HPC.NRW

NATIONALES HOCHLEISTUNGS RECHNEN

EDIH Rheinland

WEST AI KI-Servicezentrum

PPCES: Machine and Deep Learning

Case Study – PyTorch

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Introduction to PyTorch

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- **PyTorch was introduced in 2016**
  - Designed for Deep Learning workloads
  - Latest stable version: 2.2.1
  - Frontends for Python and C++
- **Extensive documentation and tutorials (here)**
  - Performance tuning guides
  - Distributed training
- **Libraries (transform, datasets, models, …)**
  - torchaudio (e.g., signal processing + sampling)
  - torchtext (e.g., tokenizers, metrics, vocabular)
  - torchvision (e.g., segmentation, video, image)

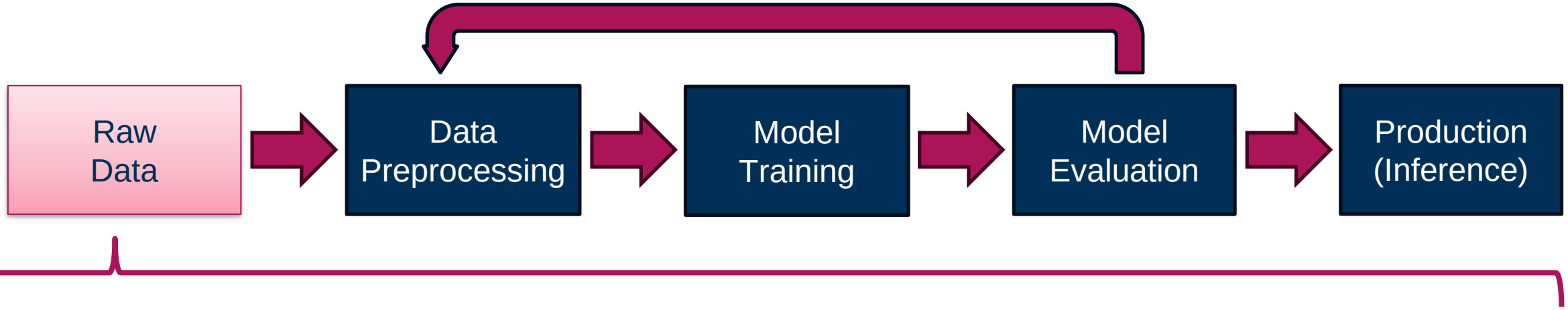
- **Key points**
  - High flexibility and freedom
  - Define layers with nn package
  - Manual training and evaluation loop
  - Stable interface

```
# create model to be trained
model = torch.nn.Sequential(
        torch.nn.Linear(3, 1),
        torch.nn.Flatten(0, 1)
    )
# model training
for t in range(n_epochs):
    y_pred = model(data)      # forward pass
    loss = loss_fn(y_pred, y) # determine loss
    optimizer.zero_grad()     # zero the gradients
    loss.backward()           # compute gradients
    optimizer.step()          # update weights
```

Deep Learning Workflow with PyTorch

- **Build your pipelines**
  - Data pipline
  - Training pipeline

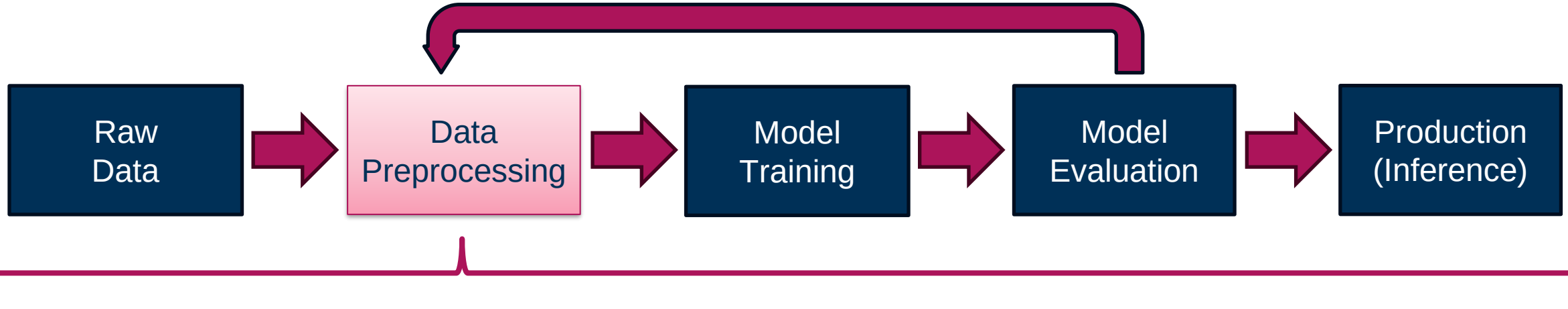
Deep Learning Workflow with PyTorch



- **Utilize your own data dataset**
  - Some interfaces work with X (features) and y (labels)
  - However, more complex data: Images, time series
  - Use `Dataset` classes from `torch.utils.data` (Link)
- **Predefined datasets for vision, audio, …**
  - ImageNet
  - CIFAR (10 and 100)
  - MNIST
  - …

`Caltech101`(root[, target_type, transform, ...])	Caltech 101 Dataset.
`Caltech256`(root[, transform, ...])	Caltech 256 Dataset.
`CelebA`(root[, split, target_type, ...])	Large-scale CelebFaces Attributes (CelebA) Dataset Dataset.
`CIFAR10`(root[, train, transform, ...])	CIFAR10 Dataset.
`CIFAR100`(root[, train, transform, ...])	CIFAR100 Dataset.
`Country211`(root[, split, transform, ...])	The Country211 Data Set from OpenAI.

Deep Learning Workflow with PyTorch



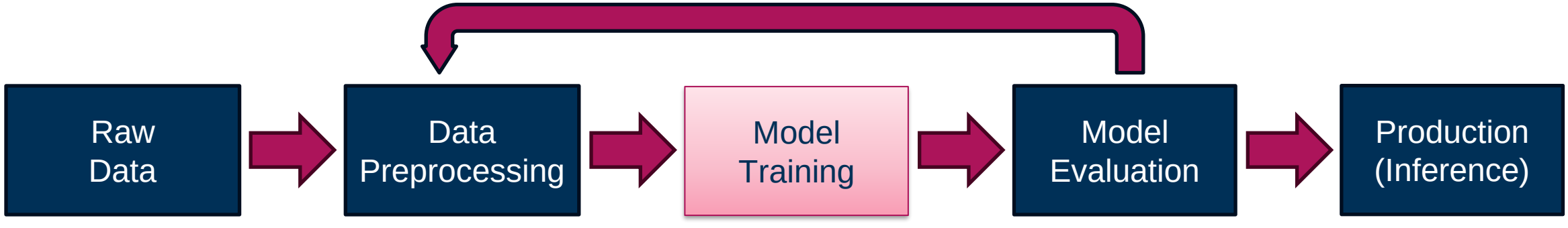
- **Various map / transformation operations available**
  - Manual data manipulations (e.g., standardization)
  - Apply raw functions in `torch.nn.functional` to tensors
  - Several transformations in `torchvision.transforms`
    - Normalize
    - RandomHorizontalFlip
    - Resize
    - Padding
    - Full list → here
  - DataLoader (batching, shuffling)

```python
import torchvision.transforms as trf

transf = trf.Compose([
    trf.RandomHorizontalFlip(),
    trf.ToTensor(),
    trf.Normalize(mean, std)
])
```

```python
import torch
# create data loader
loader = torch.utils.data.DataLoader(
    dataset,
    batch_size=32,
    shuffle=False,
    num_workers=0,
    pin_memory=False,
)
# iterate data loader
for idx, samples in enumerate(loader):
    print(batch_idx, samples)
```

Deep Learning Workflow with PyTorch



- **Loss function** (MSE, CrossEntropy, …)
- **Optimizers** (SGD, Adam, …)
- **Create or load a model**
  - Sequential API
  - Functional API: Define your own `torch.nn.Module`
  - Predefined modules (Catalogue)
    - AlexNet, ResNet, VGG, ShuffleNet, …

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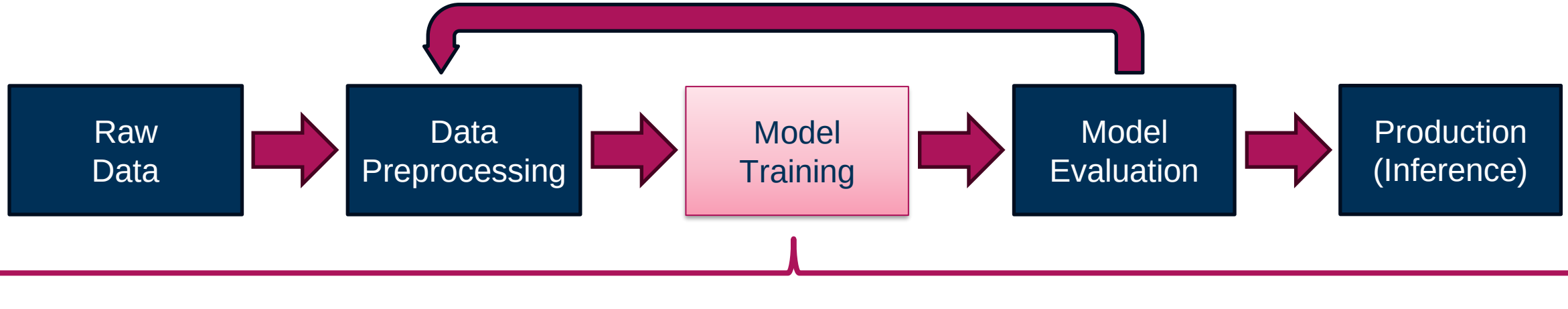
    )
```

```
import torch

class TinyModel(torch.nn.Module):
    def __init__(self):
        super(TinyModel, self).__init__()
        self.linear1 = torch.nn.Linear(100, 200)
        self.activation = torch.nn.ReLU()
        self.linear2 = torch.nn.Linear(200, 10)
        self.softmax = torch.nn.Softmax()

    def forward(self, x):
        x = self.linear1(x)
        x = self.activation(x)
        x = self.linear2(x)
        x = self.softmax(x)
        return x
```

Deep Learning Workflow with PyTorch



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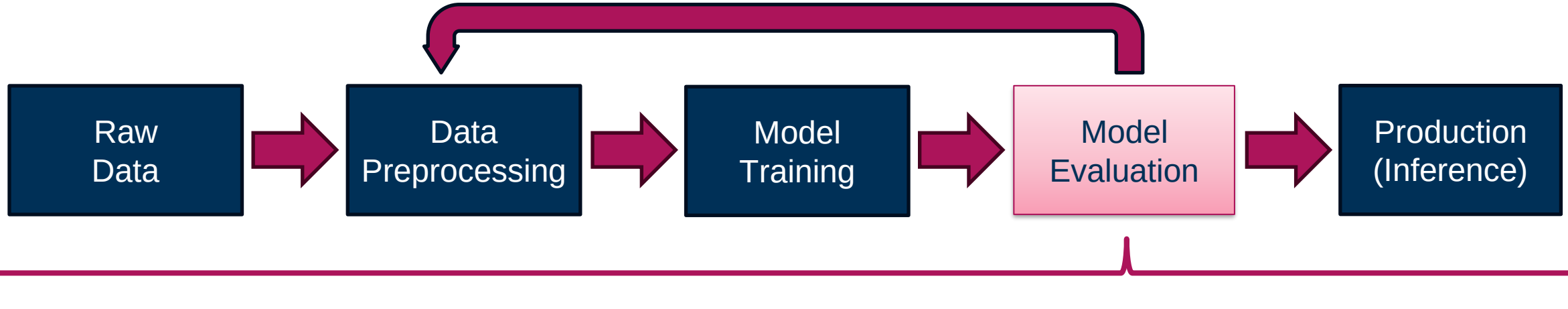
Deep Learning Workflow with PyTorch



- **Standard PyTorch:** Explicit training / test loops
  - Full control / allows customization
- **Extensions:** `torcheval` or TorchMetrics
  - BinaryAccuracy, BinaryPrecision
  - MulticlassAccuracy, MulticlassPrecision
  - MeanSquaredError, R2Score

```
# calculate accuracy in a single line
acc = (y_pred.round() == y_batch).float().mean()
```

- Metrics
  - Aggregation Metrics
  - Classification Metrics
  - Ranking Metrics
  - Regression Metrics
  - Text Metrics
  - Windowed Metrics

(Doc torcheval)

(Doc TorchMetrics)

PyTorch Lightning

Example: Classification with MNIST (Source Code)

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```
def main():
    # parsing arguments and other preparations
    ...

    # load and preprocess MNIST dataset
    loader_train, loader_test = get_data_loaders()

    # load the model
    model = Net().to(device)

    # create optimizer instance
    optimizer = optim.Adadelta(model.parameters(), lr=args.lr)

    # training
    for epoch in range(1, args.epochs + 1):
        train(args, model, device, loader_train, optimizer, epoch)
        test(model, device, loader_test)
```

Example: Classification with MNIST (Source Code)

HPC.NRW

```
def get_data_loaders(args):
    # define arguments for data loaders
    ds_kwargs = {'batch_size': args.batch_size}

    # transformation
    transform=transforms.Compose([
        transforms.ToTensor(),
        transforms.Normalize((0.1307,), (0.3081,))
    ])

    # train and test dataset
    dataset1 = datasets.MNIST('../data', train=True,  download=True, transform=transform)
    dataset2 = datasets.MNIST('../data', train=False, transform=transform)
    # create data loaders
    loader_train = torch.utils.data.DataLoader(dataset1, **ds_kwargs)
    loader_test  = torch.utils.data.DataLoader(dataset2, **ds_kwargs)
    return loader_train, loader_test
```

Example: Classification with MNIST (Source Code)

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```
class Net(nn.Module):

    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 32, 3, 1)
        self.conv2 = nn.Conv2d(32, 64, 3, 1)
        self.dropout1 = nn.Dropout(0.25)
        self.dropout2 = nn.Dropout(0.5)
        self.fc1 = nn.Linear(9216, 128)
        self.fc2 = nn.Linear(128, 10)
```

```
    def forward(self, x):
        x = self.conv1(x)
        x = F.relu(x)
        x = self.conv2(x)
        x = F.relu(x)
        x = F.max_pool2d(x, 2)
        x = self.dropout1(x)
        x = torch.flatten(x, 1)
        x = self.fc1(x)
        x = F.relu(x)
        x = self.dropout2(x)
        x = self.fc2(x)
        output = F.log_softmax(x, dim=1)
        return output
```

Example: Classification with MNIST (Source Code)

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```
def train(args, model, device, loader_train, optimizer, epoch):
    # set model into training mode
    model.train()

    # iterative over batches
    for batch_idx, (data, target) in enumerate(loader_train):
        data, target = data.to(device), target.to(device) # move them to GPU
        optimizer.zero_grad()
        output = model(data)
        loss = F.nll_loss(output, target)
        loss.backward()
        optimizer.step()

        if batch_idx % args.log_interval == 0:
            print('Train Epoch: {} [{}/{} ({:.0f}%)]\tLoss: {:.6f}'.format(
                epoch, batch_idx * len(data), len(loader_train.dataset),
                100. * batch_idx / len(loader_train), loss.item()))
```

Example: Classification with MNIST (Source Code)

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```
def test(model, device, loader_test):
    # set model into evaluation mode
    model.eval()
    test_loss, correct = 0, 0
    with torch.no_grad():
        for data, target in loader_test:
            data, target = data.to(device), target.to(device) # move them to GPU
            output = model(data)
            test_loss += F.nll_loss(output, target, reduction='sum').item()
            pred = output.argmax(dim=1, keepdim=True)
            correct += pred.eq(target.view_as(pred)).sum().item()

    test_loss /= len(loader_test.dataset)

    print('\nTest set: Average loss: {:.4f}, Accuracy: {}/{} ({:.0f}%)\n'.format(
        test_loss, correct, len(loader_test.dataset),
        100. * correct / len(loader_test.dataset)))
```