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Hands-on Al I

Unit 5 – Your first neural networks

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```
In [1]: # Required packages and the u5_utils file
import u5_utils as u5
import matplotlib.pyplot as plt
import numpy as np
import seaborn as sns
import torch

from scipy.special import expit as sigmoid

u5.check_module_versions()
# Set plotting style of seaborn related plots.
sns.set()
```

```
Installed Python version: 3.9 (\checkmark)
Installed numpy version: 1.21.1 (\checkmark)
Installed pandas version: 1.3.1 (\checkmark)
Installed scikit-learn version: 1.0 (\checkmark)
Installed matplotlib version: 3.4.3 (\checkmark)
Installed seaborn version: 0.11.2 (\checkmark)
Installed scipy version: 1.7.1 (\checkmark)
Installed torch version: 1.10.0+cpu (\checkmark)
Installed tqdm version: 4.62.1 (\checkmark)
```

Note: When specifying a seed for the sources of randomness, use the u5.set_seed(seed=XYZ) function.

Exercise 1

Following the instructions given in the lecture notebook, perform the following tasks:

• Create a dataset by sampling 50 values for x and computing $y = 0.100 + 0.200 \cdot x$, then adding some noise (variance 0.5) to y. For this, consider the function <code>get_dataset()</code> from <code>u5_utils.py</code>.

Note: For reproducibility, set a fixed seed (seed=23).

- Define a *linear* model with two coefficients *d* and *k* (polynomial of degree 1), with which we will approximate the relation between *x* and *y*.
- Define *Mean Squared Error (MSE)* as the loss function. Using the most elegant method from the lecture, find the optimum *d* and *k* minimizing the loss and print out the loss.
- Plot the resulting linear model along with the data.

1.1. Create the dataset.

1.2. Define the linear model.

```
In [3]: def model(x, d, k):
    return d + k * x
```

1.3. Define MSE as loss function. Minimize the loss and print it.

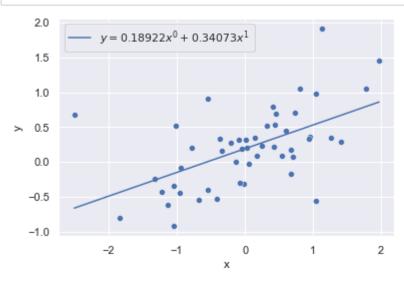
```
In [4]: def loss(dataset, d, k):
    predictions = model(dataset.x.values, d, k)
    targets = dataset.y.values
    return np.mean((targets - predictions) ** 2, axis=-1)

k, d = np.polyfit(x=dataset.x, y=dataset.y, deg=1)
loss(dataset, d, k)
```

Out[4]: 0.22078537210785434

1.4. Plot the linear model and the data.

In [5]: u5.plot_model(dataset, (d, k))



Exercise 2

• Create a dataset with two variables, x and y, where y=1 for x>0.6 and y=0 otherwise. For this, use the function <code>get_dataset_logistic()</code> from <code>u5_utils.py</code>, with 75 data points and variance 0.1. Then, plot the dataset.

Note: For reproducibility, set a fixed seed (seed=23).

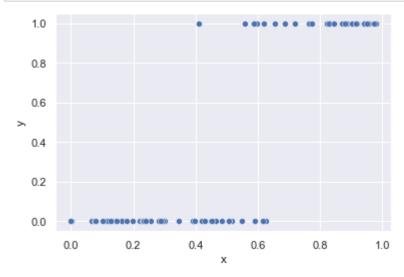
- Define a logistic model with two coefficients d and k to fit the created dataset.
- Define a suitable loss and corresponding gradient function.
- Visualize the loss landscape including the gradient arrows. For this, use the function $plot_loss_landscape()$ from $us_landscape()$ for d and k in a range from -10 to 10 each.
- Optimize the parameters d and k of the model using Gradient Descent. For this, use the function plot_gradient_descent() from u5_utils.py . As a starting point, use d=-5, k=-5, 1000 iterations (steps), a step size (learning rate) of 1.0 and a momentum of 0.0.
- Print out the optimized values for d and k as well as the loss.

2.1. Create and plot the dataset.

```
In [6]: u5.set_seed(seed=23)

dataset = u5.get_dataset_logistic(
    num_pairs=75,  # number of data points
    threshold=0.6,  # position of class boundary
    variance=0.1  # amount of noise
)

sns.scatterplot(data=dataset, x="x", y="y");
```



2.2. Define the logistic model.

```
In [7]: def model(x, d, k):
    return sigmoid(d + k * x)
```

2.3. Define the loss function and its corresponding gradient function.

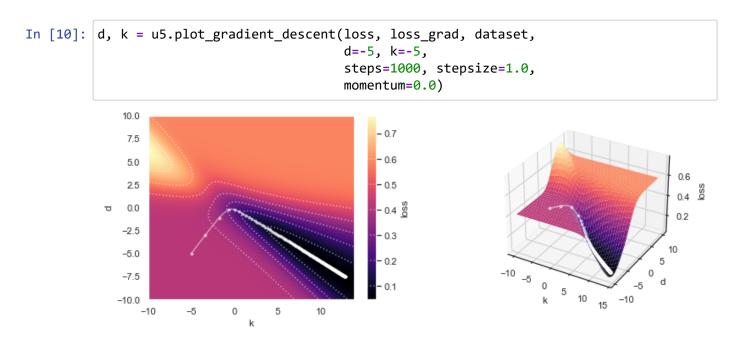
```
In [8]: def loss(dataset, d, k):
    predictions = model(dataset.x.values, d, k)
    targets = dataset.y.values
    return np.mean((predictions - targets)**2, axis=-1)

def loss_grad(dataset, d, k):
    predictions = model(dataset.x.values, d, k)
    targets = dataset.y.values
    delta = predictions - targets
    d_grad = np.mean(delta, axis=-1)
    k_grad = np.mean(dataset.x.values * delta, axis=-1)
    return d_grad, k_grad
```

2.4. Define the ranges for d and k and plot the loss landscape including the gradient arrows.

```
In [9]: d_values = np.linspace(-10, 10, 101)
          k_{values} = np.linspace(-10, 10, 101)
          landscape = u5.plot_loss_landscape(loss, dataset, d=d_values, k=k_values, grad_fr
              10.0
                                                         - 0.7
               7.5
                                                         - 0.6
               5.0
                                                                                                           0.6
               2.5
                                                         - 0.5
                                                                                                           0.4
               0.0
                                                         - 0.4 g
                                                                                                           0.2
              -2.5
                                                         - 0.3
              -5.0
                                                         - 0.2
              -7.5
                                                                                 -5
                                                                                                    -5
                                                          0.1
                                                                                                 -10
              -10.0
                                                                                             10
                  -10
                                            5
                                                    10
```

2.5. Perform gradient descent to optimize the model parameters.



2.6. Print the values found for d and k and the corresponding loss.

```
In [11]: print(f"Final: d={d:9f}, k={k:9f}, loss={loss(dataset, d, k):9f}")
```

Final: d=-7.527506, k=12.879191, loss= 0.047809

Exercise 3

Continuing with the dataset and the logistic model from Exercise 2, we will now replace the loss function with the Mean Squared Error (MSE) loss to see what happens. Since we also need its gradient, we prepared this for you.

- Visualize the loss landscape including the gradient arrows. For this, use the function $plot_loss_landscape()$ from $us_landscape()$ for d and k in a range from -10 to 10 each.
- Optimize the parameters d and k of the model using Gradient Descent. Again, use the function plot_gradient_descent() from u5_utils.py to perform the optimization. Again, start from d=-5, k=-5, do 1000 iterations (steps), use a step size (learning rate) of 1.0 and a momentum of 0.0.
- Print out the optimized values for d and k as well as the loss.
- In an extra cell, redo the optimization but change the starting position for d and k such that it finds a loss smaller than 0.1.

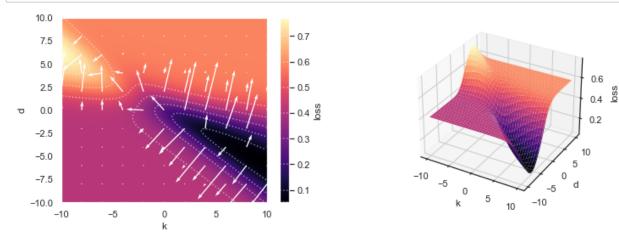
Note: Look at the loss landscape to pick the position. Remember that gradient descent can be compared to a ball rolling down a hill.

Again, print the optimized values for d and k and the loss.

```
In [12]: # MSE Loss and gradient of MSE Loss for a Logistic model
def loss(dataset, d, k):
    predictions = model(dataset.x.values, d, k)
    targets = dataset.y.values
    return np.mean((predictions - targets)**2, axis=-1)

def loss_grad(dataset, d, k):
    predictions = model(dataset.x.values, d, k)
    targets = dataset.y.values
    delta = 2 * (predictions - targets) # grad of (predictions - targets)**2
    delta *= predictions * (1 - predictions) # grad of sigmoid()
    d_grad = np.mean(delta, axis=-1)
    k_grad = np.mean(dataset.x.values * delta, axis=-1)
    return d_grad, k_grad
```

3.1. Define the ranges for d and k and plot the loss landscape including the gradient arrows.



3.2. Perform gradient descent to optimize the model parameters.

0.6

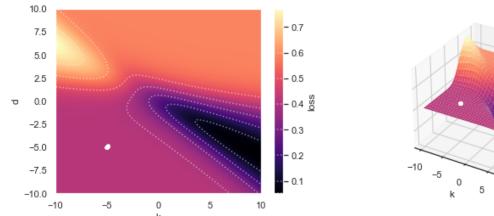
0.2

-5

-10

10

0.4 S

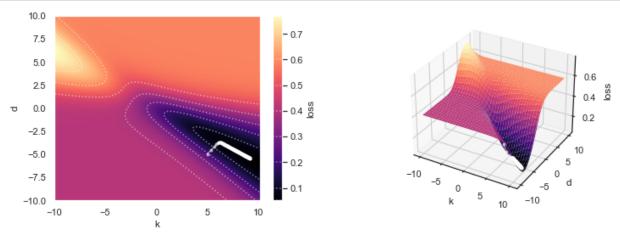


3.3. Print the values found for d and k and the corresponding loss.

```
In [15]: print(f"Final: d={d:9f}, k={k:9f}, loss={loss(dataset, d, k):9f}")
```

Final: d=-4.860773, k=-4.899753, loss= 0.413173

3.4. Perform gradient descent from a better starting position (choose yourself!).



3.5. Print the values found for d and k and the corresponding loss.

```
In [18]: print(f"Final: d={d:9f}, k={k:9f}, loss={loss(dataset, d, k):9f}")
```

Final: d=-5.433859, k= 9.183437, loss= 0.053566

Exercise 4

• Considering again the dataset from Exercises 2 & 3, implement a logistic regression model in pytorch and define a suitable loss function and optimization method. For the optimization, set learning rate = 0.1 and momentum = 0.0.

Note: For reproducibility, set a fixed seed (seed=23).

• Run the optimization (get predictions, calculate loss, compute loss gradient, perform update step) until the loss is ≤ 0.17 and print out the loss as well as the difference between the initial (randomly chosen) d (bias) and k (weight) and those achieved after optimization.

Note: Follow the lecture notebook to convert the input data and target to torch tensors for the optimization.

4.1. Define the logistic model, the loss function and the gradient descent optimizer in pytorch.

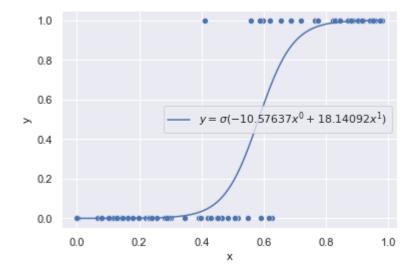
```
In [27]: u5.set_seed(seed=23)

model = torch.nn.Linear(1, 1)
    loss = torch.nn.functional.binary_cross_entropy_with_logits
    optimizer = torch.optim.SGD(model.parameters(), lr=0.1, momentum=0.0,)
```

4.2. Run the optimization until the loss is ≤ 0.17 and print the loss as well as the differences between d and k before and after this optimization.

```
In [28]: X = torch.as tensor(dataset.x.values)[:, np.newaxis]
         Y = torch.as_tensor(dataset.y.values)[:, np.newaxis]
          d, k = model.bias.item(), model.weight.item()
          error = loss(model(X), Y)
          print(f"Initial: d={d:9f}, k={k:9f}, loss={error.item():9f}")
          for _ in range(50000):
                                      # compute predictions
              preds = model(X)
              error = loss(preds, Y) # compute error
              error.backward()  # compute gradient of
optimizer.step()  # perform update step
                                      # compute gradient of the error
              optimizer.zero_grad() # reset gradients for the next iteration
          d, k = model.bias.item(), model.weight.item()
                           d={d:9f}, k={k:9f}, loss={error.item():9f}")
          print(f"Final:
          u5.plot model(dataset, (d, k), transform=sigmoid)
```

Initial: d=-0.422275, k=-0.143484, loss= 0.698535
Final: d=-10.576372, k=18.140919, loss= 0.151791



Exercise 5

With the dataset defined and plotted below (as given in the next cell), perform the following tasks:

Note: As usual, for reproducibility, set a fixed seed (seed=23).

• Implement a similar model as in Exercise 4, i.e., a logistic regression model in pytorch, considering Binary Cross-Entropy (BCE) as the loss funtion and Gradient Descent as the optimization method. For the optimization, set learning rate = 0.1 and momentum = 0.9. Then, run the optimization for 5000 steps and print out the loss.

Note: This dataset is two-dimensional, i.e., it has 2 input features called x1 and x2. They need to be combined into a single torch tensor for the optimization. You can concatenate two torch vectors into a matrix with $\frac{\mathsf{torch.stack}(\ldots,\ \mathsf{dim}=1)}{\mathsf{torch.stack}(\ldots,\ \mathsf{dim}=1)}$

(https://pytorch.org/docs/stable/generated/torch.stack.html#torch.stack), or you can directly assign the entire feature vector matrix dataset[["x1", "x2"]].values to a tensor.

Note: Your model will now need 2 input nodes to handle 2 features but still 1 output node for binary classification.

- Visualize the predictions of the model with the code provided by us. Does the model manage to separate the 2 classes? Does it look like it tried to separate them with a straight line?
- Implement a more complex model by adding a hidden layer with two nodes (the loss function
 and the Gradient Descent optimizer parameters remain the same). Then, print out the loss
 and visualize the predictions of the model with the code provided by us. Increase the number
 of nodes in the hidden layer, re-train the model and visualize the predictions until the classes
 are separated properly.

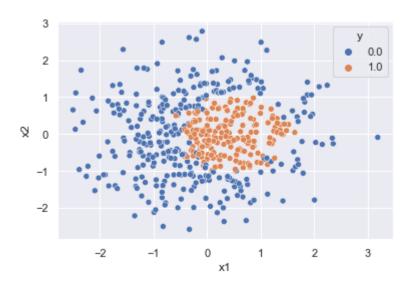
```
In [66]: # set seed for reproducibility
u5.set_seed(seed=23)

# create dataset consisting of random (x, y) pairs
dataset = u5.get_dataset_blob2d(num_samples=500, variance=0.1, threshold=1.0, off

# display the dataset
sns.scatterplot(data=dataset, x="x1", y="x2", hue="y")
dataset.head()
```

Out[66]:

	x1	x2	У
0	0.666988	-1.707695	0.0
1	0.025813	0.409163	1.0
2	-0.777619	-0.514758	0.0
3	0.948634	-0.518663	1.0
4	0.701672	-0.816038	1.0



5.1. Define the model, the loss function and the gradient descent optimizer. Run the optimization for 5000 steps and print the loss.

```
In [76]: u5.set_seed(seed=23)

model = torch.nn.Linear(2, 1)
    loss = torch.nn.functional.binary_cross_entropy_with_logits
    optimizer = torch.optim.SGD(model.parameters(), lr=0.1, momentum=0.9,)

X = torch.as_tensor(dataset[["x1", "x2"]].values)
Y = torch.as_tensor(dataset[["y"]].values)

error = loss(model(X), Y)

print(f"Initial Loss: {error.item():9f}")

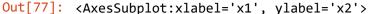
for _ in range(5000):
    preds = model(X)  # compute predictions
    error = loss(preds, Y) # compute error
    error.backward()  # compute gradient of the error
    optimizer.step()  # perform update step
    optimizer.zero_grad() # reset gradients for the next iteration

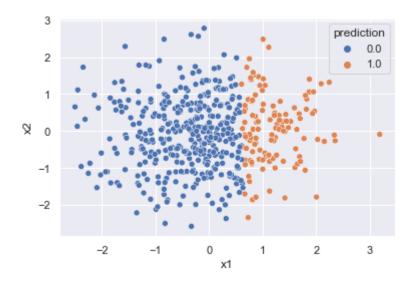
print(f"Final Loss: {error.item():9f}")
```

Initial Loss: 0.716146 Final Loss: 0.592780

Display the predictions. The following code assumes that the predictions from above are stored into a variable called preds. Adapt this if needed (or simply name your predictions above preds.).

```
In [77]: dataset["prediction"] = (preds.detach().sigmoid().numpy() > 0.5).astype(float)
sns.scatterplot(data=dataset, x="x1", y="x2", hue="prediction")
```





5.2. Does the model manage to separate the 2 classes?

5.3. Does it look like it tried to separate them with a straight line?

```
Yes
```

5.4. Define a more complex model (same loss function and gradient descent optimizer parameters). Run the optimization for 5000 steps and print the loss.

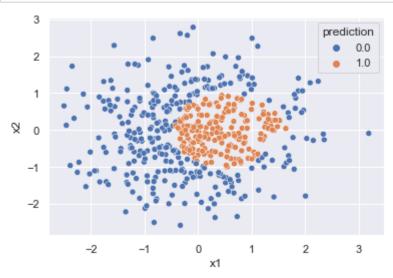
```
In [91]: u5.set_seed(seed=23)
         model = torch.nn.Sequential(torch.nn.Flatten(),
                                     torch.nn.Linear(2, 4),
                                     torch.nn.Sigmoid(),
                                     torch.nn.Linear(4, 1))
         loss = torch.nn.functional.binary_cross_entropy_with_logits
         optimizer = torch.optim.SGD(model.parameters(), lr=0.1, momentum=0.9,)
         X = torch.as_tensor(dataset[["x1", "x2"]].values)
         Y = torch.as_tensor(dataset[["y"]].values)
         error = loss(model(X), Y)
         print(f"Initial Loss: {error.item():9f}")
         for _ in range(20000):
             preds = model(X)
                                  # compute predictions
             error = loss(preds, Y) # compute error
             error.backward() # compute gradient of the error
                                # perform update step
             optimizer.step()
             optimizer.zero grad() # reset gradients for the next iteration
         print(f"Final Loss: {error.item():9f}")
```

Initial Loss: 0.671082 Final Loss: 0.096849

Display the predictions with the more complex model. The following code assumes that the predictions from above are stored into a variable called <code>preds</code>. Adapt this if needed (or simply name your predictions above <code>preds</code>).

Repeat step 5.4. until the model properly separates the two classes (a visual check is sufficient).

In [92]: dataset["prediction"] = (preds.detach().sigmoid().numpy() > 0.5).astype(float)
sns.scatterplot(data=dataset, x="x1", y="x2", hue="prediction");



Exercise 6

Following the instruction given in the lecture notebook, perform the following tasks, but this time, considering the **Fashion-MNIST** dataset. More information about the dataset can be found in this publication:

Fashion-MNIST: a Novel Image Dataset for Benchmarking Machine Learning Algorithms. Han Xiao, Kashif Rasul, Roland Vollgraf (2017). <u>arXiv:1708.07747</u> (<u>https://arxiv.org/abs/1708.07747</u>)

To load the Fashion-MNIST dataset and take a look at a preview of 5 samples, run the cell below (provided by us).

Note: The first time you run this, it will download the dataset. You may see a UserWarning: The given NumPy array is not writeable. This can be safely ignored.

• Like the MNIST dataset, the Fashion-MNIST has input images of $28 \times 28 = 784$ pixels and 10 classes. Considering this, define a Neural Network model with one hidden layer consisting of 15 nodes.

Note. For reproducibility, set a fixed seed (seed=23).

• Reload the dataset considering 15% of the samples as validation set and train the model with the following hyperparameters: batch size = 25, iterations = 5, momentum = 0.7 and learning

rate = 0.01. Use the function run_gradient_descent() from u5_utils.py.

Note. For reproducibility, set a fixed seed (seed=23). It will need to be set both before defining the model and before the optimization (which includes grabbing samples from the dataset). Otherwise, changes in the model would change the train/validation split samples, since both draw random numbers.

- Plot the training and validation losses and print out the accuracy on the test set.
- Keeping the partitioning as before, can you optimize the model in order to achieve an accuracy on the test set > 86% (there are various ways to achieve this)? Plot the training and validation losses to show that your model does not overfit to the training data and print out the accuracy on test to show that it is better than 86%.

Note. For optimization, vary the following hyperparameters: batch size, iterations, learning rate, momentum, number of layers, number of nodes and type of nonlinearity. You may also try randomly flipping training images to perform data augmentation (provided by get_dataset_mnist()). Do not vary the validation set size, as that would increase the training set size.

```
In [93]: # Load the dataset with custom batch size
         train loader, valid loader, test loader = u5.get dataset mnist(
             root="resources",
             variant="FashionMNIST",
             batch size=8,
             valid_size=0.10
         # load the first batch of data (set seed for reproducibility)
         u5.set_seed(seed=23)
         images, labels = next(iter(train loader))
         # transform the image shapes for visualization purposes
         images = np.concatenate([img.squeeze() for img in images], axis=1)
         # display the first batch of data
         with plt.style.context({"axes.grid": False, "xtick.bottom": False}):
             plt.imshow(images, cmap="binary")
             plt.xticks(14 + np.arange(len(labels)) * 28, labels.numpy())
             plt.yticks([])
```

Downloading http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/train-images-idx3-ubyte.gz (http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/train-images-idx3-ubyte.gz)

Downloading http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/train-im ages-idx3-ubyte.gz (http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/train-images-idx3-ubyte.gz) to resources\FashionMNIST\raw\train-images-idx3-ubyte.gz

```
0% | 0/26421880 [00:00<?, ?it/s]
```

Extracting resources\FashionMNIST\raw\train-images-idx3-ubyte.gz to resources\F
ashionMNIST\raw

Downloading http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/train-labels-idx1-ubyte.gz (http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/train-labels-idx1-ubyte.gz)

Downloading http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/train-labels-idx1-ubyte.gz (http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/train-labels-idx1-ubyte.gz) to resources\FashionMNIST\raw\train-labels-idx1-ubyte.gz

```
0% | 0/29515 [00:00<?, ?it/s]
```

Extracting resources\FashionMNIST\raw\train-labels-idx1-ubyte.gz to resources\F
ashionMNIST\raw

```
Downloading http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/t10k-ima ges-idx3-ubyte.gz (http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/t 10k-images-idx3-ubyte.gz)
```

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```
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```

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Downloading http://fashion-mnist.s3-website.eu-central-1.amazonaws.com/t10k-l abels-idx1-ubyte.gz (http://fashion-mnist.s3-website.eu-central-1.amazonaws.c om/t10k-labels-idx1-ubyte.gz) to resources\FashionMNIST\raw\t10k-labels-idx1-ubyte.gz

Extracting resources\FashionMNIST\raw\t10k-labels-idx1-ubyte.gz to resources\Fa
shionMNIST\raw



| 0/5148 [00:00<?, ?it/s]

0%|

6.1. Define the model with one hidden layer of 15 nodes.

```
In [114]: u5.set_seed(seed=23)
    model = torch.nn.Sequential(torch.nn.Flatten(), torch.nn.Linear(784, 15), torch.n
```

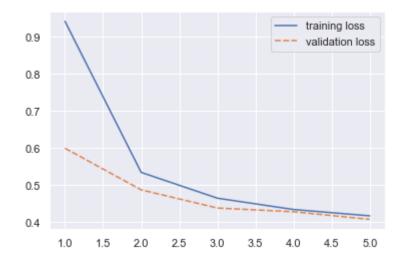
6.2. Reload the dataset with 15% validation data. Define the loss function. Run the optimization.

```
In [115]: u5.set seed(seed=23)
          train_loader, valid_loader, test_loader = u5.get_dataset_mnist(
              root="resources",
              variant="FashionMNIST",
              batch_size=25,
              valid_size=0.15)
          u5.set_seed(seed=23)
          loss = torch.nn.functional.cross_entropy
          u5.set_seed(seed=23)
          losses = u5.run_gradient_descent(
              model=model,
              loss=loss,
              training_set=train_loader,
              valid_set=valid_loader,
              iterations=5, # number of iterations/epochs over the training set
              learning_rate=0.01, # step size/learning rate
              momentum=0.7
                             # momentum
            0%|
                         | 0/51000 [00:00<?, ?it/s]
          Epoch 1 finished with training loss: 0.9420297345110015
          Epoch 2 finished with training loss: 0.5346310313206677
          Epoch 3 finished with training loss: 0.4650839749541061
          Epoch 4 finished with training loss: 0.43452410739207387
```

6.3. Plot the training and validation losses and print the accuracy on the test set.

Epoch 5 finished with training loss: 0.41743046279412277

Test set: {'loss': 0.4535802588239312, 'accuracy': 0.8419999971985817}

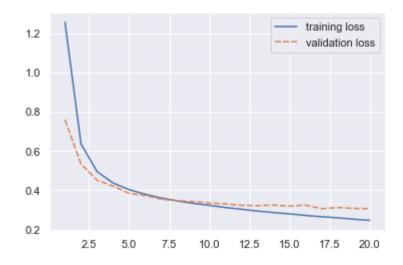


6.4. Optimize the model in order to achieve an accuracy on the test set > 86%. Plot the training and validation losses and print the accuracy on the test set.

```
model = torch.nn.Sequential(torch.nn.Flatten(),
                            torch.nn.Linear(784, 110),
                            torch.nn.Sigmoid(),
                            torch.nn.Linear(110, 50),
                            torch.nn.Sigmoid(),
                            torch.nn.Linear(50, 10)
u5.set seed(seed=23)
train_loader, valid_loader, test_loader = u5.get_dataset_mnist(
    root="resources",
    variant="FashionMNIST",
    batch_size=20,
    valid size=0.15)
u5.set_seed(seed=23)
loss = torch.nn.functional.cross entropy
u5.set seed(seed=23)
losses = u5.run_gradient_descent(
    model=model,
    loss=loss,
    training_set=train_loader,
    valid set=valid loader,
    iterations=20, # number of iterations/epochs over the training set
    learning_rate=0.01, # step size/learning rate
    momentum=0.7 # momentum
)
sns.lineplot(data=losses)
print("Test set:")
print(u5.evaluate_model(model, test_loader, loss=loss,
                        accuracy=u5.multiclass accuracy))
  0%|
               | 0/51000 [00:00<?, ?it/s]
Epoch 1 finished with training loss: 1.2563633986781626
Epoch 2 finished with training loss: 0.636404042080337
Epoch 3 finished with training loss: 0.4952621008981677
Epoch 4 finished with training loss: 0.4369803425333664
Epoch 5 finished with training loss: 0.4031957918420142
Epoch 6 finished with training loss: 0.3796805253011339
Epoch 7 finished with training loss: 0.3603389037006042
Epoch 8 finished with training loss: 0.3459714960336101
Epoch 9 finished with training loss: 0.33308531070602876
Epoch 10 finished with training loss: 0.32305818791482965
Epoch 11 finished with training loss: 0.3120996140498741
Epoch 12 finished with training loss: 0.30321346135189137
Epoch 13 finished with training loss: 0.294211783884641
Epoch 14 finished with training loss: 0.28631279002729
```

In [164]: u5.set seed(seed=23)

```
Epoch 15 finished with training loss: 0.2796084925963306
Epoch 16 finished with training loss: 0.2716696179103033
Epoch 17 finished with training loss: 0.26511403055094623
Epoch 18 finished with training loss: 0.2596839503096599
Epoch 19 finished with training loss: 0.25249143427493526
Epoch 20 finished with training loss: 0.2466835242630366
Test set:
{'loss': 0.34282448339648547, 'accuracy': 0.8781999975442887}
```



In []: