Лекция 3: PyTorch - построение моделей

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При подготовке лекции использованы материалы:

- ...

v 0.13

Разделы:

Нормализация

- к оглавлению

In [2]:

```
# загружаем стиль для оформления презентации
from IPython.display import HTML
from urllib.request import urlopen
html = urlopen("file:./lec_v2.css")
HTML(html.read().decode('utf-8'))
```

Out[2]:

Загрузка и преобразование данных

- к оглавлению

Импорты

- Нужно установить PyTorch (см предыдущую лекцию!)

In [47]:

```
import time
```

In [1]:

```
import math
import csv
import itertools as it
from collections import Counter
import numpy as np

import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline

from sklearn import datasets

#---------
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim

import torchvision
from torchvision import transforms
from torchvision.transforms.functional import normalize
import torchvision.datasets as dset

from torch.utils.data import Dataset, DataLoader
from torch.utils.data.sampler import SubsetRandomSampler, Sampler
```

Принципиальная логика организации работы с данными в PyTorch:

1. Создается объект `Dataset`
   - `Dataset` обеспечивает доступ к данным (с помощью интерфеса)
   - в параметр `transform` конструктора `Dataset` передается *вызываемый объкт* , обеспечивающий трансформацию исходных данных
2. `Dataset` передается в `DataLoader`
   - `DataLoader` обеспечивает загрузку данных батчами, распараллеливает загрузку данных и т.п.

см.:

- общая логика: [https://pytorch.org/tutorials/beginner/data_loading_tutorial.html (https://pytorch.org/tutorials/beginner/data_loading_tutorial.html)](https://pytorch.org/tutorials/beginner/data_loading_tutorial.html)
- трансформеры: [https://pytorch.org/docs/stable/torchvision/transforms.html (https://pytorch.org/docs/stable/torchvision/transforms.html)](https://pytorch.org/docs/stable/torchvision/transforms.html)
- DataLoader и то что его окружает: [https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader (https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader)](https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader)

Dataset Types

The most important argument of DataLoader constructor is **dataset**, which indicates a dataset object to load data from. PyTorch supports two different types of datasets:

- map-style datasets
  - the `__getitem__()` and `__len__()` protocols, and represents a map from (possibly non-integral) indices/keys to data samples.
  - For example, such a dataset, when accessed with `dataset[idx]`, could read the `idx`-th image and its corresponding label from a folder on the disk.
  - Note: `DataLoader` **by default constructs a index sampler that yields integral indices**. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.
- iterable-style datasets.
  - IterableDataset implements the `__iter__()` protocol, and represents an iterable over data samples. This type of datasets is particularly suitable for cases **where random reads are expensive or even improbable**, and where the batch size depends on the fetched data.
- see: [https://pytorch.org/docs/stable/data.html#torch.utils.data.Dataset (https://pytorch.org/docs/stable/data.html#torch.utils.data.Dataset)](https://pytorch.org/docs/stable/data.html#torch.utils.data.Dataset)

Далее работаем с примером: датасетом WINE.

Информация о датасете WINE: [https://archive.ics.uci.edu/ml/datasets/wine (https://archive.ics.uci.edu/ml/datasets/wine)](https://archive.ics.uci.edu/ml/datasets/wine)

In [2]:

```python
from sklearn import datasets
raw_data = datasets.load_wine()
raw_data.keys()
```

Out[2]:

```
dict_keys(['data', 'target', 'target_names', 'DESCR', 'feature_names'])
```

In [3]:

```python
print(raw_data['feature_names'])
print(raw_data['data'][:3])
print('Values: ', Counter(raw_data['target']))
```

```
['alcohol', 'malic_acid', 'ash', 'alcalinity_of_ash', 'magnesium', 'total_phe
nols', 'flavanoids', 'nonflavanoid_phenols', 'proanthocyanins', 'color_intens
ity', 'hue', 'od280/od315_of_diluted_wines', 'proline']
[[1.423e+01 1.710e+00 2.430e+00 1.560e+01 1.270e+02 2.800e+00 3.060e+00
  2.800e-01 2.290e+00 5.640e+00 1.040e+00 3.920e+00 1.065e+03]
 [1.320e+01 1.780e+00 2.140e+00 1.120e+01 1.000e+02 2.650e+00 2.760e+00
  2.600e-01 1.280e+00 4.380e+00 1.050e+00 3.400e+00 1.050e+03]
 [1.316e+01 2.360e+00 2.670e+00 1.860e+01 1.010e+02 2.800e+00 3.240e+00
  3.000e-01 2.810e+00 5.680e+00 1.030e+00 3.170e+00 1.185e+03]]
Values:  Counter({1: 71, 0: 59, 2: 48})
```

In [4]:

```python
with open('./data/wine/wine.csv') as wine_csv:
    # load data:
    wine_data = list(csv.reader(wine_csv, delimiter=','))

wine_data_it = iter(wine_data)
print('Header', list(next(wine_data_it)))
for line_n, line in enumerate(it.islice(wine_data_it, 3)):
    print(f'line: {line_n} | {line}')

print('Values: ', Counter([l[0] for l in wine_data[1:]]))
```

```
Header ['Wine', 'Alcohol', 'Malic.acid', 'Ash', 'Acl', 'Mg', 'Phenols', 'Flav
anoids', 'Nonflavanoid.phenols', 'Proanth', 'Color.int', 'Hue', 'OD', 'Prolin
e']
line: 0 | ['1', '14.23', '1.71', '2.43', '15.6', '127', '2.8', '3.06', '.28',
'2.29', '5.64', '1.04', '3.92', '1065']
line: 1 | ['1', '13.2', '1.78', '2.14', '11.2', '100', '2.65', '2.76', '.26',
'1.28', '4.38', '1.05', '3.4', '1050']
line: 2 | ['1', '13.16', '2.36', '2.67', '18.6', '101', '2.8', '3.24', '.3',
'2.81', '5.68', '1.03', '3.17', '1185']
Values:  Counter({'2': 71, '1': 59, '3': 48})
```

In [5]:

```python
# Implement a custom Dataset:
# inherit Dataset
# implement __init__ , __getitem__ , and __len__
class WineDataset(Dataset):

    def __init__(self, transform=None, verbose=False):
        # load dataset from CSV file (first row: labels)
        xy = np.loadtxt('./data/wine/wine.csv', delimiter=',', dtype=np.float32, skiprows=1

        # note that we do not convert to tensor here
        self.n_samples = xy.shape[0] # number of samples
        self.y_data = xy[:, [0]] # y in first column (shape: N*1)
        self.x_data = xy[:, 1:]
        if verbose:
            print(f'y shape:{self.y_data.shape()}')
            print(f'x shape:{self.x_data.shape()}')

        # save transformer
        self.transform = transform

    def __getitem__(self, index):
        sample = self.x_data[index], self.y_data[index]

        # apply transformer:
        if self.transform:
            sample = self.transform(sample)

        return sample

    def __len__(self):
        return self.n_samples
```

In [6]:

```
print('Without Transformation:')
dataset = WineDataset()

X, y = dataset[0]
print('X:', X, type(X), X.shape)
print('y:', y, type(y), y.shape)
```

```
Without Transformation:
X: [1.423e+01 1.710e+00 2.430e+00 1.560e+01 1.270e+02 2.800e+00 3.060e+00
 2.800e-01 2.290e+00 5.640e+00 1.040e+00 3.920e+00 1.065e+03] <class 'numpy.n
darray'> (13,)
y: [1.] <class 'numpy.ndarray'> (1,)
```

Transforms

Часто необходим некоторый препроцессинг данных получаемых из данных, оформленных в виде `Dataset`.

Мы будем реализовывать препроцессинг в виде **callable classes** вместо обычных функций, это позволит не передавать параметры трансформации при каждом вызове преобразований. Для создания вызываемых классов в них необходимо реализовать функцию вызова `__call__` и, если необходимо, конструктор `__init__`, через который можно передавать параметры трансформациия:

```
tsfm = Transform(params)
transformed_sample = tsfm(sample)
```

- В `torchvision.transforms` находится много готовых трансформеров (см. [https://pytorch.org/docs/stable/torchvision/transforms.html (https://pytorch.org/docs/stable/torchvision/transforms.html)](https://pytorch.org/docs/stable/torchvision/transforms.html)), большая часть ориентирована на преобразование изображений, но есть несколько универсальных инструментов:
  - `torchvision.transforms.Compose` - позволяет создать трансформер из нескольких трансформеров, применяемых последовательно. Пример:

```
transforms.Compose([
    transforms.CenterCrop(10),
    transforms.ToTensor()
])
```

In [7]:

```
# Custom Transforms
# implement __call__(self, sample)
class ToTensor:
    # Convert ndarrays to Tensors
    def __call__(self, sample):
        inputs, targets = sample
        return torch.from_numpy(inputs), torch.from_numpy(targets)
```

In [8]:

```
print('With Tensor Transform')
dataset = WineDataset(transform=ToTensor())

X, y = dataset[0]
print('X:', X, type(X), X.size())
print('y:', y, type(y), y.size())
```

```
With Tensor Transform
X: tensor([1.4230e+01, 1.7100e+00, 2.4300e+00, 1.5600e+01, 1.2700e+02, 2.8000
e+00,
        3.0600e+00, 2.8000e-01, 2.2900e+00, 5.6400e+00, 1.0400e+00, 3.9200e+0
0,
        1.0650e+03]) <class 'torch.Tensor'> torch.Size([13])
y: tensor([1.]) <class 'torch.Tensor'> torch.Size([1])
```

In [9]:

```
class MulTransform:
    # multiply inputs with a given factor
    def __init__(self, factor):
        self.factor = factor

    # multiply imputs by factor:
    def __call__(self, sample):
        inputs, targets = sample
        inputs *= self.factor
        return inputs, targets
```

In [10]:

```
print('With Tensor and Multiplication Transform')
# create composed transformer:
composed_tfms = torchvision.transforms.Compose([ToTensor(), MulTransform(4)])
dataset_mul = WineDataset(transform=composed_tfms)

X, y = dataset_mul[0]
print('X:', X, type(X), X.size())
print('y:', y, type(y), y.size())
```

```
With Tensor and Multiplication Transform
X: tensor([5.6920e+01, 6.8400e+00, 9.7200e+00, 6.2400e+01, 5.0800e+02, 1.1200
e+01,
        1.2240e+01, 1.1200e+00, 9.1600e+00, 2.2560e+01, 4.1600e+00, 1.5680e+0
1,
        4.2600e+03]) <class 'torch.Tensor'> torch.Size([13])
y: tensor([1.]) <class 'torch.Tensor'> torch.Size([1])
```

Имеется модуль `torchvision.transforms.functional` (обычно импортируется как `python import torch.nn.functional as F`) в котором есть множество готовых трансформеров (в основном для преобразования изображений):

- подробнее см.: [https://pytorch.org/docs/stable/torchvision/transforms.html (https://pytorch.org/docs/stable/torchvision/transforms.html)](https://pytorch.org/docs/stable/torchvision/transforms.html)

```
class Normalize(object):
    def __call__(self, tensor):
        """
        Args:
            tensor (Tensor): Tensor image of size (C, H, W) to be normalized.

        Returns:
            Tensor: Normalized Tensor image.
        """
        return F.normalize(tensor, self.mean, self.std, self.inplace)

    def __repr__(self):
        return self.__class__.__name__ + '(mean={0}, std={1})'.format(self.mean, s
elf.std)
```

DataLoader

`DataLoader` подгружает данные, предоставляемые классом `Dataset`, во время тренировки и группирует их в батчи. Он дает возможность указать `Sampler`, который выбирает, какие примеры из датасета использовать для тренировки. Этот параметр можно использовать для разделения данных на training и validation.

`torch.utils.data.DataLoader` это итератор, который обеспечивает:

- организацию данных в батчи (batching the data)
- перемешивание данных (shuffling the data)
- параллельную загрузку данных с использованием multiprocessing workers.

Основные параметры:

- `dataset` (Dataset) – dataset from which to load the data.
- `batch_size` (int, optional) – how many samples per batch to load (default: 1).
- `shuffle` (bool, optional) – set to True to have the data reshuffled at every epoch (default: False).
- `sampler` (Sampler, optional) – defines the strategy to draw samples from the dataset. If specified, shuffle must be False.
- `num_workers` (int, optional) – how many subprocesses to use for data loading. 0 means that the data will be loaded in the main process. (default: 0)

Подробнее см. в: [https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader (https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader)](https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader)

In [11]:

```
# Load whole dataset with DataLoader
# shuffle: shuffle data, good for training
# num_workers: faster loading with multiple subprocesses
# !!! IF YOU GET AN ERROR DURING LOADING, SET num_workers TO 0 !!!
train_loader = DataLoader(dataset=dataset,
                          batch_size=4,
                          shuffle=True,
                          num_workers=0)
```

In [12]:

```
dataiter = iter(train_loader)
data = dataiter.next()
features, labels = data
print('features:', features, features.shape)
print('labels:', labels, labels.shape)
```

```
features: tensor([[1.2880e+01, 2.9900e+00, 2.4000e+00, 2.0000e+01, 1.0400e+0
2, 1.3000e+00,
         1.2200e+00, 2.4000e-01, 8.3000e-01, 5.4000e+00, 7.4000e-01, 1.4200e+
00,
         5.3000e+02],
        [1.3320e+01, 3.2400e+00, 2.3800e+00, 2.1500e+01, 9.2000e+01, 1.9300e+
00,
         7.6000e-01, 4.5000e-01, 1.2500e+00, 8.4200e+00, 5.5000e-01, 1.6200e+
00,
         6.5000e+02],
        [1.3900e+01, 1.6800e+00, 2.1200e+00, 1.6000e+01, 1.0100e+02, 3.1000e+
00,
         3.3900e+00, 2.1000e-01, 2.1400e+00, 6.1000e+00, 9.1000e-01, 3.3300e+
00,
         9.8500e+02],
        [1.3050e+01, 2.0500e+00, 3.2200e+00, 2.5000e+01, 1.2400e+02, 2.6300e+
00,
         2.6800e+00, 4.7000e-01, 1.9200e+00, 3.5800e+00, 1.1300e+00, 3.2000e+
00,
         8.3000e+02]]) torch.Size([4, 13])
labels: tensor([[3.],
        [3.],
        [1.],
        [1.]]) torch.Size([4, 1])
```

In [13]:

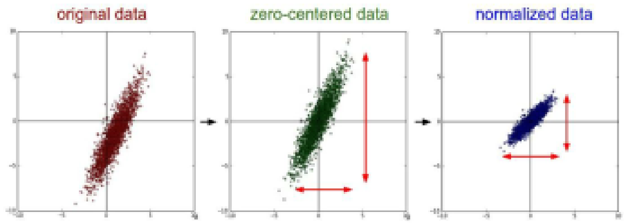
```
# Dummy Training Loop
num_epochs = 2
total_samples = len(dataset)
n_iterations = math.ceil(total_samples/4)
print(total_samples, n_iterations)

for epoch in range(num_epochs):
    for i, (inputs, targets) in enumerate(train_loader):
        # here: 178 samples, batch_size = 4, n_iters=178/4=44.5 -> 45 iterations
        # Run your training process
        if (i+1) % 5 == 0:
            print(f'Epoch: {epoch+1}/{num_epochs}, Step {i+1}/{n_iterations}| Inputs {input
```

```
178 45
Epoch: 1/2, Step 5/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4, 1])
Epoch: 1/2, Step 10/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/2, Step 15/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/2, Step 20/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/2, Step 25/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/2, Step 30/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/2, Step 35/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/2, Step 40/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/2, Step 45/45| Inputs torch.Size([2, 13]) | Labels torch.Size([4,
1])
Epoch: 2/2, Step 5/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4, 1])
Epoch: 2/2, Step 10/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 2/2, Step 15/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 2/2, Step 20/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 2/2, Step 25/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 2/2, Step 30/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 2/2, Step 35/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 2/2, Step 40/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 2/2, Step 45/45| Inputs torch.Size([2, 13]) | Labels torch.Size([4,
1])
```

Нормализация

- к оглавлению



$$x' = \frac{x - \bar{x}}{\sigma}$$

$$\sigma = \frac{\sqrt{(x - \bar{x})^2}}{N - 1}$$

Предобработка данных

In [530]:

```
bs = 4

composed_tfms = transforms.Compose([
            ToTensor()
            # don't use Normalize() for the first time
        ])

dataset = WineDataset(transform=composed_tfms)
```

In [133]:

```
# axes.ndim
```

Out[133]:

```
2
```

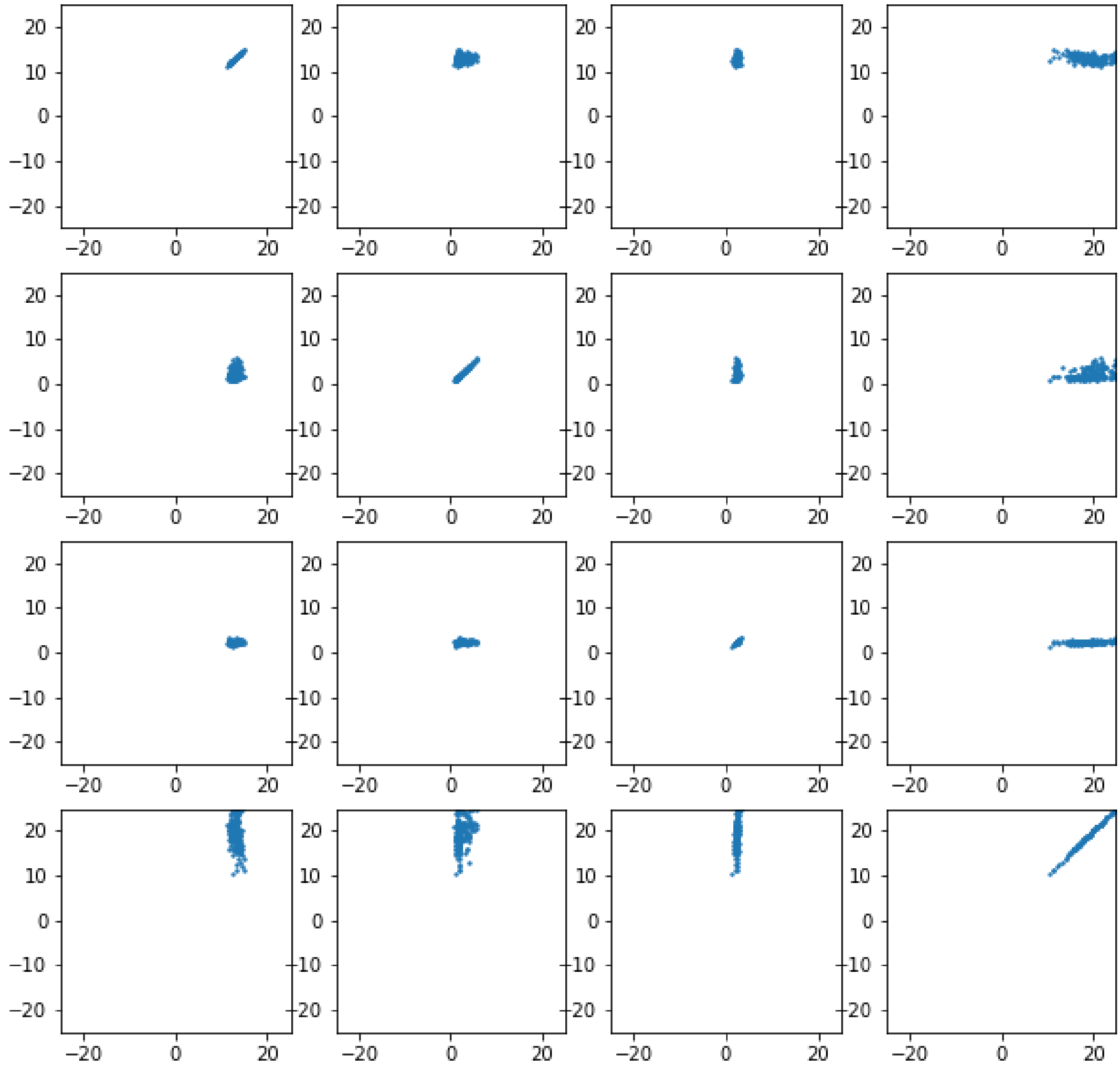
In [531]:

```
# axes.shape
```

In [184]:

```
points = dataset.x_data
fig, axes = plt.subplots(4, 4, figsize=(10, 10))
use_lim = True
lim = 25.0

for i in range(axes.shape[0]):
    for j in range(axes.shape[1]):
        ax = axes[i, j]
        if use_lim:
            ax.set_xlim([-lim, lim])
            ax.set_ylim([-lim, lim])
        ax.scatter(points[:, j], points[:, i], s = 2)
```



In [14]:

```
# получаем среднее по всему датасету:
wine_mean = dataset.x_data.mean(axis=0)
wine_mean
```

Out[14]:

```
array([1.3000614e+01, 2.3363481e+00, 2.3665185e+00, 1.9494946e+01,
       9.9741570e+01, 2.2951121e+00, 2.0292699e+00, 3.6185396e-01,
       1.5908992e+00, 5.0580897e+00, 9.5744956e-01, 2.6116843e+00,
       7.4689325e+02], dtype=float32)
```

In [15]:

```
# получаем стандартное отклонение по всему датасету:
wine_std = dataset.x_data.std(axis=0)
wine_std
```

Out[15]:

```
array([8.0954307e-01, 1.1140037e+00, 2.7357230e-01, 3.3301697e+00,
       1.4242310e+01, 6.2409055e-01, 9.9604911e-01, 1.2410324e-01,
       5.7074893e-01, 2.3117647e+00, 2.2792861e-01, 7.0799321e-01,
       3.1402167e+02], dtype=float32)
```

In [16]:

```
# Тест для фичи 0:

# r = (dataset.x_data - wine_mean)/wine_std
# r[:, 0]
```

In [17]:

```
class Normalize:
    def __init__(self, mean, std, inplace=False):
        self.mean = torch.tensor(mean)
        self.std = torch.tensor(std)
        self.inplace = inplace

    def __call__(self, sample):
        inputs, targets = sample

        if not self.inplace:
            inputs = inputs.clone()
        inputs.sub_(self.mean).div_(self.std)
        return inputs, targets
```

In [18]:

```
batch_size = 4

composed_tfms = transforms.Compose([
            ToTensor(),
            Normalize(wine_mean, wine_std)
        ])

train_ds = WineDataset(transform=composed_tfms)
train_dl = DataLoader(train_ds, batch_size=batch_size, shuffle=False)
```

In [19]:

```
dataiter = iter(train_dl)
data = dataiter.next()
features, labels = data
print('features:', features, features.shape)
print('labels:', labels, labels.shape)
```

```
features: tensor([[ 1.5186, -0.5622,  0.2320, -1.1696,  1.9139,  0.8090,  1.0
348, -0.6596,
          1.2249,  0.2517,  0.3622,  1.8479,  1.0130],
        [ 0.2463, -0.4994, -0.8280, -2.4908,  0.0181,  0.5686,  0.7336, -0.82
07,
         -0.5447, -0.2933,  0.4060,  1.1135,  0.9652],
        [ 0.1969,  0.0212,  1.1093, -0.2687,  0.0884,  0.8090,  1.2155, -0.49
84,
          2.1360,  0.2690,  0.3183,  0.7886,  1.3951],
        [ 1.6916, -0.3468,  0.4879, -0.8093,  0.9309,  2.4914,  1.4665, -0.98
19,
          1.0322,  1.1861, -0.4275,  1.1841,  2.3346]]) torch.Size([4, 13])
labels: tensor([[1.],
        [1.],
        [1.],
        [1.]]) torch.Size([4, 1])
```

In [537]:

```
# Dummy Training loop
num_epochs = 1
total_samples = len(dataset)
n_iterations = math.ceil(total_samples/4)
print(total_samples, n_iterations)

# тензор в котором накапливаются все наблюдения:
inputs_points = None
for epoch in range(num_epochs):
    for i, (inputs, targets) in enumerate(train_dl):
        # here: 178 samples, batch_size = 4, n_iters=178/4=44.5 -> 45 iterations
        # Run your training process
        if inputs_points is None:
            inputs_points = inputs.clone()
        else:
            inputs_points = torch.cat((inputs_points, inputs))

        if (i+1) % 5 == 0:
            print(f'Epoch: {epoch+1}/{num_epochs}, Step {i+1}/{n_iterations}| Inputs {input
```

```
178 45
Epoch: 1/1, Step 5/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4, 1])
Epoch: 1/1, Step 10/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/1, Step 15/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/1, Step 20/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/1, Step 25/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/1, Step 30/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/1, Step 35/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/1, Step 40/45| Inputs torch.Size([4, 13]) | Labels torch.Size([4,
1])
Epoch: 1/1, Step 45/45| Inputs torch.Size([2, 13]) | Labels torch.Size([4,
1])
```

In [538]:

```
inputs_points.size()
```

Out[538]:

```
torch.Size([178, 13])
```

In [181]:

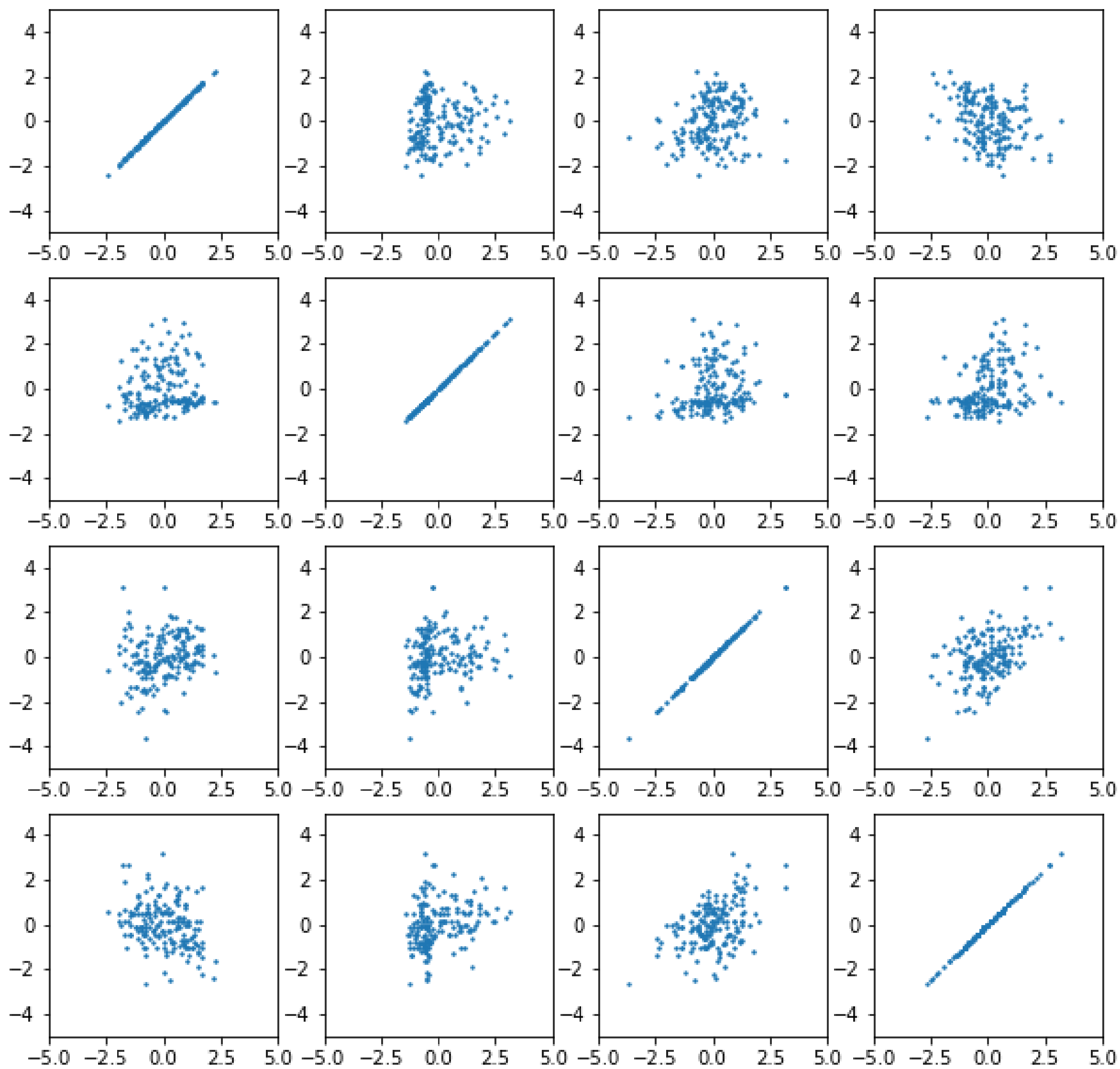
```
# Тест для фичи 0:

# inputs_points[:, 0]
```

In [539]:

```
points = inputs_points
fig, axes = plt.subplots(4, 4, figsize=(10, 10))
use_lim = True
lim = 5.0

for i in range(axes.shape[0]):
    for j in range(axes.shape[1]):
        ax = axes[i, j]
        if use_lim:
            ax.set_xlim([-lim, lim])
            ax.set_ylim([-lim, lim])
        ax.scatter(points[:, j], points[:, i], s = 2)
```



In [ ]:

```
mean, std = np.mean(image), np.std(image)
image = image - mean
image = image / std
```

In [90]:

```
dataset.x_data
```

Out[90]:

```
array([[1.423e+01, 1.710e+00, 2.430e+00, ..., 1.040e+00, 3.920e+00,
        1.065e+03],
       [1.320e+01, 1.780e+00, 2.140e+00, ..., 1.050e+00, 3.400e+00,
        1.050e+03],
       [1.316e+01, 2.360e+00, 2.670e+00, ..., 1.030e+00, 3.170e+00,
        1.185e+03],
       ...,
       [1.327e+01, 4.280e+00, 2.260e+00, ..., 5.900e-01, 1.560e+00,
        8.350e+02],
       [1.317e+01, 2.590e+00, 2.370e+00, ..., 6.000e-01, 1.620e+00,
        8.400e+02],
       [1.413e+01, 4.100e+00, 2.740e+00, ..., 6.100e-01, 1.600e+00,
        5.600e+02]], dtype=float32)
```

Batch normalization

$$x^{(k)} = \frac{x^{(k)} - \mathbb{E}\left[x^{(k)}\right]}{\sqrt{\mathrm{Var}\left[x^{(k)}\right]}}$$

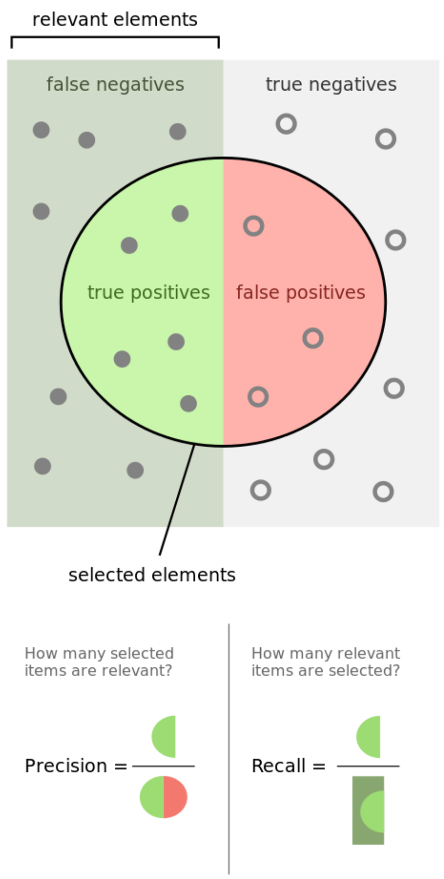
$$y^{(k)} = \gamma^k x^{(k)} + \beta^k$$

- Ускоряет и стаблизирует тренировку
- Регуляризует
- Не так важна инициализация

Оценка качества моделей

- [к оглавлению]

Типы ошибок в двухклассовой классификиации



Предобработка данных

- Правильные ответы:
  - TP - истино-положительное решение
  - TN - истино-отрицательное решение
- Ошибки:
  - FP - ложно-положительное решение (false positive) / ошибка 1го рода
  - FN - ложно-отрицательное решение (false negative) / ошибка 2го рода

Метрики качества

- Тривиальная метрика качества в двухклассовой классификации: $Accuracy = \frac{correct}{total}$.
  - Проблема: при несбалансированном наборе данных (обычно он всегда такой!) тривиальный ответ может давать высокую Accuracy.
- Улучшенные метрики качества:
  - $Precision = \frac{TP}{TP+FP}$ - точность
  - $Recall = \frac{TP}{TP+FN}$ - полнота

F-мера

- Метрика F_1 принимает значения в диапазоне от 0 до 1, учитывает с одинаковым весом точность и полноту:

$$F_1 = 2 \cdot \frac{Precision \cdot Recall}{Precision + Recall}$$

- Обобщенная формула (F-мера), в котрой точность рассматривается, как в β раз более важный параметр чем полнота:

$$F_\beta = (1+\beta^2)\cdot\frac{\text{precision}\cdot\text{recall}}{(\beta^2\cdot\text{precision})+\text{recall}}$$

Перекрестная энтропия

В задаче классификации мы хотим оценить вероятность различных исходов. Если ожидаемая вероятность исхода i это q_i при том что частота (эмпирическая оценка вероятности) исхода i в тренировочном множестве это p_i и всего в тренировочном множестве имеется N исходов тогда правдоподобие в тренировочном множестве пропорционально:

$$\prod_i q_i^{N\cdot p_i}$$

тогда логарифм правдоподобия (log-likelihood) деленный на N это:

$$\frac{1}{N}\log\prod_i q_i^{Np_i} = \sum_i p_i\log q_i = -H(p,q)$$

таким образом максимизация правдоподобия происходит при минимизации функции перекрестной энтропии (cross entropy), определяемой для дискретных случайных величин p и q по формуле:

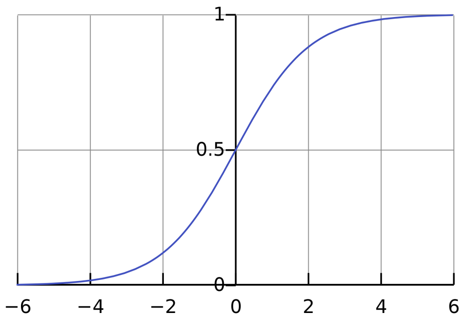
$$H(p,q) = -\sum_{x\in\mathcal{X}} p(x)\ \log q(x)$$

Т.к. в реализации задач оптимизации принято искать параметры модели, при которых достигается минимум (в нашем случае - минимум функции потерь), то обычно минимзируют функцию потерь Negative Log-likelihood:

$$\mathcal{L} = -\sum_i p_i\log q_i = H(p,q)$$

Логистическая регрессия

- Рассмотрим случай **логистической регресии** которая используется для классификации наблюдений на два класса, обозначим их 0 и 1.
- Результат модели для наблюдения, представленного вектором факторов (features) $\mathbf{x}$, может быть интерпретирован как вероятность отнесения наблюдения к одному из классов. Для этого используется **логистическая функция**: $\sigma(z) = 1/(1+e^{-z})$.



Предобработка данных

При этом z это результат преобразования входного вектора $\mathbf{x}$, чаще всего реализуемого с помощью линейной функции: $z = \mathbf{w}\cdot\mathbf{x}$.

- Тогда:
  - веротяноть значения $y = 1$ для наблюдения $\mathbf{x}$:

$$q_{y=1} \;=\; \hat{y} \;\equiv\; \sigma(\mathbf{w}\cdot\mathbf{x}) \;=\; 1/(1+e^{-\mathbf{w}\cdot\mathbf{x}})$$

  - и, соответственно, вероятность значения $y = 0$:

$$q_{y=0} \;=\; 1 - \hat{y}$$

- **Ex:** Например, мы имеем N наблюдений имеющих индексы $n = 1, \dots, N$ и линейную функцию преобразования входного вектора, тогда среднее значение функции потерь:

$$\mathcal{L}(\mathbf{w}) \;=\; \frac{1}{N}\sum_{n=1}^{N} H(p_n, q_n) \;=\; -\frac{1}{N}\sum_{n=1}^{N}\bigg[y_n \log \hat{y}_n + (1-y_n)\log(1-\hat{y}_n)\bigg]\,,$$

где при использовании ленейной функции преобразования имеем
$\hat{y}_n = \sigma(z) = \sigma(\mathbf{w}\cdot\mathbf{x}_n) = 1/(1+e^{-\mathbf{w}\cdot\mathbf{x}_n})$

In [185]:

```
wine_mean, wine_std
```

Out[185]:

```
(array([1.3000614e+01, 2.3363481e+00, 2.3665185e+00, 1.9494946e+01,
        9.9741570e+01, 2.2951121e+00, 2.0292699e+00, 3.6185396e-01,
        1.5908992e+00, 5.0580897e+00, 9.5744956e-01, 2.6116843e+00,
        7.4689325e+02], dtype=float32),
 array([8.0954307e-01, 1.1140037e+00, 2.7357230e-01, 3.3301697e+00,
        1.4242310e+01, 6.2409055e-01, 9.9604911e-01, 1.2410324e-01,
        5.7074893e-01, 2.3117647e+00, 2.2792861e-01, 7.0799321e-01,
        3.1402167e+02], dtype=float32))
```

In [220]:

```
torch.cuda.is_available()
```

Out[220]:

```
False
```

Решение задачи двухклассовой классификации

- к оглавлению

```
Используем:
* результат $z$ преобразования входного вектора $\mathbf{x}$, (чаще всего реализуемого с
помощью линейной функции: $z = \mathbf{w}\cdot\mathbf{x}$) направляем на сигмоиду:
https://pytorch.org/docs/master/generated/torch.nn.Sigmoid.html
* В качестве функции ошибки используем Binary Cross Entropy:
https://pytorch.org/docs/stable/nn.html#torch.nn.BCELoss , используем усреднение по мини
батчу (значение по умолчанию для параметра reduction = 'mean').
```

In [20]:

```
# Device configuration
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')

# parameters:
positive_class_label = 3.0

# Hyper-parameters #1
batch_size = 20
shuffle_dataset = True

class TwoClass:
    def __init__(self, positive_label, inplace=False):
        self.positive_label = positive_label

    def __call__(self, sample):
        inputs, targets = sample
        targets_tc = torch.empty(targets.size())
        targets_tc[targets == self.positive_label] = 1.0
        targets_tc[targets != self.positive_label] = 0.0
#         print(inputs, targets_tc)
        return inputs, targets_tc


composed_tfms = transforms.Compose([
            ToTensor(),
            Normalize(wine_mean, wine_std),
            TwoClass(positive_label=positive_class_label)
        ])

train_ds = WineDataset(transform=composed_tfms)
train_dl = DataLoader(train_ds, batch_size=batch_size, shuffle=shuffle_dataset)


# Get features size:
dataiter = iter(train_dl)
data = dataiter.next()
# print(f'data: {data}')
# features, labels = data
inputs, targets = data

# Hyper-parameters #2
input_size = inputs.shape[1] # use features size
hidden_size = 50
num_classes = 2
print(f'input_size:{input_size}, hidden_size:{hidden_size}, num_classes:{num_classes}')

num_epochs = 30
learning_rate = 0.001


# print('inputs:', inputs, features.shape)
# print('targets:', targets, targets.shape)
# ----------

# Fully connected neural network with one hidden layer
class NNTwoClases(nn.Module):
    def __init__(self, input_size, hidden_size):
        super(NNTwoClases, self).__init__()
        self.input_size = input_size
```

```python
        self.l1 = nn.Linear(input_size, hidden_size)
        self.relu = nn.ReLU()
        self.l2 = nn.Linear(hidden_size, 1) # класса 2 вероятность y^ - одна
        self.sigmoid = nn.Sigmoid()

    def forward(self, x):
        out = self.l1(x)
        out = self.relu(out)
        out = self.l2(out)
        out = self.sigmoid(out)
        return out

model = NNTwoClases(input_size, hidden_size).to(device)

# Loss and optimizer
# see: https://pytorch.org/docs/stable/nn.html#torch.nn.BCELoss
criterion = nn.BCELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)

# Train the model
n_total_steps = len(train_loader)
for epoch in range(num_epochs):
    for i, (inputs, targets_) in enumerate(train_dl):
        inputs = inputs.to(device)
        targets_ = targets_.to(device)

        # Forward pass
        outputs = model(inputs)
#         print(outputs, targets_)
        loss = criterion(outputs, targets_)

        # zero grad before new step
        optimizer.zero_grad()
        # Backward and optimize
        loss.backward()
        optimizer.step()

        if (i+1) % 2 == 0:
            print (f'Epoch [{epoch+1}/{num_epochs}], Step [{i+1}/{n_total_steps}], Loss: {l
```

```
input_size:13, hidden_size:50, num_classes:2
Epoch [1/30], Step [2/45], Loss: 0.7495
Epoch [1/30], Step [4/45], Loss: 0.7350
Epoch [1/30], Step [6/45], Loss: 0.8554
Epoch [1/30], Step [8/45], Loss: 0.7801
Epoch [2/30], Step [2/45], Loss: 0.6953
Epoch [2/30], Step [4/45], Loss: 0.6888
Epoch [2/30], Step [6/45], Loss: 0.6180
Epoch [2/30], Step [8/45], Loss: 0.6512
Epoch [3/30], Step [2/45], Loss: 0.6157
Epoch [3/30], Step [4/45], Loss: 0.5729
Epoch [3/30], Step [6/45], Loss: 0.5860
Epoch [3/30], Step [8/45], Loss: 0.6395
Epoch [4/30], Step [2/45], Loss: 0.5780
Epoch [4/30], Step [4/45], Loss: 0.5651
Epoch [4/30], Step [6/45], Loss: 0.5414
Epoch [4/30], Step [8/45], Loss: 0.4955
Epoch [5/30], Step [2/45], Loss: 0.4989
Epoch [5/30], Step [4/45], Loss: 0.5098
```

Добавляем train/test split:

Разделим данные на training и test с использованием классов `SubsetRandomSampler` и `DataLoader` .

`DataLoader` подгружает данные, предоставляемые классом `Dataset` , во время тренировки и группирует их в батчи. Он дает возможность указать `Sampler` (в нашем случае `SubsetRandomSampler`), который выбирает, какие примеры из датасета использовать для тренировки. Мы используем это, чтобы разделить данные на training и test.

Подробнее: [https://pytorch.org/tutorials/beginner/data_loading_tutorial.html (https://pytorch.org/tutorials/beginner/data_loading_tutorial.html)](https://pytorch.org/tutorials/beginner/data_loading_tutorial.html)

In [227]:

```
# dataset = list(range(178))
# validation_split = .2
# random_seed= 42
# shuffle_dataset = True

# dataset_size = len(dataset)
# indices = list(range(dataset_size))
# split = int(np.floor(validation_split * dataset_size))
# if shuffle_dataset :
#     np.random.seed(random_seed)
#     np.random.shuffle(indices)
# train_indices, val_indices = indices[split:], indices[:split]

# # train_indices, val_indices
```

In [25]:

```
#LOAD DATA

# Device configuration
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')

# parameters:
positive_class_label = 3.0

# Hyper-parameters #1
batch_size = 20
test_split = .2
random_seed= 42
shuffle_dataset = True

composed_tfms = transforms.Compose([
            ToTensor(),
            Normalize(wine_mean, wine_std),
            TwoClass(positive_label=positive_class_label)
        ])

dataset = WineDataset(transform=composed_tfms)

# Creating data indices for training and test splits:
dataset_size = len(dataset)
indices = list(range(dataset_size))
split = int(np.floor(test_split * dataset_size))
if shuffle_dataset :
    np.random.seed(random_seed)
    np.random.shuffle(indices)

train_indices, test_indices = indices[split:], indices[:split]

# Creating PT data samplers and loaders:
train_sampler = SubsetRandomSampler(train_indices)
test_sampler = SubsetRandomSampler(test_indices)

train_dl = torch.utils.data.DataLoader(dataset, batch_size=batch_size,
                                           sampler=train_sampler)
test_dl = torch.utils.data.DataLoader(dataset, batch_size=batch_size,
                                                sampler=test_sampler)

# Get inputs(features) size:
dataiter = iter(train_dl)
data = dataiter.next()
# features, labels = data
inputs, targets = data
# print(f'inputs: {inputs.shape}, {inputs}, targets: {targets.shape}, {targets}')

# parameters:
dataset_num_classes = 2
dataset_input_size = inputs.shape[1]
```

In [26]:

```
# len(train_indices), len(test_indices)
```

In [27]:

```python
# DEFINE MODEL

# Hyper-parameters #2
input_size = dataset_input_size # use inputs size
hidden_size = 50 # 20 | 50
num_classes = dataset_num_classes # 2
print(f'input_size:{input_size}, hidden_size:{hidden_size}, num_classes:{num_classes}')

num_epochs = 60
learning_rate = 0.001

# Fully connected neural network with one hidden layer
class NNTwoClases(nn.Module):
    def __init__(self, input_size, hidden_size):
        super(NNTwoClases, self).__init__()
        self.input_size = input_size
        self.l1 = nn.Linear(input_size, hidden_size)
        self.relu = nn.ReLU() # on|off
        self.l2 = nn.Linear(hidden_size, 1) # класса 2 вероятность y^ - одна
        self.sigmoid = nn.Sigmoid()

    def forward(self, x):
        out = self.l1(x)
        out = self.relu(out) # on|off
        out = self.l2(out)
        out = self.sigmoid(out)
        return out

model = NNTwoClases(input_size, hidden_size).to(device)

# Loss and optimizer
# see: https://pytorch.org/docs/stable/nn.html#torch.nn.BCELoss
criterion = nn.BCELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
```

```
input_size:13, hidden_size:50, num_classes:2
```

In [28]:

```
# TRAINING THE NETWORK
def train(model, device, train_dl, optimizer):
    #set model in train() mode:
    model.train()

    total_loss = 0.0
    total_samples = 0.0
    correct_samples = 0.0

    for i, (inputs, targets) in enumerate(train_dl):
        inputs, targets = inputs.to(device), targets.to(device)

        # Forward pass
        outputs = model(inputs)
        loss = criterion(outputs, targets)

        # Backward and optimize
        # zero grad before new step
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        # calculating the total_loss for checking
        total_loss += loss

        # PREDICTIONS
        total_samples += targets.shape[0]
        predictions = outputs.round()
        correct_samples += torch.sum(predictions==targets)
#         if i ==0:
#             print(f'outputs: {outputs}, predictions:{predictions}, targets:{targets}, cor

    train_accuracy = float(correct_samples) / total_samples

    return total_loss, train_accuracy
```

In [29]:

```
# TESTING THE MODEL
def test(model, device, test_dl):
    #set model in eval() mode (it skips Dropout etc):
    model.eval()

    total_samples = 0.0
    correct_samples = 0.0

    # set the requires_grad flag to false as we are in the test mode
    with torch.no_grad():
        for i, (inputs, targets) in enumerate(test_dl):
            #LOAD THE DATA IN A BATCH
            inputs, targets = inputs.to(device), targets.to(device)

            # apply model to input data
            outputs = model(inputs)

            #PREDICTIONS
            total_samples += targets.shape[0]
            predictions = outputs.round()
            correct_samples += torch.sum(predictions==targets)

    test_accuracy = correct_samples / total_samples

    return test_accuracy
```

In [30]:

```
# Train the model
n_total_steps = len(train_loader)
for epoch in range(num_epochs):
    total_loss, train_accuracy = train(model, device, train_dl, optimizer)
    test_accuracy = test(model, device, test_dl)
    print (f'Epoch [{epoch+1}/{num_epochs}], Loss: {total_loss:.4f}, Train acc: {train_accu
```

```
Epoch [1/60], Loss: 5.4664, Train acc: 0.5944, Test acc: 0.8286
Epoch [2/60], Loss: 5.0799, Train acc: 0.7972, Test acc: 0.9429
Epoch [3/60], Loss: 4.5665, Train acc: 0.9161, Test acc: 0.9714
Epoch [4/60], Loss: 4.1883, Train acc: 0.9650, Test acc: 1.0000
Epoch [5/60], Loss: 3.8292, Train acc: 0.9790, Test acc: 1.0000
Epoch [6/60], Loss: 3.4566, Train acc: 0.9860, Test acc: 1.0000
Epoch [7/60], Loss: 3.2074, Train acc: 0.9860, Test acc: 1.0000
Epoch [8/60], Loss: 2.9398, Train acc: 0.9860, Test acc: 1.0000
Epoch [9/60], Loss: 2.5663, Train acc: 0.9860, Test acc: 1.0000
Epoch [10/60], Loss: 2.3269, Train acc: 0.9860, Test acc: 1.0000
Epoch [11/60], Loss: 2.2346, Train acc: 0.9860, Test acc: 1.0000
Epoch [12/60], Loss: 1.9347, Train acc: 0.9860, Test acc: 1.0000
Epoch [13/60], Loss: 1.8830, Train acc: 0.9860, Test acc: 1.0000
Epoch [14/60], Loss: 1.5720, Train acc: 0.9930, Test acc: 1.0000
Epoch [15/60], Loss: 1.4696, Train acc: 0.9930, Test acc: 1.0000
Epoch [16/60], Loss: 1.3034, Train acc: 0.9930, Test acc: 1.0000
Epoch [17/60], Loss: 1.2106, Train acc: 0.9860, Test acc: 1.0000
Epoch [18/60], Loss: 1.1196, Train acc: 0.9930, Test acc: 1.0000
Epoch [19/60], Loss: 1.0060, Train acc: 0.9930, Test acc: 1.0000
Epoch [20/60], Loss: 1.0122, Train acc: 0.9930, Test acc: 1.0000
Epoch [21/60], Loss: 0.8501, Train acc: 0.9930, Test acc: 1.0000
Epoch [22/60], Loss: 0.8039, Train acc: 0.9930, Test acc: 1.0000
Epoch [23/60], Loss: 0.8261, Train acc: 0.9930, Test acc: 1.0000
Epoch [24/60], Loss: 0.7375, Train acc: 0.9930, Test acc: 1.0000
Epoch [25/60], Loss: 0.7203, Train acc: 0.9930, Test acc: 1.0000
Epoch [26/60], Loss: 0.6068, Train acc: 0.9930, Test acc: 1.0000
Epoch [27/60], Loss: 0.5874, Train acc: 0.9930, Test acc: 1.0000
Epoch [28/60], Loss: 0.5480, Train acc: 0.9930, Test acc: 1.0000
Epoch [29/60], Loss: 0.5097, Train acc: 0.9930, Test acc: 1.0000
Epoch [30/60], Loss: 0.5061, Train acc: 0.9930, Test acc: 1.0000
Epoch [31/60], Loss: 0.4763, Train acc: 0.9930, Test acc: 1.0000
Epoch [32/60], Loss: 0.4572, Train acc: 0.9930, Test acc: 1.0000
Epoch [33/60], Loss: 0.4224, Train acc: 0.9930, Test acc: 1.0000
Epoch [34/60], Loss: 0.4069, Train acc: 0.9930, Test acc: 1.0000
Epoch [35/60], Loss: 0.3965, Train acc: 0.9930, Test acc: 1.0000
Epoch [36/60], Loss: 0.3881, Train acc: 0.9930, Test acc: 1.0000
Epoch [37/60], Loss: 0.3503, Train acc: 0.9930, Test acc: 1.0000
Epoch [38/60], Loss: 0.3362, Train acc: 0.9930, Test acc: 1.0000
Epoch [39/60], Loss: 0.3390, Train acc: 0.9930, Test acc: 1.0000
Epoch [40/60], Loss: 0.3132, Train acc: 0.9930, Test acc: 1.0000
Epoch [41/60], Loss: 0.3889, Train acc: 0.9930, Test acc: 1.0000
Epoch [42/60], Loss: 0.2962, Train acc: 0.9930, Test acc: 1.0000
Epoch [43/60], Loss: 0.2796, Train acc: 0.9930, Test acc: 1.0000
Epoch [44/60], Loss: 0.2756, Train acc: 0.9930, Test acc: 1.0000
Epoch [45/60], Loss: 0.2591, Train acc: 0.9930, Test acc: 1.0000
Epoch [46/60], Loss: 0.2502, Train acc: 0.9930, Test acc: 1.0000
Epoch [47/60], Loss: 0.2609, Train acc: 0.9930, Test acc: 1.0000
Epoch [48/60], Loss: 0.2434, Train acc: 0.9930, Test acc: 1.0000
Epoch [49/60], Loss: 0.2276, Train acc: 0.9930, Test acc: 1.0000
Epoch [50/60], Loss: 0.2262, Train acc: 0.9930, Test acc: 1.0000
Epoch [51/60], Loss: 0.2179, Train acc: 0.9930, Test acc: 1.0000
```

```
Epoch [52/60], Loss: 0.2233, Train acc: 0.9930, Test acc: 1.0000
Epoch [53/60], Loss: 0.2027, Train acc: 0.9930, Test acc: 1.0000
Epoch [54/60], Loss: 0.2130, Train acc: 0.9930, Test acc: 1.0000
Epoch [55/60], Loss: 0.1923, Train acc: 1.0000, Test acc: 1.0000
Epoch [56/60], Loss: 0.1872, Train acc: 1.0000, Test acc: 1.0000
Epoch [57/60], Loss: 0.1932, Train acc: 1.0000, Test acc: 1.0000
Epoch [58/60], Loss: 0.1779, Train acc: 1.0000, Test acc: 1.0000
Epoch [59/60], Loss: 0.1795, Train acc: 1.0000, Test acc: 1.0000
Epoch [60/60], Loss: 0.3433, Train acc: 1.0000, Test acc: 1.0000
```

Обобщение на задачу многоклассовой классификаци

- к оглавлению

- **Def:** Функяия **softmax** (или _normalized exponential function_) — это обобщение логистической функции для многомерного случая.
  - Функция преобразует вектор $\mathbf{z}$ размерности K в вектор σ той же размерности, где каждая координата σ_i полученного вектора представлена вещественным числом в интервале $[0, 1]$:
  $$\sigma(\mathbf{z})_i = \frac{e^{z_i}}{\sum\limits_{k=1}^{K} e^{z_k}}$$
  - Легко показать, что:
    - сумма координат равна $\sum_{k=1}^{K} \sigma(\mathbf{z})_k = 1$.
    - и каждое из значений $\sigma(\mathbf{z})_i \in [0, 1]$.
  - Таким образом, функция берет на вход вектор $\mathbf{z}$ содержащий значения, которые могут выходить за интервал $[0, 1]$ преобразуя их вектор σ, который может рассматриваться как вероятности K значений дискретной случайной величины.
  - При этом, наибольшее значение среди K компонент вектора $\mathbf{z}$ осатется наибольшей в векторе σ (соотношение максимального компонента к остальным увеличвиается т.к.: $\sigma(\mathbf{z})_i/\sigma(\mathbf{z})_j = e^{z_i - z_j} > 1$, если $z_i > z_j$

- Применяя softmax в функции потерь negative log-likelihood получим:

$$\mathcal{L} = -\sum_i p_i \log q_i = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \ln y_{nk} = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk} \frac{e^{z_{nk}}}{\sum\limits_{i=1}^{K} e^{z_{ni}}} = -\sum_{n=1}^{N} \frac{e^{z_{nk(n)}}}{\sum\limits_{i=1}^{K} e^{z_{ni}}}$$

где, при использовании ленейной функции преобразования входного вектора $\mathbf{x}$ в z, имеем $z_{nk} = \sigma(\mathbf{w}_k \cdot \mathbf{x}_n)$

In [38]:

```
#LOAD DATA

# Device configuration
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')

# Hyper-parameters #1
batch_size = 20
validation_split = .2
random_seed= 42
shuffle_dataset = True

composed_tfms = transforms.Compose([
            ToTensor(),
            Normalize(wine_mean, wine_std) # without TwoClass
        ])

dataset = WineDataset(transform=composed_tfms)

# Creating data indices for training and test splits:
dataset_size = len(dataset)
indices = list(range(dataset_size))
split = int(np.floor(validation_split * dataset_size))
if shuffle_dataset :
    np.random.seed(random_seed)
    np.random.shuffle(indices)

train_indices, test_indices = indices[split:], indices[:split]

# Creating PT data samplers and loaders:
train_sampler = SubsetRandomSampler(train_indices)
test_sampler = SubsetRandomSampler(test_indices)

train_dl = torch.utils.data.DataLoader(dataset, batch_size=batch_size,
                                           sampler=train_sampler)
test_dl = torch.utils.data.DataLoader(dataset, batch_size=batch_size,
                                                sampler=test_sampler)

# Get inputs(features) size:
dataiter = iter(train_dl)
data = dataiter.next()
# features, labels = data
inputs, targets = data
# print(f'inputs: {inputs.shape}, {inputs}, targets: {targets.shape}, {targets}')

# parameters:
dataset_num_classes = 3
dataset_input_size = inputs.shape[1]
```

Решаем задачу многоклассовой классификации

- Используем CrossEntropyLoss: [https://pytorch.org/docs/stable/nn.html#crossentropyloss (https://pytorch.org/docs/stable/nn.html#crossentropyloss)](https://pytorch.org/docs/stable/nn.html#crossentropyloss)
    - This criterion combines `nn.LogSoftmax()` and `nn.NLLLoss()` in one single class.
    - Input: (N, C)(N,C) where C = number of classes

- Target: (N)(N) where each value is $0 \le \text{targets}[i] \le C-1$
- Default: `reduction='mean'`

In [39]:

```
# DEFINE MODEL

# Hyper-parameters #2
input_size = dataset_input_size # use inputs(features) size
hidden_size = 50
num_classes = dataset_num_classes # (не можем получить из минибатча)
print(f'input_size:{input_size}, hidden_size:{hidden_size}, num_classes:{num_classes}')

num_epochs = 60
learning_rate = 0.001

# Fully connected neural network with one hidden layer
class NClases(nn.Module):
    def __init__(self, input_size, hidden_size, num_classes): # new parameter: num_classes
        super(NClases, self).__init__()
        self.input_size = input_size
        self.l1 = nn.Linear(input_size, hidden_size)
        self.relu = nn.ReLU() # on|off
        self.l2 = nn.Linear(hidden_size, num_classes)

    def forward(self, x):
        out = self.l1(x)
        out = self.relu(out) # on|off
        out = self.l2(out)
        # no activation and no softmax at the end
        return out

model = NClases(input_size, hidden_size, num_classes).to(device)

# Loss and optimizer
# criterion = nn.BCELoss()
criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
```

```
input_size:13, hidden_size:50, num_classes:3
```

- `torch.max()` : `torch.max(input, dim, keepdim=False, out=None) -> (Tensor, LongTensor)`
  - parameters:
    - `input (Tensor)` – the input tensor.
    - `dim (int)` – the dimension to reduce.
    - `keepdim (bool)` – whether the output tensor has dim retained or not. Default: False.
    - `out (tuple, optional)` – the result tuple of two output tensors (max, max_indices)
  - returns namedtuple `(values, indices)`
    - `values` is the maximum value of each row of the input tensor in the given dimension dim.
    - `indices` is the index location of each maximum value found (argmax).

In [40]:

```
# TRAINING THE NETWORK
def train(model, device, train_dl, optimizer):
    #set model in train() mode:
    model.train()

    total_loss = 0.0
    total_samples = 0.0
    correct_samples = 0.0

    for i, (inputs, targets) in enumerate(train_dl):
        inputs, targets = inputs.to(device), targets.to(device)
        targets = targets.squeeze().to(torch.long)-1 # target mast be 1-D tensor

        # Forward pass
        outputs = model(inputs)
        loss = criterion(outputs, targets.squeeze())

        # Backward and optimize
        # zero grad before new step
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        # calculating the total_loss for checking
        total_loss += loss

        # PREDICTIONS
        total_samples += targets.shape[0]
        _, predictions_indices = torch.max(outputs, 1) # dim=1 - dimension to reduce
        correct_samples += torch.sum(predictions_indices==targets)
#         if i == 0:
#             print(f'outputs: {outputs}, predictions_indices:{predictions_indices}, \
#             targets:{targets}, correct_samples:{correct_samples}, total_samples: {total_s

    train_accuracy = float(correct_samples) / total_samples

    return total_loss, train_accuracy
```

In [41]:

```python
# TESTING THE MODEL
def test(model, device, test_dl):
    #set model in eval() mode (it skips Dropout etc):
    model.eval()

    total_samples = 0.0
    correct_samples = 0.0

    # set the requires_grad flag to false as we are in the test mode
    with torch.no_grad():
        for i, (inputs, targets) in enumerate(test_dl):
            #LOAD THE DATA IN A BATCH
            inputs, targets = inputs.to(device), targets.to(device)
            targets = targets.squeeze().to(torch.long)-1 # target mast be 1-D tensor

            # apply model to input data
            outputs = model(inputs)

            #PREDICTIONS
            total_samples += targets.shape[0]
            _, predictions_indices = torch.max(outputs, 1) # dim=1 - dimension to reduce
            correct_samples += torch.sum(predictions_indices==targets)

    test_accuracy = correct_samples / total_samples

    return test_accuracy
```

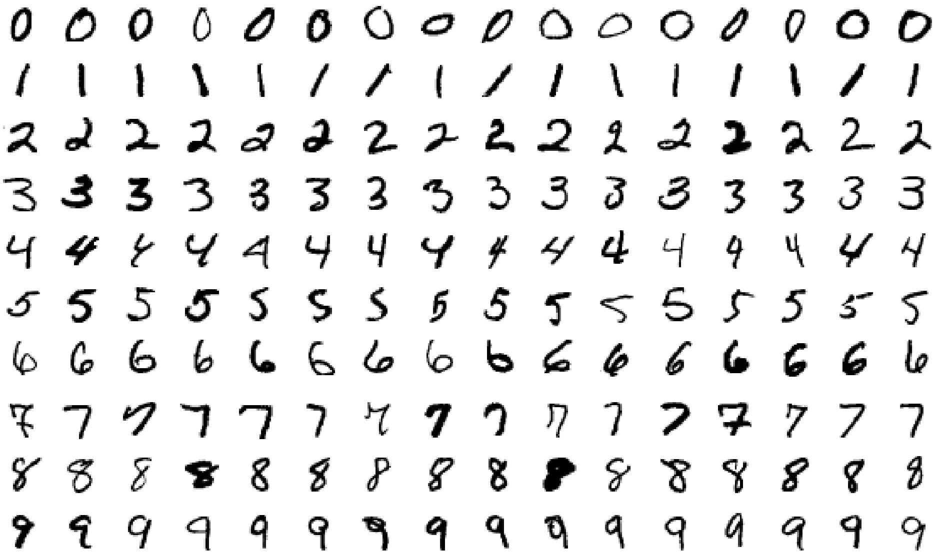
In [42]:

```python
# Train the model
n_total_steps = len(train_loader)
for epoch in range(num_epochs):
    total_loss, train_accuracy = train(model, device, train_dl, optimizer)
    test_accuracy = test(model, device, test_dl)
    print (f'Epoch [{epoch+1}/{num_epochs}], Loss: {total_loss:.4f}, Train acc: {train_accu
```

```
Epoch [40/60], Loss: 0.4045, Train acc: 0.9930, Test acc: 1.0000
Epoch [41/60], Loss: 0.5643, Train acc: 0.9930, Test acc: 1.0000
Epoch [42/60], Loss: 0.3527, Train acc: 0.9930, Test acc: 1.0000
Epoch [43/60], Loss: 0.6883, Train acc: 0.9930, Test acc: 1.0000
Epoch [44/60], Loss: 0.4221, Train acc: 0.9930, Test acc: 1.0000
Epoch [45/60], Loss: 0.3322, Train acc: 0.9930, Test acc: 1.0000
Epoch [46/60], Loss: 0.3677, Train acc: 1.0000, Test acc: 1.0000
Epoch [47/60], Loss: 0.3023, Train acc: 1.0000, Test acc: 1.0000
Epoch [48/60], Loss: 0.2996, Train acc: 1.0000, Test acc: 1.0000
Epoch [49/60], Loss: 0.2730, Train acc: 1.0000, Test acc: 1.0000
Epoch [50/60], Loss: 0.2866, Train acc: 0.9930, Test acc: 1.0000
Epoch [51/60], Loss: 0.2647, Train acc: 0.9930, Test acc: 1.0000
Epoch [52/60], Loss: 0.2690, Train acc: 0.9930, Test acc: 1.0000
Epoch [53/60], Loss: 0.3243, Train acc: 1.0000, Test acc: 1.0000
Epoch [54/60], Loss: 0.2467, Train acc: 1.0000, Test acc: 1.0000
Epoch [55/60], Loss: 0.2481, Train acc: 1.0000, Test acc: 1.0000
Epoch [56/60], Loss: 0.2190, Train acc: 1.0000, Test acc: 1.0000
Epoch [57/60], Loss: 0.2259, Train acc: 1.0000, Test acc: 1.0000
Epoch [58/60], Loss: 0.2108, Train acc: 1.0000, Test acc: 1.0000
Epoch [59/60], Loss: 0.2068, Train acc: 1.0000, Test acc: 1.0000
```

Многоклассовая классификация на датасете MNIST

https://en.wikipedia.org/wiki/MNIST_database (https://en.wikipedia.org/wiki/MNIST_database)



Примеры изображений из MNIST

In [43]:

```
#LOAD DATA

# Device configuration
device = torch.device('cuda' if torch.cuda.is_available() else 'cpu')

# parameters:
positive_class_label = 3.0

# Hyper-parameters #1
batch_size = 100 # big batches
validation_split = .2
random_seed= 42
shuffle_dataset = True

# MNIST dataset
train_dataset = torchvision.datasets.MNIST(root='./data',
                                           train=True,
                                           transform=transforms.ToTensor(),
                                           download=True)

train_batch_qty = math.ceil(len(train_dataset)/batch_size)

test_dataset = torchvision.datasets.MNIST(root='./data',
                                          train=False,
                                          transform=transforms.ToTensor())
test_batch_qty = math.ceil(len(test_dataset)/batch_size)

# Data loader
train_dl = torch.utils.data.DataLoader(dataset=train_dataset,
                                           batch_size=batch_size,
                                           shuffle=shuffle_dataset)

test_dl = torch.utils.data.DataLoader(dataset=test_dataset,
                                          batch_size=batch_size,
                                          shuffle=False)

# # Get inputs(features) size:
# dataiter = iter(train_dl)
# data = dataiter.next()
# # features, labels = data
# inputs, targets = data
# # print(f'inputs: {inputs.shape}, {inputs}, targets: {targets.shape}, {targets}')

# parameters:
dataset_num_classes = 10
# dataset_input_size = inputs.shape[1]
dataset_input_size = 28 * 28 # 28x28=784
```

In [48]:

```
# DEFINE MODEL

# Hyper-parameters #2
input_size = dataset_input_size # use inputs(features) size
hidden_size = 500
num_classes = dataset_num_classes # (не можем получить из минибатча)
print(f'input_size:{input_size}, hidden_size:{hidden_size}, num_classes:{num_classes}')

num_epochs = 10
learning_rate = 0.001

# Create fully connected neural network with one hidden layer:
model = NClases(input_size, hidden_size, num_classes).to(device)

# Loss and optimizer
# criterion = nn.BCELoss()
criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
```

```
input_size:784, hidden_size:500, num_classes:10
```

In [49]:

```
#  tqdm import tqdm
# import tqdm.notebook.tqdm
from tqdm.notebook import tqdm
import sys
```

In [50]:

```
for i in tqdm(range(100)):
    time.sleep(0.03)
```

100% 100/100 [00:17<00:00, 5.84it/s]

In [51]:

```
# TRAINING THE NETWORK
def train(model, device, train_dl, optimizer):
    #set model in train() mode:
    model.train()

    total_loss = 0.0
    total_samples = 0.0
    correct_samples = 0.0

    for i, (inputs, targets) in tqdm(enumerate(train_dl), total=train_batch_qty, desc='Trai
        inputs, targets = inputs.to(device), targets.to(device)
        inputs = inputs.reshape(-1, 28*28).to(device)
#         print(inputs.size(), targets.size(), targets)
#         assert False

        # Forward pass
        outputs = model(inputs)
        loss = criterion(outputs, targets.squeeze())

        # Backward and optimize
        # zero grad before new step
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        # calculating the total_loss for checking
        total_loss += loss

        # PREDICTIONS
        total_samples += targets.shape[0]
        _, predictions_indices = torch.max(outputs, 1) # dim=1 - dimension to reduce
        correct_samples += torch.sum(predictions_indices==targets)
#         if i == 0:
#             print(f'outputs: {outputs}, predictions_indices:{predictions_indices}, \
#             targets:{targets}, correct_samples:{correct_samples}, total_samples: {total_s

    train_accuracy = float(correct_samples) / total_samples

    return total_loss, train_accuracy
```

In [52]:

```
# TESTING THE MODEL
def test(model, device, test_dl):
    #set model in eval() mode (it skips Dropout etc):
    model.eval()

    total_samples = 0.0
    correct_samples = 0.0

    # set the requires_grad flag to false as we are in the test mode
    with torch.no_grad():
        for i, (inputs, targets) in tqdm(enumerate(test_dl), total=test_batch_qty, desc='Te
            #LOAD THE DATA IN A BATCH
            inputs, targets = inputs.to(device), targets.to(device)
            inputs = inputs.reshape(-1, 28*28).to(device)

            # apply model to input data
            outputs = model(inputs)

            #PREDICTIONS
            total_samples += targets.shape[0]
            _, predictions_indices = torch.max(outputs, 1) # dim=1 - dimension to reduce
            correct_samples += torch.sum(predictions_indices==targets)

    test_accuracy = correct_samples / total_samples

    return test_accuracy
```

In [53]:

```
# Train the model
n_total_steps = len(train_loader)
for epoch in range(num_epochs):
    total_loss, train_accuracy = train(model, device, train_dl, optimizer)
    test_accuracy = test(model, device, test_dl)
    print (f'Epoch [{epoch+1}/{num_epochs}], Loss: {total_loss:.4f}, Train acc: {train_accu
```

Training minibatch loop : 100% 600/600 [00:15<00:00, 39.02it/s]

Testing minibatch loop:: 100% 100/100 [00:18<00:00, 5.40it/s]

```
Epoch [1/10], Loss: 174.7974, Train acc: 0.9190, Test acc: 0.9538
```

Training minibatch loop : 100% 600/600 [00:16<00:00, 36.45it/s]

Testing minibatch loop:: 100% 100/100 [00:02<00:00, 47.09it/s]

```
Epoch [2/10], Loss: 70.6127, Train acc: 0.9654, Test acc: 0.9728
```

Training minibatch loop : 100% 600/600 [00:16<00:00, 36.01it/s]

Testing minibatch loop:: 100% 100/100 [00:02<00:00, 46.06it/s]

```
Epoch [3/10], Loss: 46.1081, Train acc: 0.9772, Test acc: 0.9761
```

Training minibatch loop : 100% 600/600 [00:16<00:00, 36.47it/s]

Testing minibatch loop:: 100% 100/100 [00:18<00:00, 5.35it/s]

```
Epoch [4/10], Loss: 32.0094, Train acc: 0.9843, Test acc: 0.9773
```

Training minibatch loop : 100% 600/600 [00:16<00:00, 36.42it/s]

Testing minibatch loop:: 100% 100/100 [00:02<00:00, 47.99it/s]

```
Epoch [5/10], Loss: 24.0859, Train acc: 0.9879, Test acc: 0.9759
```

Training minibatch loop : 100% 600/600 [00:19<00:00, 31.52it/s]

Testing minibatch loop:: 100% 100/100 [00:02<00:00, 47.33it/s]

```
Epoch [6/10], Loss: 18.6134, Train acc: 0.9910, Test acc: 0.9784
```

Training minibatch loop : 100% 600/600 [00:16<00:00, 36.92it/s]

Testing minibatch loop:: 100% 100/100 [00:18<00:00, 5.34it/s]

```
Epoch [7/10], Loss: 13.5114, Train acc: 0.9940, Test acc: 0.9805
```

Training minibatch loop : 100% 600/600 [00:16<00:00, 36.16it/s]

Testing minibatch loop:: 100% 100/100 [00:02<00:00, 47.47it/s]

```
Epoch [8/10], Loss: 9.9926, Train acc: 0.9951, Test acc: 0.9804
```

Training minibatch loop : 100% 600/600 [00:17<00:00, 34.27it/s]

Testing minibatch loop:: 100% 100/100 [00:02<00:00, 48.97it/s]

```
Epoch [9/10], Loss: 8.5921, Train acc: 0.9961, Test acc: 0.9810
```

Training minibatch loop : 100% 600/600 [00:17<00:00, 35.14it/s]

Testing minibatch loop:: 100% 100/100 [00:02<00:00, 47.62it/s]

```
Epoch [10/10], Loss: 6.1767, Train acc: 0.9974, Test acc: 0.9801
```

In [ ]: