In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.nn.init as init


from torch.utils.data import Dataset, DataLoader
```

Data generation: You are tasked with generating simulated data to represent microscopic images of subjects, some of whom have been diagnosed with cancer. The data generation process involves creating a 32x32 matrix for each subject to simulate microscopic images, using the following specifications: For each subject, a label yi indicates the presence (1) or absence (0) of cancer. This label is generated using a Bernoulli distribution with a probability of 0.5. The image matrix $\boldsymbol{Xi}$ for each subject is produced as $\boldsymbol{Xi} = \boldsymbol{Bi} + \boldsymbol{\epsilon i}$, where $\boldsymbol{Bi}$ represents the signal matrix and ϵi is random noise following a normal distribution $N(0, 0.04)$. The signal matrix $\boldsymbol{Bi}$ is generated by first determining the number of macrovesicle pixels mi using a Poisson distribution with parameters dependent on the subject's cancer status, and then randomly assigning these pixels in the matrix:

Determine the number of macrovesicle pixels m_i using a poisson distribution with parameters dependent on subject cancer status, and then randomly assigning these pixels in the matrix:

• Generate number of macrovesicle pixels mi: mi follows Poisson distribution with parameter $\mu c yi + \mu n(1 - yi)$. In other words, if the i th subject has cancer, its associated mi follows Poisson(μc); Otherwise, its associated mi follows Poisson(μn). For this simulation, we consider μn = 5, and μc = 10, 20, 30, respectively.

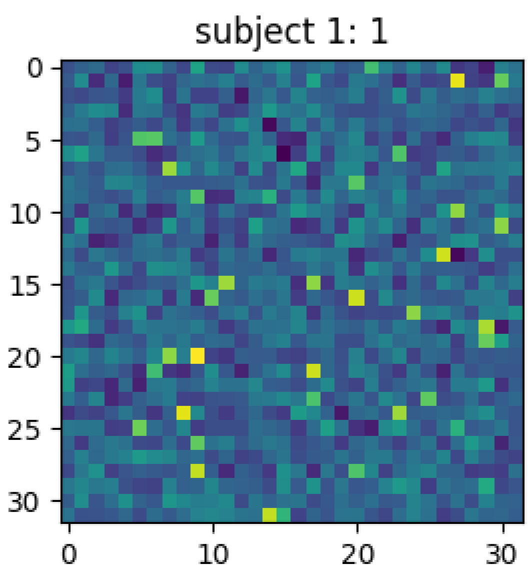
• Randomly select mi pixels from $\boldsymbol{Bi}$ as 1, and set all other pixels as 0.

In [2]:
```
def simulateData(n, mu_c, mu_n):

    y = np.random.choice([0, 1], size = n, p = [0.5, 0.5])
    m_i = np.random.poisson(lam = mu_c, size = n) * y + np.random.poisson(lam = mu_n,

    simulated_data = np.zeros([n, 32, 32])
    for i in range(n):
        random_indices = np.random.choice(32 * 32, m_i[i], replace = False)
        row_indices, col_indices = np.unravel_index(random_indices, (32, 32))
        Bi = np.zeros([32, 32])
        Bi[row_indices, col_indices] = 1
        epsilon_i = np.random.normal(loc = 0, scale = np.sqrt(0.04), size = (32, 32))
        simulated_data[i] = Bi + epsilon_i

    return y, simulated_data
```

In [3]:
```
n = [200, 500, 1000, 200, 500, 1000, 200, 500, 1000]
mu_n = [5, 5, 5, 5, 5, 5, 5, 5, 5]
mu_c = [10, 10, 10, 20, 20, 20, 30, 30, 30]
```

In [4]:
```
simulated_datasets_list = []
simulated_y_list = []
for i in range(9):

    y, simulated_data = simulateData(n = n[i],
                                     mu_c = mu_c[i],
                                     mu_n = mu_n[i])

    simulated_datasets_list.append(simulated_data)
    simulated_y_list.append(y)
```

In [5]:
```
subject = 0
plt.figure(figsize=(3, 3))
plt.imshow(simulated_datasets_list[8][subject, :, :])
plt.title('subject ' + str(subject + 1) + ': ' + str(y[subject]))
plt.show()
```



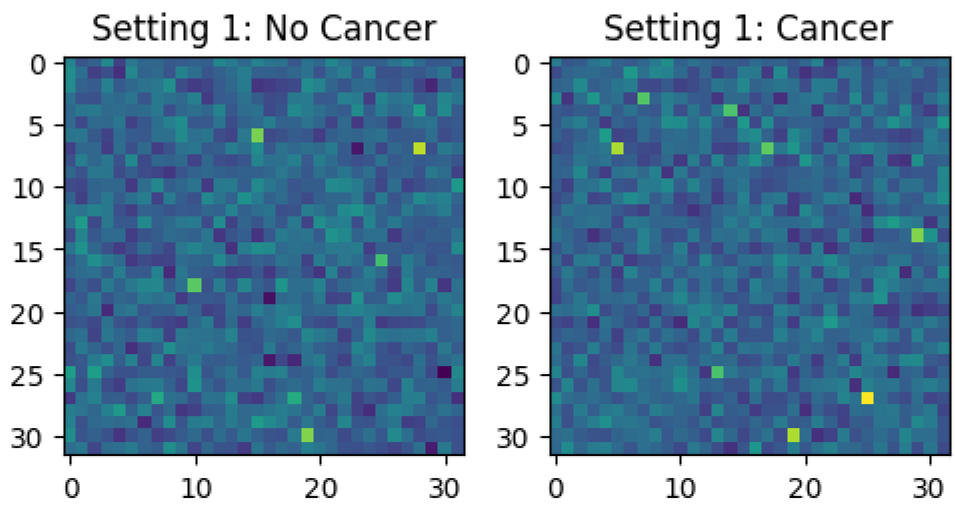
Question 1

Data visualization: Visualize the generated images for settings 1, 4, and 7. For each setting, display one image from a subject without cancer yi = 0 and one from a subject with cancer yi = 1. In total, six images should be visualized, highlighting the differences in the simulated microscopic images between normal and cancerous subjects.

Setting 1: (N μn μc) = (200 5 10)

In [6]:
```
setting1_data = simulated_datasets_list[0]
setting1_y = simulated_y_list[0]

indices_0_y = np.where(setting1_y == 0)
setting1_example_0 = setting1_data[indices_0_y][0, :, :]

indices_1_y = np.where(setting1_y == 1)
setting1_example_1 = setting1_data[indices_1_y][0, :, :]

min_range = np.min([setting1_example_0.min(), setting1_example_1.min()])
```

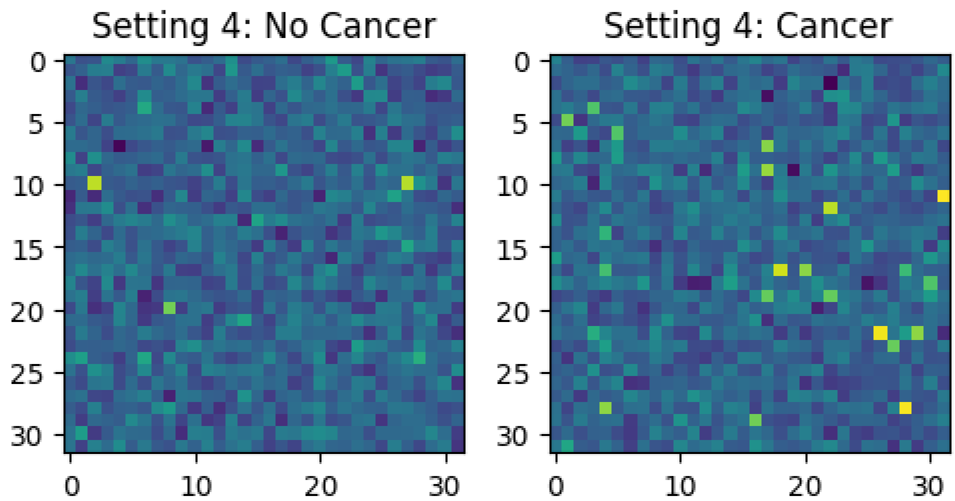
```
max_range = np.max([setting1_example_0.max(), setting1_example_1.max()])

plt.figure(figsize=(5, 5))
plt.subplot(1, 2, 1)
plt.imshow(setting1_example_0, vmin=min_range, vmax=max_range)
plt.title('Setting 1: No Cancer')

plt.subplot(1, 2, 2)
plt.imshow(setting1_example_1, vmin=min_range, vmax=max_range)
plt.title('Setting 1: Cancer')

plt.tight_layout()
```



Setting 4: (N μn μc) = (200 5 20)

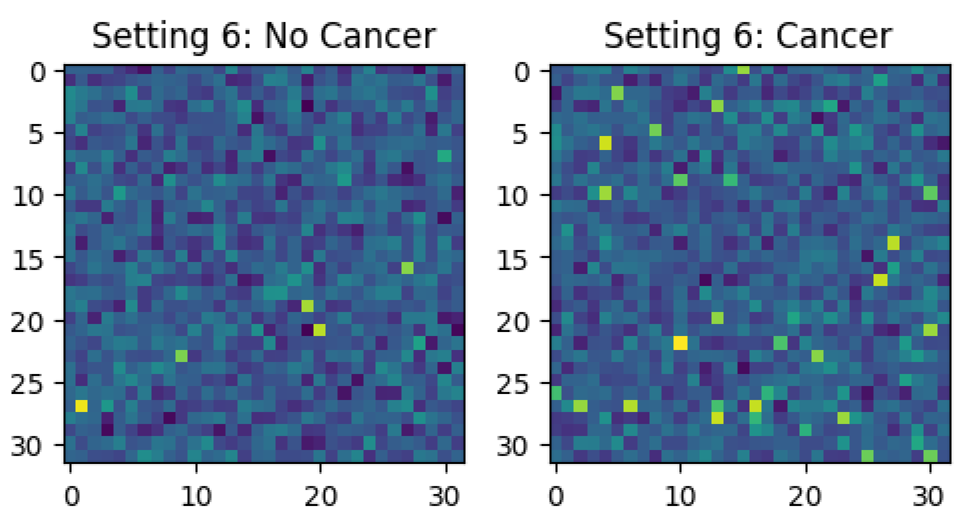
In [7]:

```
setting4_data = simulated_datasets_list[3]
setting4_y = simulated_y_list[3]

indices_0_y = np.where(setting4_y == 0)
setting4_example_0 = setting4_data[indices_0_y][0, :, :]

indices_1_y = np.where(setting4_y == 1)
setting4_example_1 = setting4_data[indices_1_y][0, :, :]

min_range = np.min([setting4_example_0.min(), setting4_example_1.min()])
max_range = np.max([setting4_example_0.max(), setting4_example_1.max()])

plt.figure(figsize=(5, 5))
plt.subplot(1, 2, 1)
plt.imshow(setting4_example_0, vmin=min_range, vmax=max_range)
plt.title('Setting 4: No Cancer')

plt.subplot(1, 2, 2)
plt.imshow(setting4_example_1, vmin=min_range, vmax=max_range)
plt.title('Setting 4: Cancer')
plt.tight_layout()
```



Setting 7: (N μn μc) = (200 5 30)

In [8]:
```
setting7_data = simulated_datasets_list[6]
setting7_y = simulated_y_list[6]

indices_0_y = np.where(setting7_y == 0)
setting7_example_0 = setting7_data[indices_0_y][0, :, :]

indices_1_y = np.where(setting7_y == 1)
setting7_example_1 = setting7_data[indices_1_y][0, :, :]

min_range = np.min([setting7_example_0.min(), setting7_example_1.min()])
max_range = np.max([setting7_example_0.max(), setting7_example_1.max()])

plt.figure(figsize=(5, 5))
plt.subplot(1, 2, 1)
plt.imshow(setting7_example_0, vmin=min_range, vmax=max_range)
plt.title('Setting 6: No Cancer')

plt.subplot(1, 2, 2)
plt.imshow(setting7_example_1, vmin=min_range, vmax=max_range)
plt.title('Setting 6: Cancer')
plt.tight_layout()
```



Question 2

CNN training: Train a Convolutional Neural Network on the simulated data for each of the nine simulation settings. The goal is to use the CNN to predict the cancer status yi based on the simulated images Xi . Additionally, generate a test set of 1000 subjects using the same data generation process and evaluate the CNN's performance in terms of classification accuracy. You are free to build a CNN with arbitrary hyperparameter setting. Conduct at least 10 independent experiments for each setting by generating new datasets each time, and report the hyperparameters for the CNN, the mean and standard deviation of the classification accuracy achieved by your CNN model.

Data Simulation: Train, Validation, and Test sets

Make test set for each one now. I am also going to make a validation set, the same size as the training set!

In [9]:
```
n_test = 1000
n = [200, 500, 1000, 200, 500, 1000, 200, 500, 1000]
mu_n = [5, 5, 5, 5, 5, 5, 5, 5, 5]
mu_c = [10, 10, 10, 20, 20, 20, 30, 30, 30]
```

In [10]:
```
simulated_val_datasets_list = []
simulated_val_y_list = []
for i in range(9):

    y, simulated_data = simulateData(n = n[i],
                                     mu_c = mu_c[i],
                                     mu_n = mu_n[i])

    simulated_val_datasets_list.append(simulated_data)
    simulated_val_y_list.append(y)
simulated_datasets_list[0].shape, simulated_val_datasets_list[0].shape
```

Out[10]:
```
((200, 32, 32), (200, 32, 32))
```

In [11]:
```
simulated_test_datasets_list = []
simulated_test_y_list = []
for i in range(9):
    y, simulated_data = simulateData(n = n_test,
                                     mu_c = mu_c[i],
                                     mu_n = mu_n[i])

    simulated_test_datasets_list.append(simulated_data)
    simulated_test_y_list.append(y)

simulated_datasets_list[0].shape, simulated_test_datasets_list[0].shape
```

Out[11]:
```
((200, 32, 32), (1000, 32, 32))
```

Example image to see how a single data sample will look like going through the models.

In [12]:
```
exampleImg = simulated_datasets_list[0][0, :, :].reshape([1, 1, 32, 32])
exampleImg = torch.from_numpy(exampleImg).float()
exampleImg.shape
```

Out[12]:
```
torch.Size([1, 1, 32, 32])
```

Going to be making and testing different models!

MODEL 0 - Baseline Model!

In [13]:
```
model0 = torch.nn.Sequential()
model0.add_module('conv1', torch.nn.Conv2d(in_channels=1, out_channels=2, kernel_size
model0.add_module('relu1', torch.nn.ReLU())
model0.add_module('pool1', torch.nn.MaxPool2d(kernel_size = 2))


model0.add_module('Flatten', torch.nn.Flatten())

model0.add_module('fc1', torch.nn.Linear(512, 10))
model0.add_module('relu1', torch.nn.ReLU())
model0.add_module('fc2', torch.nn.Linear(10, 1))

model0.add_module('sigmoid', torch.nn.Sigmoid())

print(model0(exampleImg).shape)
```

```
torch.Size([1, 1])
```

MODEL 1

In [14]:
```
model1 = torch.nn.Sequential()
model1.add_module('conv1', torch.nn.Conv2d(in_channels=1, out_channels=2, kernel_size
model1.add_module('relu1', torch.nn.ReLU())
model1.add_module('pool1', torch.nn.MaxPool2d(kernel_size = 2))

model1.add_module('conv2', torch.nn.Conv2d(in_channels=2, out_channels=4, kernel_size
model1.add_module('relu2', torch.nn.ReLU())
model1.add_module('pool2', torch.nn.MaxPool2d(kernel_size = 2))

model1.add_module('Flatten', torch.nn.Flatten())

model1.add_module('fc1', torch.nn.Linear(256, 10))
model1.add_module('relu7', torch.nn.ReLU())
model1.add_module('fc2', torch.nn.Linear(10, 1))

model1.add_module('sigmoid', torch.nn.Sigmoid())

print(model1(exampleImg).shape)
```

```
torch.Size([1, 1])
```

MODEL 2

In [15]:
```
model2 = torch.nn.Sequential()
model2.add_module('conv1', torch.nn.Conv2d(in_channels=1, out_channels=2, kernel_size
model2.add_module('relu1', torch.nn.ReLU())
model2.add_module('pool1', torch.nn.MaxPool2d(kernel_size = 2))
```

```
model2.add_module('conv2', torch.nn.Conv2d(in_channels=2, out_channels=4, kernel_size
model2.add_module('relu2', torch.nn.ReLU())
model2.add_module('pool2', torch.nn.MaxPool2d(kernel_size = 2))


model2.add_module('conv3', torch.nn.Conv2d(in_channels=4, out_channels=8, kernel_size
model2.add_module('relu3', torch.nn.ReLU())
model2.add_module('pool3', torch.nn.MaxPool2d(kernel_size = 2))


model2.add_module('Flatten', torch.nn.Flatten())

model2.add_module('fc1', torch.nn.Linear(128, 10))
model2.add_module('relu7', torch.nn.ReLU())
model2.add_module('fc2', torch.nn.Linear(10, 1))

model2.add_module('sigmoid', torch.nn.Sigmoid())

print(model2(exampleImg).shape)
```

```
torch.Size([1, 1])
```

MODEL 3

In [16]:

```
model3 = torch.nn.Sequential()
model3.add_module('conv1', torch.nn.Conv2d(in_channels=1, out_channels=32, kernel_size
model3.add_module('relu1', torch.nn.ReLU())
model3.add_module('pool1', torch.nn.MaxPool2d(kernel_size = 2))

model3.add_module('conv2', torch.nn.Conv2d(in_channels=32, out_channels=64, kernel_siz
model3.add_module('relu2', torch.nn.ReLU())
model3.add_module('pool2', torch.nn.MaxPool2d(kernel_size = 2))

model3.add_module('Flatten', torch.nn.Flatten())

model3.add_module('fc1', torch.nn.Linear(4096, 10))
model3.add_module('relu7', torch.nn.ReLU())
model3.add_module('fc2', torch.nn.Linear(10, 1))

model3.add_module('sigmoid', torch.nn.Sigmoid())

print(model3(exampleImg).shape)
```

```
torch.Size([1, 1])
```

DataLoaders for training and validation sets

In [17]:

```
class dataSetPytorch(Dataset):
    def __init__(self, x, y):
        self.x = torch.from_numpy(x.reshape([-1, 1, 32, 32])).float()
        self.y = torch.from_numpy(y)
    def __len__(self):
        return len(self.x)
    def __getitem__(self, idx):
        return self.x[idx], self.y[idx]

# Setting 1: train and validation loader data.
```

```
datasetSetting1_train = dataSetPytorch(simulated_datasets_list[0], simulated_y_list[0]
dataLoader_setting1_train = DataLoader(datasetSetting1_train, batch_size=25, shuffle =

datasetSetting1_validation = dataSetPytorch(simulated_val_datasets_list[0], simulated_
dataLoader_setting1_validation = DataLoader(datasetSetting1_validation, batch_size=25,

# Setting 9: train and validation loader data.
datasetSetting9_train = dataSetPytorch(simulated_datasets_list[8], simulated_y_list[8]
dataLoader_setting9_train = DataLoader(datasetSetting9_train, batch_size=25, shuffle =

datasetSetting9_validation = dataSetPytorch(simulated_val_datasets_list[8], simulated_
dataLoader_setting9_validation = DataLoader(datasetSetting9_validation, batch_size=25,
```

In [18]:

```
datax, labely = next(iter(dataLoader_setting9_train))
print(datax.shape, labely.shape)
model0(datax).shape
```

```
torch.Size([25, 1, 32, 32]) torch.Size([25])
```

Out[18]:

```
torch.Size([25, 1])
```

Training the models

In [19]:

```
def reset_weights(model):
    for m in model.modules():
        if isinstance(m, nn.Conv2d) or isinstance(m, nn.Linear):
            init.xavier_uniform_(m.weight)
    return
```

In [20]:

```
def train(name, model, train_dl, valid_dl, num_epochs = 200):
    # reinitialize weights!
    reset_weights(model)

    loss_fn = torch.nn.BCELoss()
    optimizer = torch.optim.Adam(model.parameters(), lr = 0.001)
    loss_hist_train = [0] * num_epochs
    accuracy_hist_train = [0] * num_epochs
    loss_hist_valid = [0] * num_epochs
    accuracy_hist_valid = [0] * num_epochs

    best_loss = torch.inf

    for epoch in range(num_epochs):
        model.train()

        for x_batch, y_batch in train_dl:
            pred = model(x_batch)[:, 0]
            loss = loss_fn(pred, y_batch.float())
#             print("pred", pred, "observed", y_batch)
            loss.backward()
            optimizer.step()
            optimizer.zero_grad()
            loss_hist_train[epoch] += loss.item() * y_batch.size(0)

            is_correct = ((pred >= 0.5).float() == y_batch).float()
#             print(is_correct)
            accuracy_hist_train[epoch] += is_correct.sum()
        loss_hist_train[epoch] /= len(train_dl.dataset)
        accuracy_hist_train[epoch] /= len(train_dl.dataset)
```

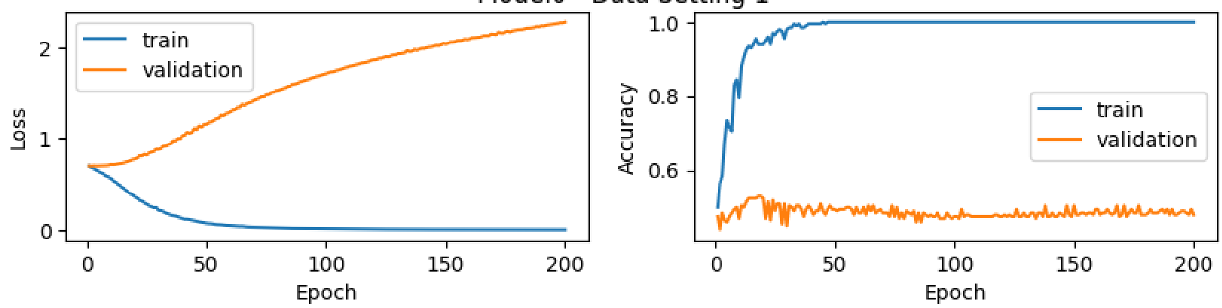
```
        model.eval()
        with torch.no_grad():
            for x_batch, y_batch in valid_dl:
                pred = model(x_batch)[:, 0]
                loss = loss_fn(pred, y_batch.float())
                loss_hist_valid[epoch] += loss.item() * y_batch.size(0)

                is_correct = ((pred >= 0.5).float() == y_batch).float()
                accuracy_hist_valid[epoch] += is_correct.sum()
        loss_hist_valid[epoch] /= len(valid_dl.dataset)
        accuracy_hist_valid[epoch] /= len(valid_dl.dataset)


    return loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid


def plotModelPerformance(modelNum, dataSettingNum, loss_hist_train, loss_hist_valid,
                         accuracy_hist_train, accuracy_hist_valid):
    epochsX = np.arange(len(loss_hist_train)) + 1
    plt.figure(figsize=(10, 2))
    plt.subplot(1, 2, 1)
    plt.plot(epochsX, loss_hist_train, label = "train")
    plt.plot(epochsX, loss_hist_valid, label = "validation")

    plt.ylabel('Loss')
    plt.xlabel('Epoch')
    plt.legend()

    plt.subplot(1, 2, 2)
    epochsX = np.arange(len(accuracy_hist_train)) + 1
    plt.plot(epochsX, accuracy_hist_train, label = "train")
    plt.plot(epochsX, accuracy_hist_valid, label = "validation")
    plt.ylabel('Accuracy')
    plt.xlabel('Epoch')
    plt.legend()

    plt.suptitle("Model" + str(modelNum) + " - Data Setting " + str(dataSettingNum))
    plt.show()
    return
```

In [21]:

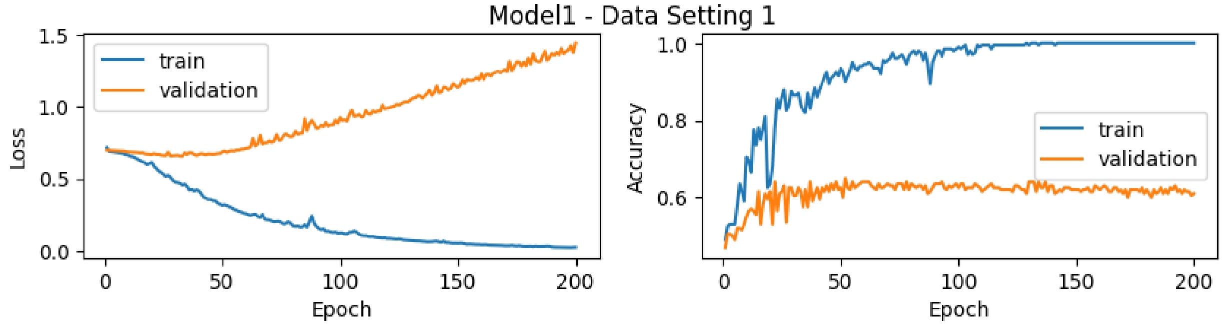
```
loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid = train("mo
                                                                                    dat
                                                                                    dat
                                                                                    num
plotModelPerformance(modelNum = 0, dataSettingNum = 1, loss_hist_train = loss_hist_tra
                         accuracy_hist_train = accuracy_hist_train, accuracy_hist_vali


loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid = train("mo
                                                                                    dat
                                                                                    dat
                                                                                    num
plotModelPerformance(modelNum = 1, dataSettingNum = 1, loss_hist_train = loss_hist_tra
                         accuracy_hist_train = accuracy_hist_train, accuracy_hist_vali

loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid = train("mo
                                                                                    dat
```

```
                                                                                   dat
                                                                                   num
plotModelPerformance(modelNum = 2, dataSettingNum = 1, loss_hist_train = loss_hist_tra
                     accuracy_hist_train = accuracy_hist_train, accuracy_hist_vali

loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid = train("mo
                                                                                   dat
                                                                                   dat
                                                                                   num
plotModelPerformance(modelNum = 3, dataSettingNum = 1, loss_hist_train = loss_hist_tra
                     accuracy_hist_train = accuracy_hist_train, accuracy_hist_vali
```

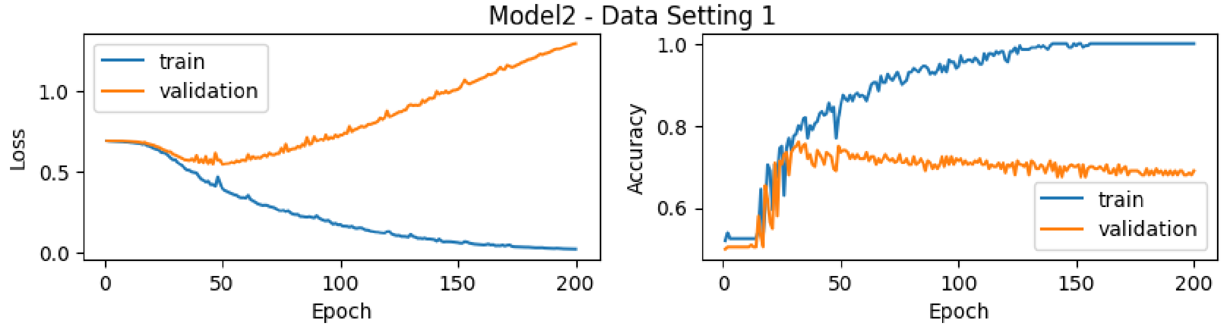
Model0 - Data Setting 1



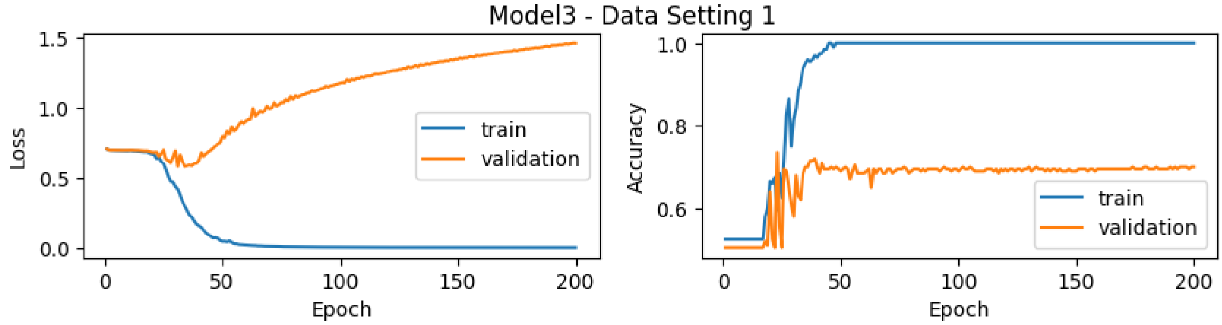
Model1 - Data Setting 1



Model2 - Data Setting 1

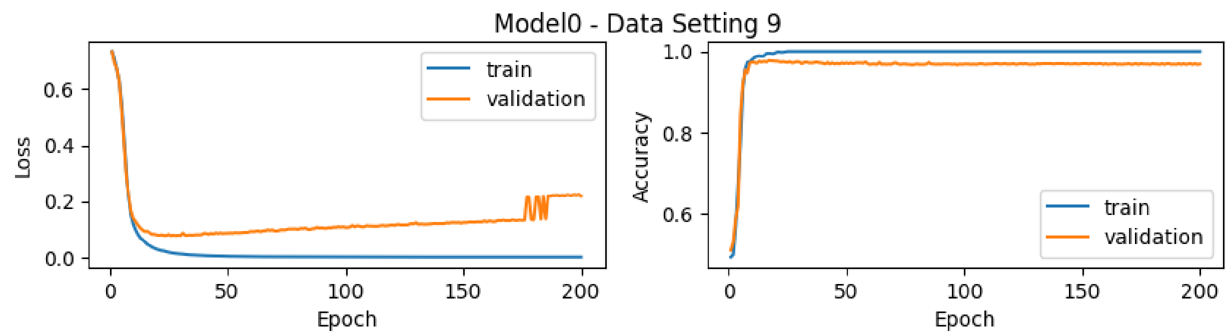


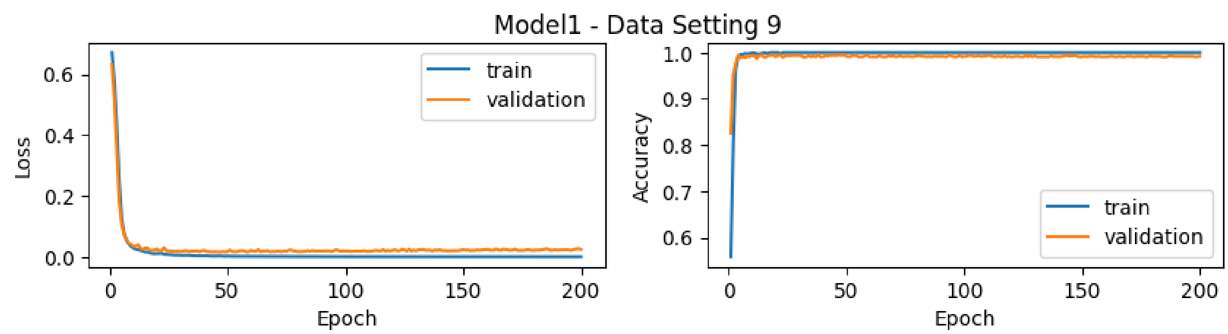
Model3 - Data Setting 1

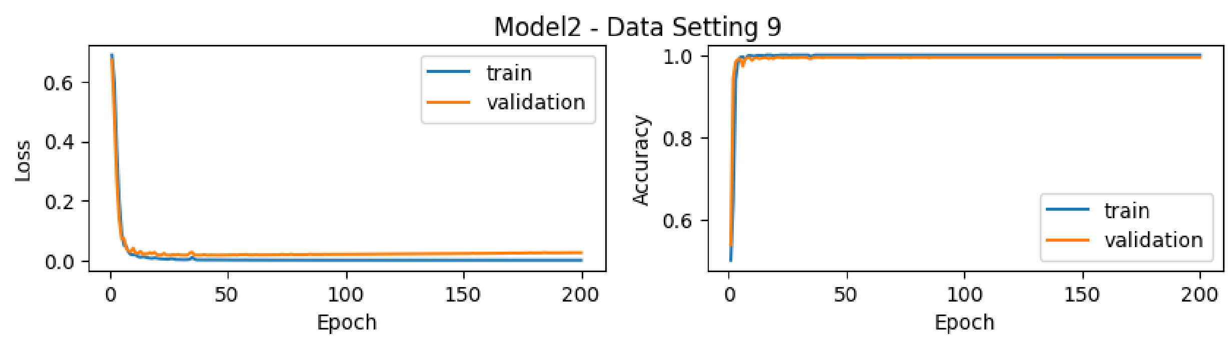


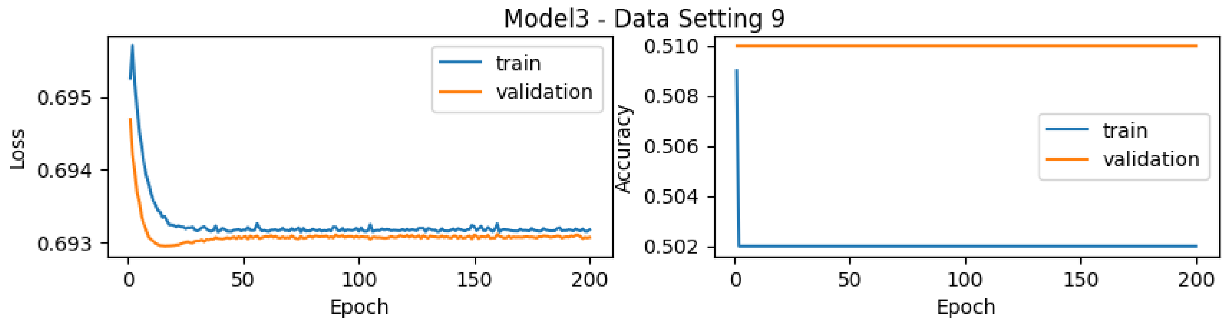
In [22]:
```
loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid = train("mo
                                                                                   dat
                                                                                   dat
```

```
                                                                                        num
plotModelPerformance(modelNum = 0, dataSettingNum = 9, loss_hist_train = loss_hist_tra
                         accuracy_hist_train = accuracy_hist_train, accuracy_hist_vali


loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid = train("mo
                                                                                        dat
                                                                                        dat
                                                                                        num
plotModelPerformance(modelNum = 1, dataSettingNum = 9, loss_hist_train = loss_hist_tra
                         accuracy_hist_train = accuracy_hist_train, accuracy_hist_vali

loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid = train("mo
                                                                                        dat
                                                                                        dat
                                                                                        num
plotModelPerformance(modelNum = 2, dataSettingNum = 9, loss_hist_train = loss_hist_tra
                         accuracy_hist_train = accuracy_hist_train, accuracy_hist_vali

loss_hist_train, loss_hist_valid, accuracy_hist_train, accuracy_hist_valid = train("mo
                                                                                        dat
                                                                                        dat
                                                                                        num
plotModelPerformance(modelNum = 3, dataSettingNum = 9, loss_hist_train = loss_hist_tra
                         accuracy_hist_train = accuracy_hist_train, accuracy_hist_vali
```








Model3 - Data Setting 9
Loss
Epoch
train
validation
Accuracy
Epoch
train
validation
0.693
0.694
0.695
0.502
0.504
0.506
0.508
0.510
0
50
100
150
200

In [ ]: