Notebook

November 9, 2025

1 Binary classification

[1]:
```
import torch
import torch.nn as nn
import torchmetrics
from torch.utils.data import Dataset
import pandas as pd
import wandb
```

1.1 Config

[2]:
```
import torch.nn as nn



BATCH_SIZE = 32
LR = 0.001
CLASSES = 2

MAX_EPOCHS = 50
POS_WEIGHT = 2
LOSS_FUNCTION = nn.BCEWithLogitsLoss(pos_weight=torch.Tensor([POS_WEIGHT]))
TRAIN_VAL_TEST_SPLIT = [0.9, 0.05, 0.05]
DROPOUT_COEF = 0.35


SAVE_BEST_MODEL = True
IS_MULTICLASS = True if CLASSES > 2 else False
NUM_OF_WORKERS = 0

REDUCE_LR_PATIENCE = 10
EARLY_STOPPING_PATIENCE = 10
```

1.2 WANDB Init

[3]:
```
wandb.init(project="zneus-project-1-binary", name=f"Basic model with BatchNorm␣
↪POS_WEIGHT={POS_WEIGHT} and layer and dropouts")
```

```python
# Config hyperparameters
config = wandb.config
config.pos_weight = POS_WEIGHT
config.batch_size = BATCH_SIZE
config.learning_rate = LR
config.max_epochs = MAX_EPOCHS
config.dropout_coef = DROPOUT_COEF
config.desc = "MLP: (512, BatchNorm,ReLU,Dropout) (256,BatchNorm, ReLU,Dropout)␣
↪(128,BatchNorm, ReLU, Dropout) (1)"
config.loss_function = "BinaryCrossentropy with logits"
config.reduce_lr_patience = REDUCE_LR_PATIENCE
config.early_stopping_patience = EARLY_STOPPING_PATIENCE
```

```
wandb: Currently logged in as: amal-akhmadinurov
(amal-akhmadinurov-stu) to https://api.wandb.ai. Use
`wandb login --relogin` to force relogin

wandb: setting up run uxk5kttc

wandb: Tracking run with wandb version 0.22.3

wandb: Run data is saved locally in
/Users/amalahmadinurov/Desktop/Subjects_ZS_2025/ZNEUS/zneus-

project-1/wandb/run-20251109_195651-uxk5kttc
wandb: Run `wandb offline` to turn off syncing.

wandb: Syncing run Basic model with BatchNorm POS_WEIGHT=2 and

layer and dropouts

wandb:  View project at␣
↪https://wandb.ai/amal-akhmadinurov-stu/zneus-project-1-binary

wandb:  View run at␣
↪https://wandb.ai/amal-akhmadinurov-stu/zneus-project-1-binary/runs/uxk5kttc
```

1.3 Define Dataset

[4]:
```python
class SteelPlateDataset(Dataset):

    def __init__(self, dataset_path):
        super().__init__()
        self.path = dataset_path
        self.df = pd.read_csv(self.path)

        self.features = self.df.drop(["Class", *("Pastry Z_Scratch K_Scratch␣
↪Stains Dirtiness Bumps".split(" "))] ,axis= 1).values.tolist() # V28 V29 V30␣
↪V31 V32 V33
        self.labels = self.df["Class"].to_list()
```

```python
    def __getitem__(self, index):

        return torch.tensor(self.features[index]), torch.tensor(self.
 ↪labels[index])
    def __len__(self):
        return len(self.labels)
```

1.4 Create datasets

[5]:
```python
torch.manual_seed(42)


dataset = SteelPlateDataset("data/norm_multiclass_data.csv")

train_dataset, val_dataset, test_dataset = torch.utils.data.
 ↪random_split(dataset, TRAIN_VAL_TEST_SPLIT)
```

1.5 Define device

[6]:
```python
if torch.cuda.is_available():
    device_name = "cuda"
elif torch.backends.mps.is_available():
    device_name = "mps"
else:
    device_name = "cpu"
```

1.6 Define EarlyStopping class

[7]:
```python
import torch

class EarlyStopping:
    def __init__(self, patience=5, min_delta=0.0):
        """
        Args:
            patience (int): How many epochs to wait after last improvement.
            min_delta (float): Minimum change to qualify as an improvement.
        """
        self.patience = patience
        self.min_delta = min_delta
        self.counter = 0
        self.best_loss = None
        self.early_stop = False

    def __call__(self, val_loss):
        if self.best_loss is None:
            self.best_loss = val_loss
```

```
        elif val_loss > self.best_loss - self.min_delta:
            self.counter += 1
            if self.counter >= self.patience:
                self.early_stop = True
        else:
            self.best_loss = val_loss
            self.counter = 0
```

1.7 Define model

[8]:
```
from torchmetrics.classification import Accuracy, BinaryPrecision
from torch.optim.lr_scheduler import ReduceLROnPlateau
import torch
import torch.nn as nn

class MyModel(nn.Module):
    def __init__(self, input_size, lr=0.001, loss_fn=nn.BCELoss(),␣
 ↪num_classes=2, reduce_lr_patience=10, early_stopping_patience=10):
        super().__init__()
        self.accuracy = Accuracy(task="binary")
        # Use BinaryPrecision for positive class
        self.precision_pos = BinaryPrecision()  # Precision for positive class␣
 ↪(label 1)
        self.precision_neg = BinaryPrecision()  # Precision for negative class␣
 ↪(label 0)
        self.loss_fn = loss_fn

        self.model = nn.Sequential(
            nn.Linear(input_size, 512),
            nn.BatchNorm1d(512),
            nn.ReLU(),
            nn.Dropout(DROPOUT_COEF),

            nn.Linear(512, 256),
            nn.BatchNorm1d(256),
            nn.ReLU(),
            nn.Dropout(DROPOUT_COEF),

            nn.Linear(256, 128),
            nn.BatchNorm1d(128),
            nn.ReLU(),
            nn.Dropout(DROPOUT_COEF),


            nn.Linear(128, 1)
        )
        self.to(device_name)
```

```
        self.optimizer = torch.optim.Adam(self.parameters(), lr=lr)
        self.early_stopping = EarlyStopping(patience=early_stopping_patience,␣
↪min_delta=0.01)
        self.scheduler = ReduceLROnPlateau(self.optimizer, mode='min', factor=0.
↪5, patience=reduce_lr_patience)

    def forward(self, x):
        return self.model(x)

    def evaluate(self, dataloader):
        self.eval()
        eval_loss = 0
        self.precision_pos.reset()
        self.precision_neg.reset()
        self.accuracy.reset()

        with torch.no_grad():
            for batch in dataloader:
                x = batch[0].to(device_name)
                y = batch[1].to(device_name)
                output = self.forward(x)
                output = torch.sigmoid(output).squeeze(1)
                y = y.float()

                loss = self.loss_fn(output, y)
                eval_loss += loss.item()

                # Update metrics
                self.accuracy(output, y)
                self.precision_pos(output, y)  # Positive class precision
                self.precision_neg(1 - output, 1 - y)  # Negative class␣
↪precision

        self.train()
        return (eval_loss / len(dataloader), self.accuracy.compute(),
                torch.tensor([self.precision_neg.compute(), self.precision_pos.
↪compute()]))

    def fit(self, train_dataloader, val_dataloader, epochs=10):
        self.train()
        best_val_loss = 9999

        for i in range(epochs):
            self.accuracy.reset()
            self.precision_pos.reset()
            self.precision_neg.reset()
```

```
        epoch_loss = 0

        for batch in train_dataloader:
            x = batch[0].to(device_name)
            y = batch[1].to(device_name)
            output = self.forward(x)
            output = torch.sigmoid(output).squeeze(1)
            y = y.float()

            loss = self.loss_fn(output, y)
            epoch_loss += loss.item()

            # Update metrics
            self.accuracy(output, y)
            self.precision_pos(output, y)  # Positive class
            self.precision_neg(1 - output, 1 - y)  # Negative class

            self.zero_grad()
            loss.backward()
            self.optimizer.step()

        epoch_loss /= len(train_dataloader)
        epoch_acc = self.accuracy.compute()
        epoch_precision = torch.tensor([self.precision_neg.compute(), self.precision_pos.compute()])

        val_loss, val_acc, val_precision = self.evaluate(val_dataloader)

        if best_val_loss > val_loss:
            best_val_loss = val_loss
            torch.save(self.state_dict(), "best-model-binary.pth")

        self.scheduler.step(val_loss)

        wandb.log({
            "epoch": i,
            "Train Loss": epoch_loss,
            "Train Acc": epoch_acc,
            "Train Positive Precision": epoch_precision[1].item(),
            "Train Negative Precision": epoch_precision[0].item(),
            "Val Loss": val_loss,
            "Val Acc": val_acc,
            "Val Positive Precision": val_precision[1].item(),
            "Val Negative Precision": val_precision[0].item(),
            "LR": self.optimizer.param_groups[0]['lr']
        })
```

```
            print(f"Epoch {i+1} Loss:{epoch_loss:.4f} Accuracy:{epoch_acc:.4f} "
                  f"Positive Precision:{epoch_precision[1].item():.4f} Negative␣
↪Precision:{epoch_precision[0].item():.4f} "
                  f"Val Loss:{val_loss:.4f} Val Accuracy:{val_acc:.4f} "
                  f"Val Positive Precision:{val_precision[1].item():.4f} Val␣
↪Negative Precision:{val_precision[0].item():.4f} "
                  f"LR = {self.optimizer.param_groups[0]['lr']}")
            self.early_stopping(val_loss)
            if self.early_stopping.early_stop:
                print("Early stopping")
                break
        wandb.finish()
```

1.8 Create dataloaders

[9]:
```
from torch.utils.data import DataLoader

train_dataloader = DataLoader(
    train_dataset,
    batch_size=BATCH_SIZE,
    shuffle=True,  # Default shuffling for training
    num_workers=NUM_OF_WORKERS
)
val_dataloader = DataLoader(
    val_dataset,
    batch_size=BATCH_SIZE,
    shuffle=False,  # No shuffling for validation
    num_workers=NUM_OF_WORKERS
)
test_dataloader = DataLoader(
    test_dataset,
    batch_size=BATCH_SIZE,
    shuffle=False,  # No shuffling for test
    num_workers=NUM_OF_WORKERS
)

# Print dataset sizes
print(f"Train dataset size: {len(train_dataset)}")
print(f"Validation dataset size: {len(val_dataset)}")
print(f"Test dataset size: {len(test_dataset)}")
```

```
Train dataset size: 1452
Validation dataset size: 81
Test dataset size: 80
```

1.9 Create model

[10]:
```
model = MyModel(
    input_size=len(dataset.features[0]),
    num_classes=CLASSES,
    loss_fn=LOSS_FUNCTION,
    lr=LR,
    reduce_lr_patience=REDUCE_LR_PATIENCE,
    early_stopping_patience=EARLY_STOPPING_PATIENCE
)
```

1.10 Train model

[11]:
```
model.fit(train_dataloader, val_dataloader, epochs=MAX_EPOCHS)
```

```
Epoch 1 Loss:0.9208 Accuracy:0.6398 Positive Precision:0.5017 Negative
Precision:0.7343 Val Loss:0.8914 Val Accuracy:0.7407 Val Positive
Precision:0.7692 Val Negative Precision:0.7273 LR = 0.001

Epoch 2 Loss:0.8741 Accuracy:0.7273 Positive Precision:0.6443 Negative
Precision:0.7642 Val Loss:0.8612 Val Accuracy:0.7407 Val Positive
Precision:0.7692 Val Negative Precision:0.7273 LR = 0.001

Epoch 3 Loss:0.8533 Accuracy:0.7472 Positive Precision:0.6688 Negative
Precision:0.7846 Val Loss:0.8567 Val Accuracy:0.7407 Val Positive
Precision:0.7692 Val Negative Precision:0.7273 LR = 0.001

Epoch 4 Loss:0.8418 Accuracy:0.7596 Positive Precision:0.6789 Negative
Precision:0.8010 Val Loss:0.8359 Val Accuracy:0.7778 Val Positive
Precision:0.7576 Val Negative Precision:0.7917 LR = 0.001

Epoch 5 Loss:0.8400 Accuracy:0.7652 Positive Precision:0.6885 Negative
Precision:0.8039 Val Loss:0.8552 Val Accuracy:0.7531 Val Positive
Precision:0.7778 Val Negative Precision:0.7407 LR = 0.001

Epoch 6 Loss:0.8363 Accuracy:0.7748 Positive Precision:0.7200 Negative
Precision:0.7994 Val Loss:0.8325 Val Accuracy:0.7654 Val Positive
Precision:0.7353 Val Negative Precision:0.7872 LR = 0.001

Epoch 7 Loss:0.8368 Accuracy:0.7576 Positive Precision:0.6755 Negative
Precision:0.7998 Val Loss:0.8401 Val Accuracy:0.7654 Val Positive
Precision:0.7500 Val Negative Precision:0.7755 LR = 0.001

Epoch 8 Loss:0.8268 Accuracy:0.7865 Positive Precision:0.7189 Negative
Precision:0.8210 Val Loss:0.8227 Val Accuracy:0.8025 Val Positive
Precision:0.7879 Val Negative Precision:0.8125 LR = 0.001

Epoch 9 Loss:0.8271 Accuracy:0.7741 Positive Precision:0.6982 Negative
Precision:0.8136 Val Loss:0.8372 Val Accuracy:0.7654 Val Positive
Precision:0.7353 Val Negative Precision:0.7872 LR = 0.001

Epoch 10 Loss:0.8253 Accuracy:0.7707 Positive Precision:0.6992 Negative
Precision:0.8062 Val Loss:0.8218 Val Accuracy:0.7901 Val Positive
```

Precision:0.8000 Val Negative Precision:0.7843 LR = 0.001

Epoch 11 Loss:0.8189 Accuracy:0.7851 Positive Precision:0.7205 Negative Precision:0.8173 Val Loss:0.8300 Val Accuracy:0.7901 Val Positive Precision:0.8000 Val Negative Precision:0.7843 LR = 0.001

Epoch 12 Loss:0.8256 Accuracy:0.7755 Positive Precision:0.7010 Negative Precision:0.8140 Val Loss:0.8312 Val Accuracy:0.7778 Val Positive Precision:0.7742 Val Negative Precision:0.7800 LR = 0.001

Epoch 13 Loss:0.8197 Accuracy:0.7837 Positive Precision:0.7249 Negative Precision:0.8118 Val Loss:0.8124 Val Accuracy:0.8148 Val Positive Precision:0.7778 Val Negative Precision:0.8444 LR = 0.001

Epoch 14 Loss:0.8203 Accuracy:0.7865 Positive Precision:0.7352 Negative Precision:0.8101 Val Loss:0.8235 Val Accuracy:0.7778 Val Positive Precision:0.7576 Val Negative Precision:0.7917 LR = 0.001

Epoch 15 Loss:0.8167 Accuracy:0.7913 Positive Precision:0.7247 Negative Precision:0.8257 Val Loss:0.8246 Val Accuracy:0.7901 Val Positive Precision:0.7812 Val Negative Precision:0.7959 LR = 0.001

Epoch 16 Loss:0.8177 Accuracy:0.7886 Positive Precision:0.7339 Negative Precision:0.8144 Val Loss:0.8223 Val Accuracy:0.7901 Val Positive Precision:0.8000 Val Negative Precision:0.7843 LR = 0.001

Epoch 17 Loss:0.8128 Accuracy:0.7955 Positive Precision:0.7385 Negative Precision:0.8234 Val Loss:0.8276 Val Accuracy:0.7778 Val Positive Precision:0.7429 Val Negative Precision:0.8043 LR = 0.001

Epoch 18 Loss:0.8186 Accuracy:0.7824 Positive Precision:0.7103 Negative Precision:0.8199 Val Loss:0.8218 Val Accuracy:0.7778 Val Positive Precision:0.7742 Val Negative Precision:0.7800 LR = 0.001

Epoch 19 Loss:0.8201 Accuracy:0.7851 Positive Precision:0.7126 Negative Precision:0.8233 Val Loss:0.8251 Val Accuracy:0.7901 Val Positive Precision:0.7812 Val Negative Precision:0.7959 LR = 0.001

Epoch 20 Loss:0.8100 Accuracy:0.7948 Positive Precision:0.7312 Negative Precision:0.8273 Val Loss:0.8160 Val Accuracy:0.8025 Val Positive Precision:0.7879 Val Negative Precision:0.8125 LR = 0.001

Epoch 21 Loss:0.8110 Accuracy:0.7961 Positive Precision:0.7390 Negative Precision:0.8243 Val Loss:0.8270 Val Accuracy:0.8025 Val Positive Precision:0.8065 Val Negative Precision:0.8000 LR = 0.001

Epoch 22 Loss:0.8202 Accuracy:0.7803 Positive Precision:0.7020 Negative Precision:0.8227 Val Loss:0.8355 Val Accuracy:0.7531 Val Positive Precision:0.7419 Val Negative Precision:0.7600 LR = 0.001

wandb: updating run metadata

Epoch 23 Loss:0.8119 Accuracy:0.7899 Positive Precision:0.7227 Negative Precision:0.8246 Val Loss:0.8323 Val Accuracy:0.7778 Val Positive

```
Precision:0.7576 Val Negative Precision:0.7917 LR = 0.001
Early stopping
```

```
wandb: uploading wandb-summary.json

wandb: uploading history steps 0-22, summary

wandb:
wandb: Run history:
wandb:                       LR
wandb:                Train Acc
wandb:               Train Loss
wandb: Train Negative Precision
wandb: Train Positive Precision
wandb:                  Val Acc
wandb:                 Val Loss
wandb:   Val Negative Precision
wandb:   Val Positive Precision
wandb:                    epoch
wandb:
wandb: Run summary:
wandb:                       LR 0.001
wandb:                Train Acc 0.78994
wandb:               Train Loss 0.81187
wandb: Train Negative Precision 0.82463
wandb: Train Positive Precision 0.72267
wandb:                  Val Acc 0.77778
wandb:                 Val Loss 0.83227
wandb:   Val Negative Precision 0.79167
wandb:   Val Positive Precision 0.75758
wandb:                    epoch 22
wandb:

wandb:  View run Basic model with BatchNorm POS_WEIGHT=2 and
layer and dropouts at:
↪https://wandb.ai/amal-akhmadinurov-stu/zneus-project-1-binary/runs/uxk5kttc
wandb:  View project at:
↪https://wandb.ai/amal-akhmadinurov-stu/zneus-project-1-binary
wandb: Synced 4 W&B file(s), 0 media file(s), 0 artifact file(s)
and 0 other file(s)

wandb: Find logs at:
./wandb/run-20251109_195651-uxk5kttc/logs
```

[12]:

```python
val_loss, val_acc, val_precision = model.evaluate(val_dataloader)
print(f"Val Loss:{val_loss} Val Accuracy:{val_acc.item()} Val Negative
↪Precision:{val_precision[0].item()} Val Positive Precision:{val_precision[1].
↪item()}")
```

```
Val Loss:0.8322668870290121 Val Accuracy:0.7777777910232544 Val Negative
```

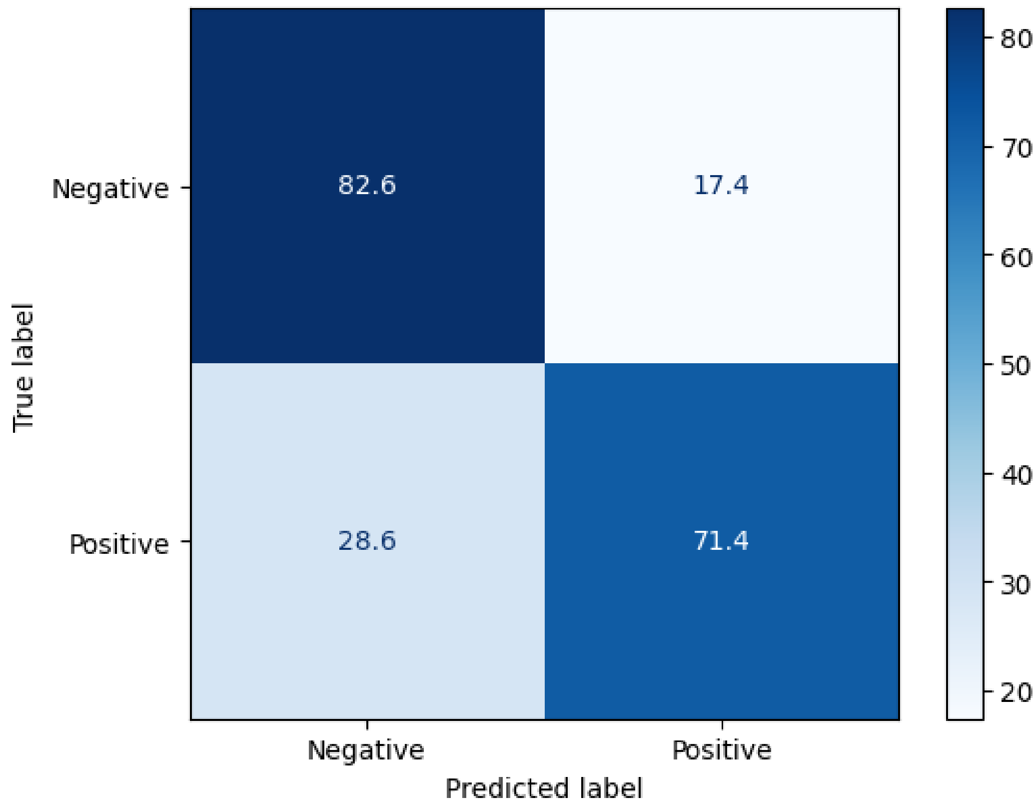
Precision:0.7916666865348816 Val Positive Precision:0.7575757503509521

1.11 Confusion Matrix on validation set

[13]:
```python
import numpy as np

import matplotlib.pyplot as plt
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay

# Example data (each pixel has an integer class label)
val_dataloader = DataLoader(
    val_dataset,
    batch_size=len(val_dataset),
    shuffle=True,  # Use sampler instead of shuffle
    num_workers=NUM_OF_WORKERS
)

features, ground_truth = next(iter(val_dataloader))

images = features.to(device_name)
model.eval()
predictions = model(images)
predictions = (torch.sigmoid(predictions) > 0.5).float()
y_true = ground_truth.numpy()
y_pred = predictions.detach().cpu().int().numpy()


cm = confusion_matrix(y_true, y_pred, labels=[0,1])
print(cm)
cm_percent = cm.astype('float') / cm.sum(axis=1, keepdims=True) * 100
disp = ConfusionMatrixDisplay(confusion_matrix=cm_percent,
                              display_labels=["Negative","Positive"])

disp.plot(cmap='Blues', values_format='.1f')
```

```
[[38  8]
 [10 25]]
```

[13]: <sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x11f5d9010>



[14]:
```
model.load_state_dict(torch.load("best-model-binary.pth",␣
↪map_location=device_name))
```

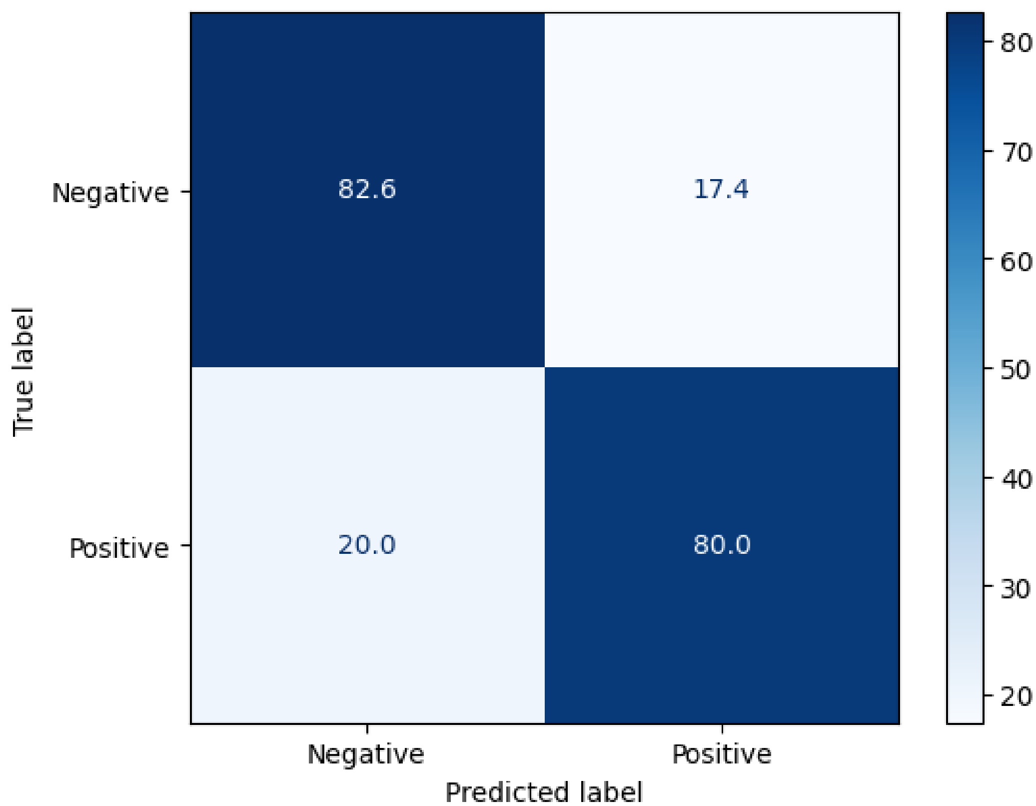
[14]: <All keys matched successfully>

[15]:
```
import numpy as np

import matplotlib.pyplot as plt
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay

# Example data (each pixel has an integer class label)
val_dataloader = DataLoader(
    val_dataset,
    batch_size=len(val_dataset),
    shuffle=True,  # Use sampler instead of shuffle
    num_workers=NUM_OF_WORKERS
)

features, ground_truth = next(iter(val_dataloader))

images = features.to(device_name)
```

```
model.eval()
predictions = model(images)
predictions = (torch.sigmoid(predictions) > 0.5).float()
y_true = ground_truth.numpy()
y_pred = predictions.detach().cpu().int().numpy()


cm = confusion_matrix(y_true, y_pred, labels=[0,1])
print(cm)
cm_percent = cm.astype('float') / cm.sum(axis=1, keepdims=True) * 100
disp = ConfusionMatrixDisplay(confusion_matrix=cm_percent,
                              display_labels=["Negative","Positive"])

disp.plot(cmap='Blues', values_format='.1f')
```

```
[[38  8]
 [ 7 28]]
```

[15]: <sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x1389db4d0>



1.12 Test on the test set (only for final evaluation)

1.12.1 Test set class distribution

[16]:
```
from collections import Counter

labels = [label.item() for _, label in test_dataset]
class_counts = Counter(labels)

print("\nClass Distribution:")
print("-" * 30)
class_names = ["No", "Yes"]
for cls, count in sorted(class_counts.items()):
    print(f"Class {class_names[int(cls)]} | Count: {count}")
print("-" * 30)
```

```
Class Distribution:
------------------------------
Class No | Count: 52
Class Yes | Count: 28
------------------------------
```

[17]:
```
test_loss, test_acc, test_precision = model.evaluate(test_dataloader)
print(f"Test Loss:{test_loss} Test Accuracy:{test_acc.item()} Test Negative␣
↪Precision:{test_precision[0].item()} Test Positive Precision:
↪{test_precision[1].item()}")
```

```
Test Loss:0.8151968320210775 Test Accuracy:0.800000011920929 Test Negative
Precision:0.8103448152542114 Test Positive Precision:0.7727272510528564
```

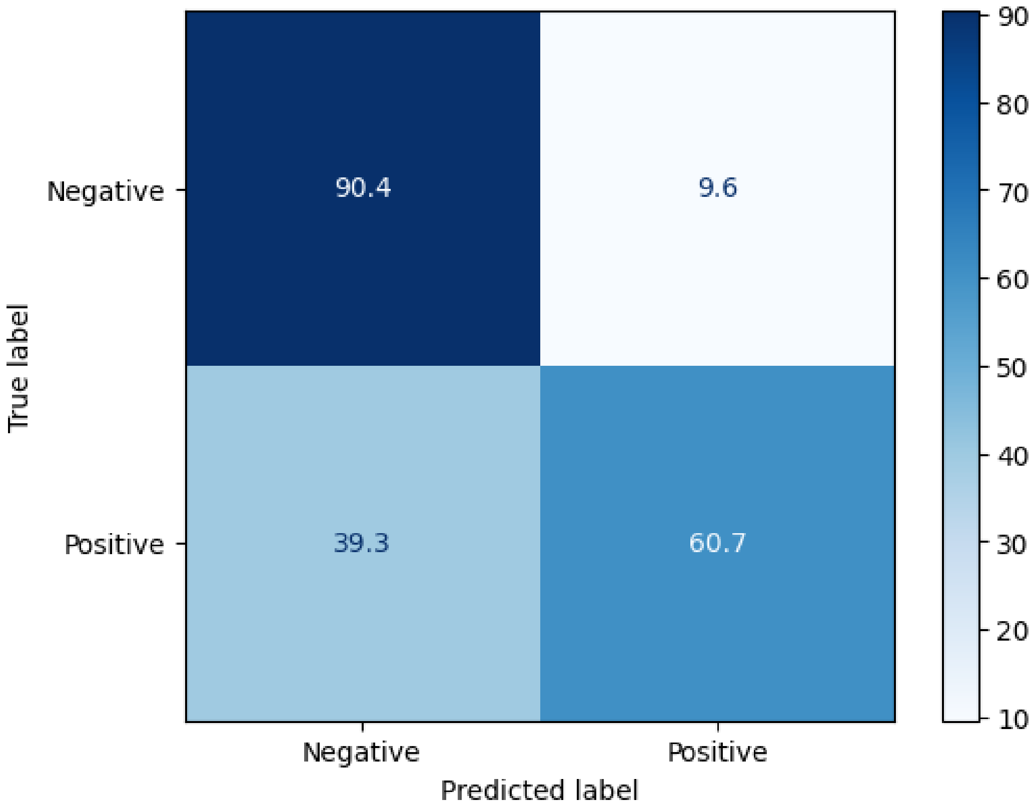
1.12.2 Confusion Matrix

[18]:
```
import numpy as np

import matplotlib.pyplot as plt
from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay

# Example data (each pixel has an integer class label)
test_dataloader = DataLoader(
    test_dataset,
    batch_size=len(test_dataset),

    num_workers=NUM_OF_WORKERS
)
```

```python
features, ground_truth = next(iter(test_dataloader))

images = features.to(device_name)
model.eval()
predictions = model(images)
predictions = (torch.sigmoid(predictions) > 0.5).float()
y_true = ground_truth.numpy()
y_pred = predictions.detach().cpu().int().numpy()


cm = confusion_matrix(y_true, y_pred, labels=[0,1])
print(cm)
cm_percent = cm.astype('float') / cm.sum(axis=1, keepdims=True) * 100
disp = ConfusionMatrixDisplay(confusion_matrix=cm_percent,
                          display_labels=["Negative","Positive"])

disp.plot(cmap='Blues', values_format='.1f')
```

```
[[47  5]
 [11 17]]
```

```
[18]: <sklearn.metrics._plot.confusion_matrix.ConfusionMatrixDisplay at 0x11f5bccd0>
```



90.4
9.6
39.3
60.7
Negative
Positive
True label
Negative
Positive
Predicted label
90
80
70
60
50
40
30
20
10


```
[ ]:
```