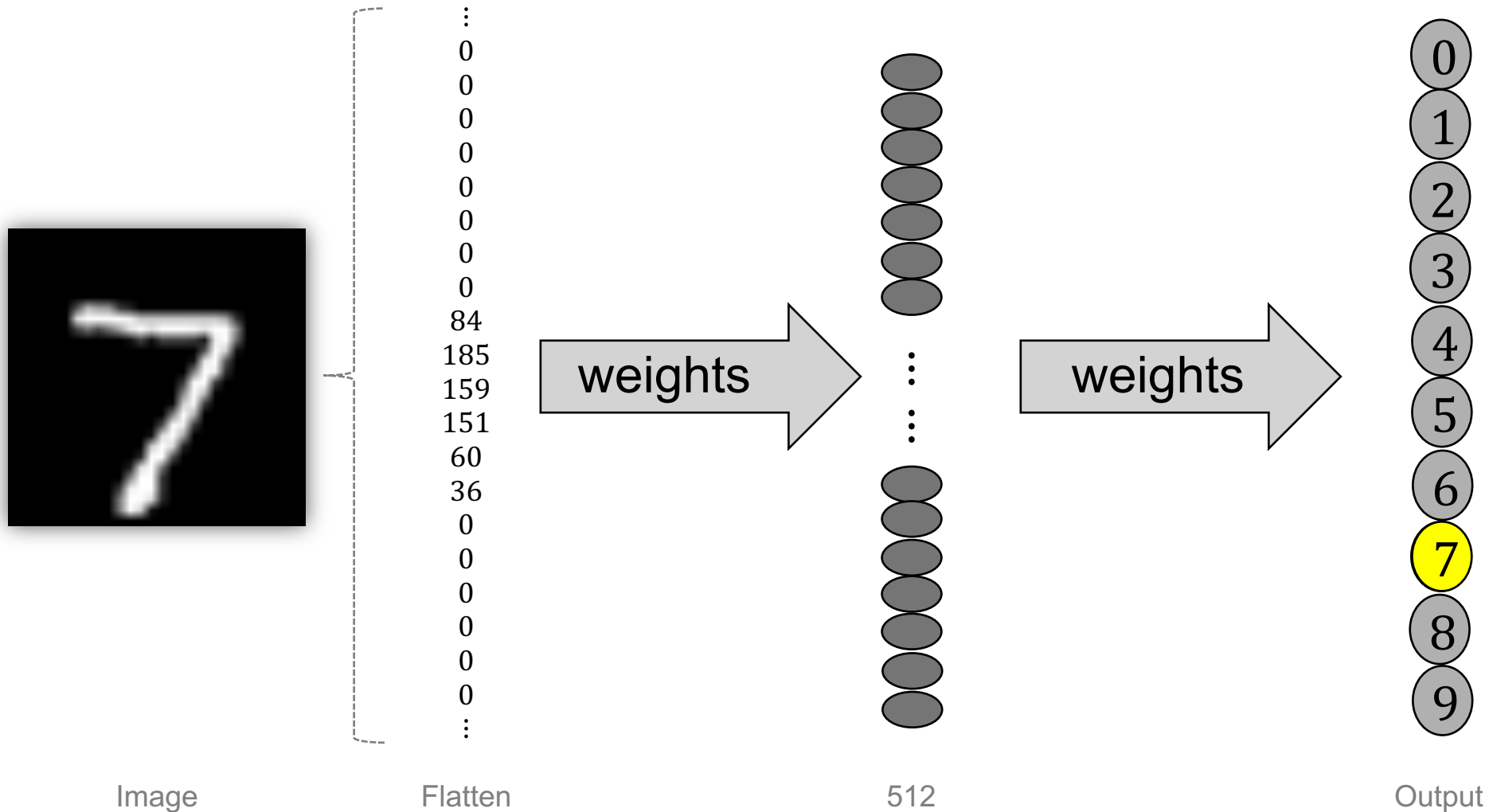


- Image dimensions: 28×28
- Each pixel $p \in [0, 255]$
- 60,000 training examples
- 10,000 test examples

Source: Modified version of [this](#). [License](#).

Examples

A basic network for classification



Examples

MNIST classification with `tf.keras`: Code

```
1. import tensorflow as tf
2. mnist = tf.keras.datasets.mnist
3. (x_train, y_train), (x_test, y_test) = mnist.load_data()
4. x_train, x_test = x_train / 255.0, x_test / 255.0
5. model = tf.keras.models.Sequential([
    tf.keras.layers.Flatten(),
    tf.keras.layers.Dense(512, activation=tf.nn.relu),
    tf.keras.layers.Dense(10, activation=tf.nn.softmax)
])
6. optimizer = tf.keras.optimizers.Adam()
7. epochs = 4
```

```
8. model.compile(
    optimizer=optimizer,
    loss='sparse_categorical_crossentropy',
    metrics=['accuracy']
)
9. model.fit(
    x=x_train,
    y=y_train,
    batch_size=32,
    epochs=epochs
)
```

`dl_on_supercomputers/course_material/examples/mnist_single_gpu.py`

Examples

MNIST classification with tf.keras: Output

```
$ python -u mnist_single_gpu.py
```

```
Epoch 1/4
```

```
60000/60000 [=====] - 8s 131us/sample - loss: 0.2006 - acc: 0.9404
```

```
Epoch 2/4
```

```
60000/60000 [=====] - 7s 120us/sample - loss: 0.0815 - acc: 0.9749
```

```
Epoch 3/4
```

```
60000/60000 [=====] - 7s 120us/sample - loss: 0.0548 - acc: 0.9831
```

```
Epoch 4/4
```

```
60000/60000 [=====] - 7s 119us/sample - loss: 0.0376 - acc: 0.9879
```

```
Test loss: 0.06436453427168308
```

```
Test accuracy: 0.9805
```

```
1. score = model.evaluate(x=x_test, y=y_test, verbose=0)
2. print(f'Test loss: {score[0]}')
3. print(f'Test accuracy: {score[1]}')
```

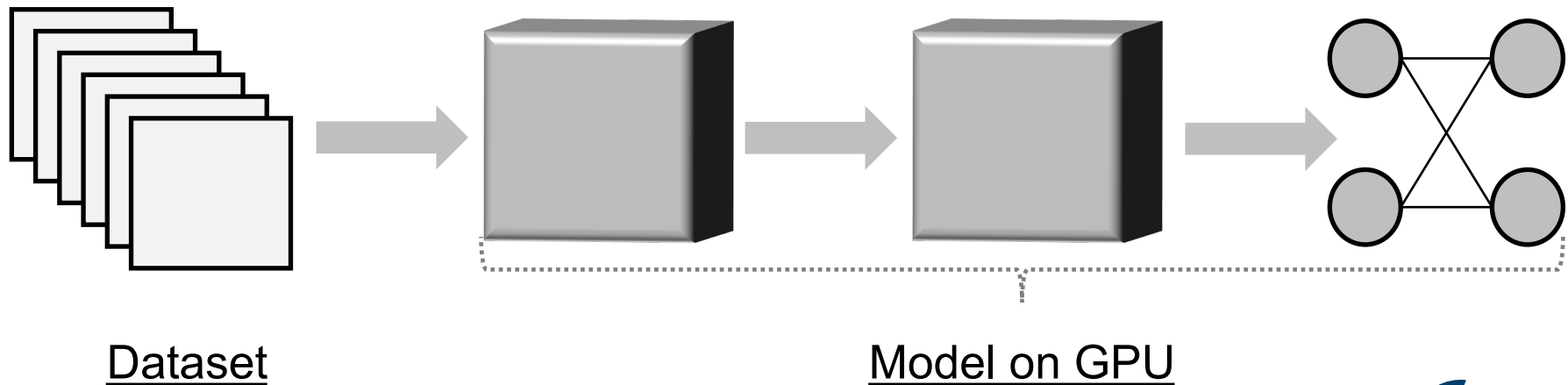
Agenda

1. Concepts: Fundamentals
 - i. Supervised learning
 - ii. Artificial Neural Networks
 - iii. Error backpropagation
2. Code examples: Training with one GPU
 - i. Handwritten digit recognition
 - ii. The MNIST dataset
 - iii. Implementation with `tf.keras`
3. Concepts: Distributed training
 - i. Why use distributed training?
 - ii. Model parallelism
 - iii. Data parallelism
 - iv. Gradient aggregation
4. Pit stop: Parallel computing
 - i. Shared memory vs. Distributed memory
 - ii. The hpc4neuro Python library
5. Back to distributed training: Examples
 - i. MNIST classification: Epoch distributed
 - ii. Handling custom data
 - iii. Distributing training data
6. The “Deep Learning on Supercomputers” tutorial
 - i. Introduction
 - ii. Running code samples on JUWELS
 - iii. Job configuration
7. Conclusion

Distributed training

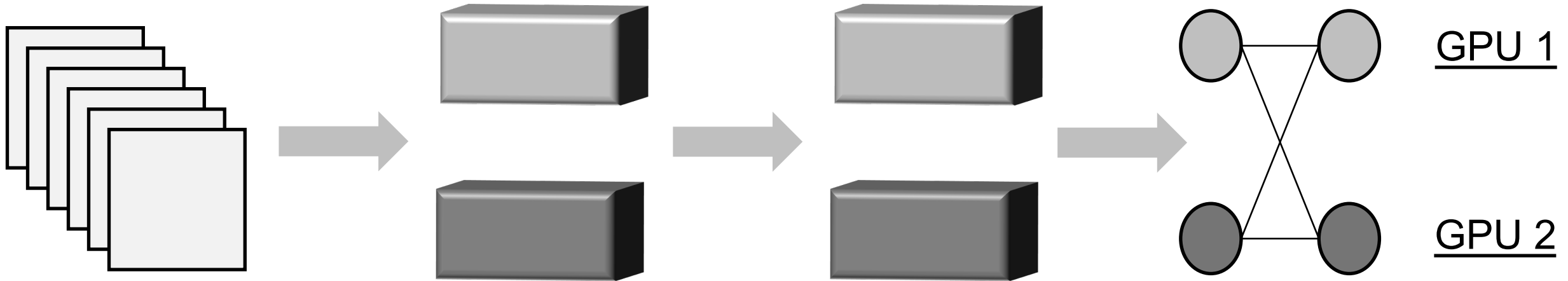
Motivation

1. Train faster
 - i. Large dataset size
 - a. Distribute epochs
 - b. Distribute training/validation data
 - ii. Compute intensive model
2. Increase the effective batch size
3. Use a dataset with very large instances
4. Use a very large model



Distributed training

Model Parallel

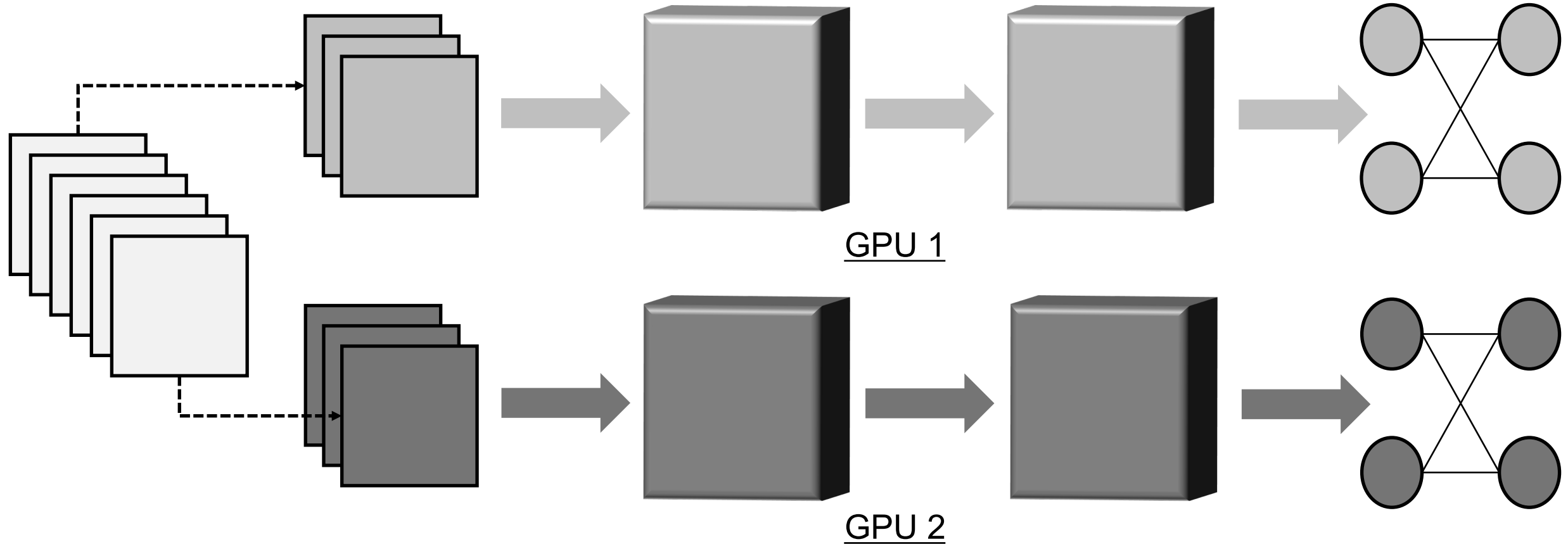


- Other methods
 - Layer Pipelining
 - Hybrid Parallelism

Ben-Nun, T., and Hoefler, T. Demystifying Parallel and Distributed Deep Learning: An In-Depth Concurrency Analysis. CoRR abs/1802.09941 (Feb. 2018)

Distributed training

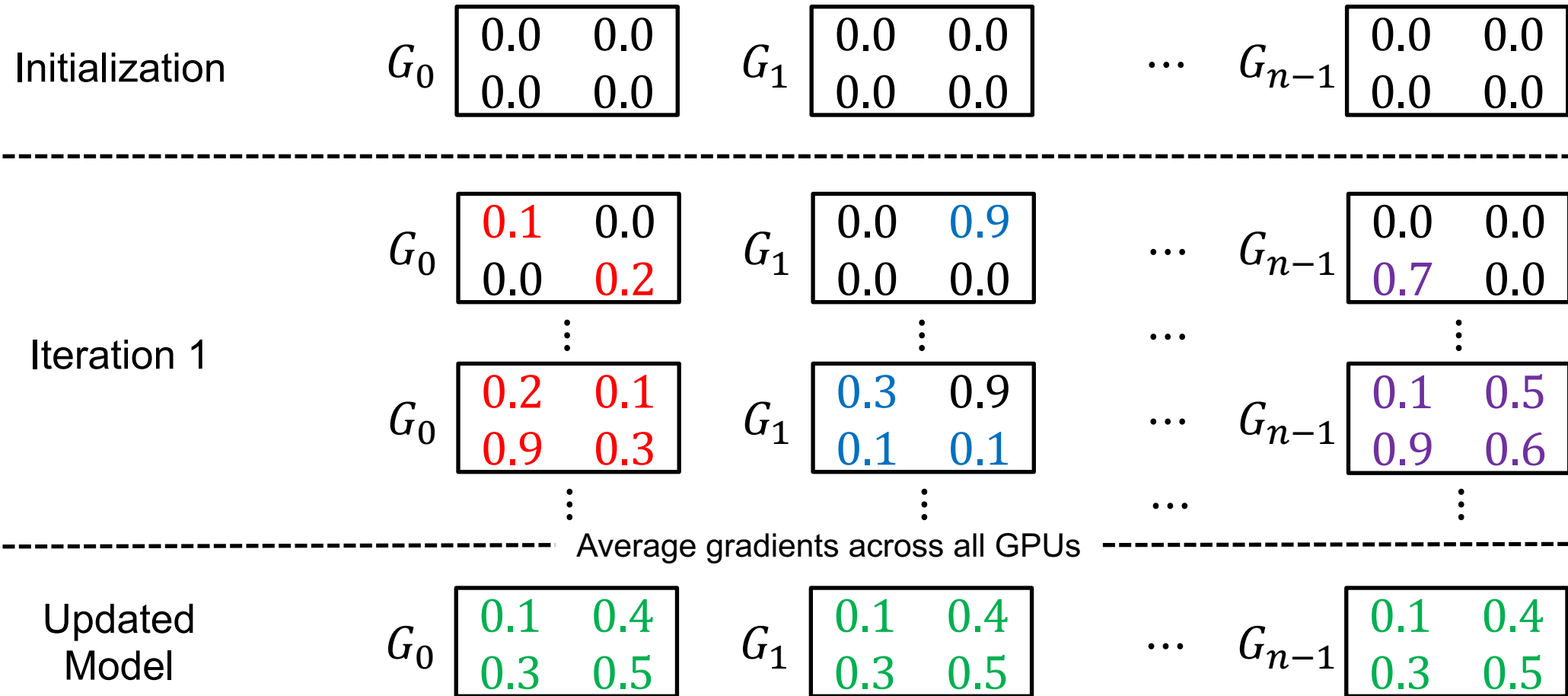
Data Parallel



Ben-Nun, T., and Hoefler, T. Demystifying Parallel and Distributed Deep Learning: An In-Depth Concurrency Analysis. CoRR abs/1802.09941 (Feb. 2018)

Distributed training

Gradient averaging in data parallel training

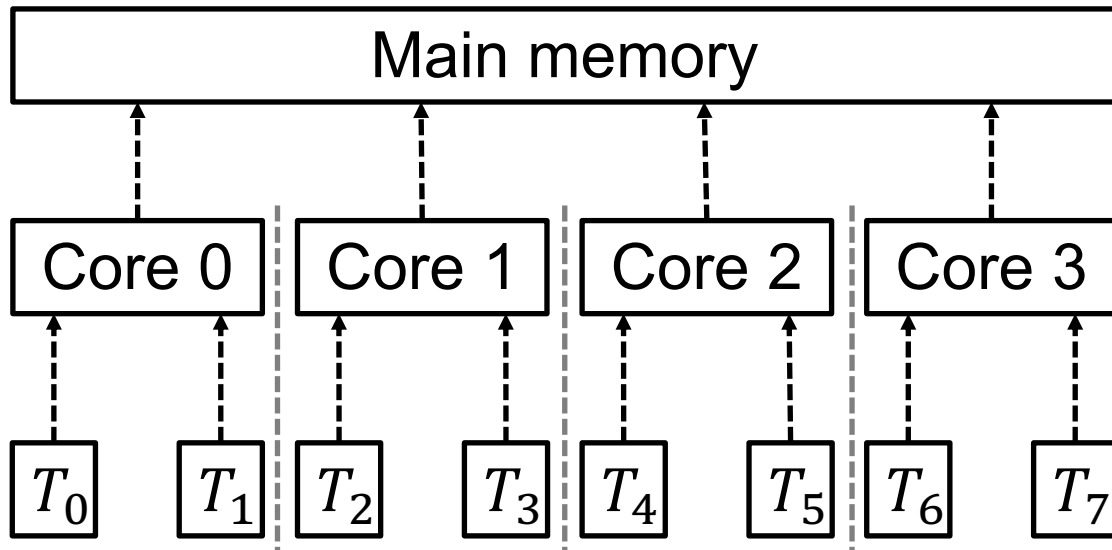


Agenda

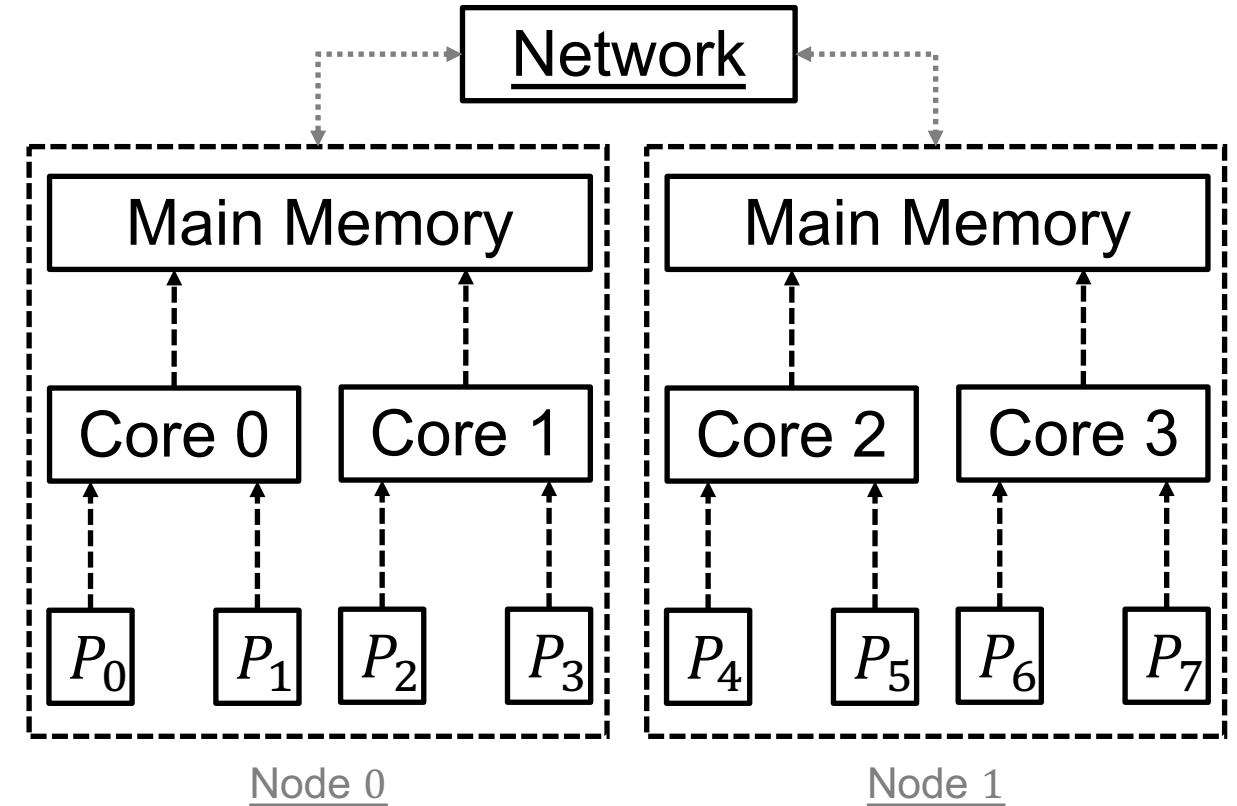
1. Concepts: Fundamentals
 - i. Supervised learning
 - ii. Artificial Neural Networks
 - iii. Error backpropagation
2. Code examples: Training with one GPU
 - i. Handwritten digit recognition
 - ii. The MNIST dataset
 - iii. Implementation with `tf.keras`
3. Concepts: Distributed training
 - i. Why use distributed training?
 - ii. Model parallelism
 - iii. Data parallelism
 - iv. Gradient aggregation
4. Pit stop: Parallel computing
 - i. Shared memory vs. Distributed memory
 - ii. The `hpc4neuro` Python library
5. Back to distributed training: Examples
 - i. MNIST classification: Epoch distributed
 - ii. Handling custom data
 - iii. Distributing training data
6. The “Deep Learning on Supercomputers” tutorial
 - i. Introduction
 - ii. Running code samples on JUWELS
 - iii. Job configuration
7. Conclusion

Parallel computing: Very briefly

Shared memory vs. Distributed memory



Threading: OpenMP, Intel TBB, etc.



Message passing: MPI, NCCL, etc.

hpc4neuro Python Utilities

DataDistributor (1)

```
1. import os
2.
3. def get_filenames(path):
4.     return os.listdir(path)
5.
6. filenames = get_filenames('.')
7. print(f'Filenames: {filenames}')
```

```
1. import os
2. from mpi4py import MPI
3. from hpc4neuro.distribution import DataDistributor
4.
5. @DataDistributor(MPI.COMM_WORLD, shutdown_on_error=True)
6. def get_filenames(path):
7.     return os.listdir(path)
8.
9. filenames = get_filenames('.')
10. print(f'{MPI.COMM_WORLD.Get_rank()} -- Filenames: {filenames}')
```

```
python -m hpc4neuro.examples.distribution.sequential_filenames
```

```
Filenames: ['errors.py', '__init__.py', 'utils',
'tutorials', '__pycache__']
```

```
mpirun -np 4 python -m hpc4neuro.examples.distribution.static_filenames_decorator
```

```
0 -- Filenames: ['errors.py', '__pycache__']
1 -- Filenames: ['__init__.py']
2 -- Filenames: ['utils']
3 -- Filenames: ['tutorials']
```

hpc4neuro/examples/sequential_filenames.py

hpc4neuro/examples/static_filenames_decorator.py

hpc4neuro Python Utilities

DataDistributor (2)

```
1. import os
2.
3. filenames = os.listdir('.')
4. print(f'Filenames: {filenames}')
```

```
1. import os
2. from mpi4py import MPI
3. from hpc4neuro.distribution import DataDistributor
4.
5. dist_decorator = DataDistributor(MPI.COMM_WORLD, shutdown_on_error=True)
6. get_rank_local_filenames = dist_decorator(os.listdir)
7.
8. filenames = get_rank_local_filenames('.')
9. print(f'{MPI.COMM_WORLD.Get_rank()} -- Filenames: {filenames}')
```

hpc4neuro/examples/dynamic_filenames_decorator.py

Agenda

1. Concepts: Fundamentals
 - i. Supervised learning
 - ii. Artificial Neural Networks
 - iii. Error backpropagation
2. Code examples: Training with one GPU
 - i. Handwritten digit recognition
 - ii. The MNIST dataset
 - iii. Implementation with `tf.keras`
3. Concepts: Distributed training
 - i. Why use distributed training?
 - ii. Model parallelism
 - iii. Data parallelism
 - iv. Gradient aggregation
4. Pit stop: Parallel computing
 - i. Shared memory vs. Distributed memory
 - ii. The `hpc4neuro` Python library
5. Back to distributed training: Examples
 - i. MNIST classification: Epoch distributed
 - ii. Handling custom data
 - iii. Distributing training data
6. The “Deep Learning on Supercomputers” tutorial
 - i. Introduction
 - ii. Running code samples on JUWELS
 - iii. Job configuration
7. Conclusion

Back to distributed training: Examples

Distributed training with Horovod: Code (1)

```
1. import tensorflow as tf
```

Single GPU

```
1. import tensorflow as tf
2. import math
3. import horovod.tensorflow.keras as hvd
4. from tensorflow.python.keras import backend as K
5. hvd.init()
6. config = tf.ConfigProto()
7. config.gpu_options.visible_device_list = str(hvd.local_rank())
8. K.set_session(tf.Session(config=config))
```

Distributed

`dl_on_supercomputers/course_material/examples/mnist_epoch_distributed.py`

Back to distributed training: Examples

Distributed training with Horovod: Code (2)

```
2. mnist = tf.keras.datasets.mnist
3. (x_train, y_train), (x_test, y_test) = mnist.load_data()
4. x_train, x_test = x_train / 255.0, x_test / 255.0
5. model = tf.keras.models.Sequential([
    tf.keras.layers.Flatten(),
    tf.keras.layers.Dense(512, activation=tf.nn.relu),
    tf.keras.layers.Dense(10, activation=tf.nn.softmax)
])
6. optimizer = tf.keras.optimizers.Adam()
7. epochs = 4
```

Single GPU

```
9. mnist = tf.keras.datasets.mnist
10. (x_train, y_train), (x_test, y_test) = mnist.load_data()
11. x_train, x_test = x_train / 255.0, x_test / 255.0
12. model = tf.keras.models.Sequential([
    tf.keras.layers.Flatten(),
    tf.keras.layers.Dense(512, activation=tf.nn.relu),
    tf.keras.layers.Dense(10, activation=tf.nn.softmax)
])
13. optimizer = tf.keras.optimizers.Adam()
14. optimizer = hvd.DistributedOptimizer(optimizer)
15. epochs = int(math.ceil(4.0 / hvd.size()))
```

Distributed

Back to distributed training: Examples

Distributed training with Horovod: Code (3)

```
8. model.compile(  
    optimizer=optimizer,  
    loss='sparse_categorical_crossentropy',  
    metrics=['accuracy']  
)  
  
9. model.fit(  
    x=x_train,  
    y=y_train,  
    batch_size=32,  
    epochs=epochs  
)
```

Single GPU

```
16. model.compile(  
    optimizer=optimizer,  
    loss='sparse_categorical_crossentropy',  
    metrics=['accuracy']  
)  
  
17. callbacks = [hvd.callbacks.BroadcastGlobalVariablesCallback(0)]  
  
18. model.fit(  
    x=x_train,  
    y=y_train,  
    batch_size=32,  
    epochs=epochs,  
    callbacks=callbacks  
)
```

Distributed

Back to distributed training: Examples

Distributed training with Horovod: Output

```
$ mpirun -np 1 python -u mnist_epoch_distributed.py

Epoch 1/4
60000/60000 [=====] - 8s 125us/sample - loss: 0.2004 - acc: 0.9410
Epoch 2/4
60000/60000 [=====] - 7s 121us/sample - loss: 0.0786 - acc: 0.9763
Epoch 3/4
60000/60000 [=====] - 7s 121us/sample - loss: 0.0519 - acc: 0.9836
Epoch 4/4
60000/60000 [=====] - 7s 121us/sample - loss: 0.0374 - acc: 0.9879

Test loss: 0.0761936013394734
Test accuracy: 0.9773
```

Back to distributed training: Examples

Training with custom data I/O: Code snippet

```
1. def get_filenames(path):
2.     absolute_path = os.path.join(os.path.abspath(f'{path}/x'))
3.     return os.listdir(absolute_path)
4.
5. def main():
6.     data_dir = 'data/mnist/partitioned'
7.     train_filenames = get_filenames(f'{data_dir}/train')
8.     test_filenames = get_filenames(f'{data_dir}/test')
9.
10.    x_train, y_train = load_dataset(f'{data_dir}/train', train_filenames)
11.    x_test, y_test = load_dataset(f'{data_dir}/test', test_filenames)
12.
13.    x_train, x_test = x_train / 255.0, x_test / 255.0
```

Back to distributed training: Examples

Input data distribution for Horovod: Code snippet

```
1. def main():
2.     initialize_hvd_and_mpi()
3.     is_root = hvd.rank() == 0
4.
5.     dist_decorator = DataDistributor(mpi_comm=mpi4py.MPI.COMM_WORLD, shutdown_on_error=True)
6.     get_rank_local_filenames = dist_decorator(get_filenames)
7.
8.     data_dir = 'data/mnist/partitioned'
9.     train_filenames = get_rank_local_filenames(f'{data_dir}/train')
10.    x_train, y_train = load_dataset(f'{data_dir}/train', train_filenames)
11.    x_train = x_train / 255.0
12.    if is_root:
13.        test_filenames = get_filenames(f'{data_dir}/test')
14.        x_test, y_test = load_dataset(f'{data_dir}/test', test_filenames)
15.        x_test = x_test / 255.0
16.    else:
17.        x_test, y_test = None, None
```

```
1. def get_filenames(path):
2.     absolute_path = os.path.join(os.path.abspath(f'{path}/x'))
3.     return os.listdir(absolute_path)
```

dl_on_supercomputers/horovod_data_distributed/mnist_data_distributed.py

Agenda

1. Concepts: Fundamentals
 - i. Supervised learning
 - ii. Artificial Neural Networks
 - iii. Error backpropagation
2. Code examples: Training with one GPU
 - i. Handwritten digit recognition
 - ii. The MNIST dataset
 - iii. Implementation with `tf.keras`
3. Concepts: Distributed training
 - i. Why use distributed training?
 - ii. Model parallelism
 - iii. Data parallelism
 - iv. Gradient aggregation
4. Pit stop: Parallel computing
 - i. Shared memory vs. Distributed memory
 - ii. The hpc4neuro Python library
5. Back to distributed training: Examples
 - i. MNIST classification: Epoch distributed
 - ii. Handling custom data
 - iii. Distributing training data
6. The “Deep Learning on Supercomputers” tutorial
 - i. Introduction
 - ii. Running code samples on JUWELS
 - iii. Job configuration
7. Conclusion

Getting started with Deep learning on Supercomputers

The tutorial

https://gitlab.version.fz-juelich.de/hpc4ns/dl_on_supercomputers

Getting started with Deep learning on Supercomputers

The tutorial: Logging in to JUWELS

```
{ ~ } » ssh khalid1@juwels.fz-juelich.de
Last login: Tue Nov 26 11:27:09 2019
*****
* Welcome to                                                                    *
*                                                                              *
*      _ _ _ _ \ / _ _ | | _ _ _ _ _ _ _ _ _ _ Juelich Wizard              *
*      _ _ _ _ \ / _ _ | | _ _ _ _ _ _ _ _ _ _   for                      *
*      _ _ _ _ \ / _ _ | | _ _ _ _ _ _ _ _ _ _ European Leadership        *
*      _ _ _ _ \ / _ _ | | _ _ _ _ _ _ _ _ _ _ Science                     *
*                                                                              *
*****
                                                                    2019-03-11T12:00+0200

### Known Issues ###
An up-to-date list of known issues on the system is maintained at

https://apps.fz-juelich.de/jsc/hps/juwels/known-issues.html
*****
[khalid1@juwels04 ~]$
```

Getting started with Deep learning on Supercomputers

The tutorial: Environment setup and Repository cloning

```
[khalid1@juwels04 ~]$ jutil env activate -p cslns -A slns
[khalid1@juwels04 cslns]$ cd $PROJECT/khalid1/juwels
[khalid1@juwels04 juwels]$ module load git-lfs
[khalid1@juwels04 juwels]$ git lfs install
Git LFS initialized.
[khalid1@juwels04 juwels]$ git lfs clone https://gitlab.version.fz-juelich.de/hpc4ns/dl_on_supercomputers.git
Cloning into 'dl_on_supercomputers'...
remote: Enumerating objects: 142, done.
remote: Counting objects: 100% (142/142), done.
remote: Compressing objects: 100% (110/110), done.
remote: Total 434 (delta 46), reused 110 (delta 31)
Receiving objects: 100% (434/434), 103.63 KiB | 0 bytes/s, done.
Resolving deltas: 100% (222/222), done.
[khalid1@juwels04 juwels]$ 0% (43/43), 193 MB | 29 MB/s
[khalid1@juwels04 juwels]$
```

Getting started with Deep learning on Supercomputers

The tutorial: Starting and monitoring the training job

```
[khalid1@juwels04 juwels]$ cd dl_on_supercomputers/horovod/keras
[khalid1@juwels04 keras]$ sbatch submit_job_juwels.sh
Submitted batch job 1885056
[khalid1@juwels04 keras]$ squeue -u khalid1
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	ODELIST(REASON)
1885056	develgpu	HOROVOD_	khalid1	CF	0:07	2	jwc09n[006,009]

```
[khalid1@juwels04 keras]$ tail -f output_1885056.out
Using /p/project/cslns/khalid1/juwels/dl_on_supercomputers/datasets as the data directory.
x_train shape: (60000, 28, 28, 1)
60000 train samples
10000 test samples
Train on 60000 samples, validate on 10000 samples
Epoch 1/12
 128/60000 [.....] - ETA: 44:55 - loss: 2.3016 - acc: 0.1016
...
60000/60000 [=====] - 3s 42us/step - loss: 0.0273 - acc: 0.9914
Test loss: 0.02779148665768025
Test accuracy: 0.9911
```

Getting started with Deep learning on Supercomputers

The tutorial: Job script `submit_job_juwels.sh`

```
# Slurm job configuration
#SBATCH --nodes=2
#SBATCH --ntasks=8
#SBATCH --ntasks-per-node=4
#SBATCH --output=output_%j.out
#SBATCH --error=error_%j.er
#SBATCH --time=00:10:00
#SBATCH --job-name=HOROVOD_KERAS_MNIST
#SBATCH --gres=gpu:4 --partition=develgpus
#SBATCH --mail-type=ALL
#SBATCH --mail-user=<...>
```

```
# Load the required modules
module load GCC/8.3.0
module load TensorFlow/1.13.1-GPU-Python-3.6.8
module load Keras/2.2.4-GPU-Python-3.6.8

# Run the program
srun python -u mnist.py
```

Agenda

1. Concepts: Fundamentals
 - i. Supervised learning
 - ii. Artificial Neural Networks
 - iii. Error backpropagation
2. Code examples: Training with one GPU
 - i. Handwritten digit recognition
 - ii. The MNIST dataset
 - iii. Implementation with `tf.keras`
3. Concepts: Distributed training
 - i. Why use distributed training?
 - ii. Model parallelism
 - iii. Data parallelism
 - iv. Gradient aggregation
4. Pit stop: Parallel computing
 - i. Shared memory vs. Distributed memory
 - ii. The hpc4neuro Python library
5. Back to distributed training: Examples
 - i. MNIST classification: Epoch distributed
 - ii. Handling custom data
 - iii. Distributing training data
6. The “Deep Learning on Supercomputers” tutorial
 - i. Introduction
 - ii. Running code samples on JUWELS
 - iii. Job configuration
7. Conclusion

Conclusion

Summary

Key points

- There is more to distributed training than speedup, e.g., effective batch size can be increased
- The supercomputers can be utilized for data parallel training with relative ease
- Tensorflow and Horovod are already available on JUWELS and JURECA
- Combining the material presented here with the “DL on Supercomputers” tutorial is a good place to start
- A good foundation in parallel programming, especially with MPI, can go a long way

Support

- All SC related issues: sc@fz-juelich.de
- Tutorial and hpc4neuro: slns@fz-juelich.de

Useful resources

- On the next slide

[Thank you!](#)

Appendix

Useful links

1. Getting started with Deep Learning on Supercomputers

- https://gitlab.version.fz-juelich.de/hpc4ns/dl_on_supercomputers#getting-started-with-deep-learning-on-supercomputers

2. The hpc4neuro Python library

- <https://gitlab.version.fz-juelich.de/hpc4ns/hpc4neuro#the-hpc4neuro-library-of-python-utilities>

3. Horovod

- <https://github.com/horovod/horovod>

4. The MPI tutorial

- <https://mpitutorial.com/>

5. MPI4Py

- <https://mpi4py.readthedocs.io/en/stable/>