MSBD566_Predictive_Final

December 12, 2025

0.1 MSBD566 - Final Project

0.2 Esmeralda Garcia

Data Source: https://www.kaggle.com/datasets/samiraalipour/genomics-of-drug-sensitivity-in-cancer-gdsc?resource=download&select=GDSC_DATASET.csv

[8]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler, OneHotEncoder
from sklearn.impute import SimpleImputer
from sklearn.decomposition import PCA
from sklearn.metrics import classification_report, confusion_matrix

import tensorflow as tf
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Dropout
from tensorflow.keras.utils import to_categorical

pd.set_option("display.max_columns", 100)
plt.rcParams["figure.dpi"] = 120

print("TensorFlow version:", tf.__version__)
```

```
TensorFlow version: 2.11.0
```

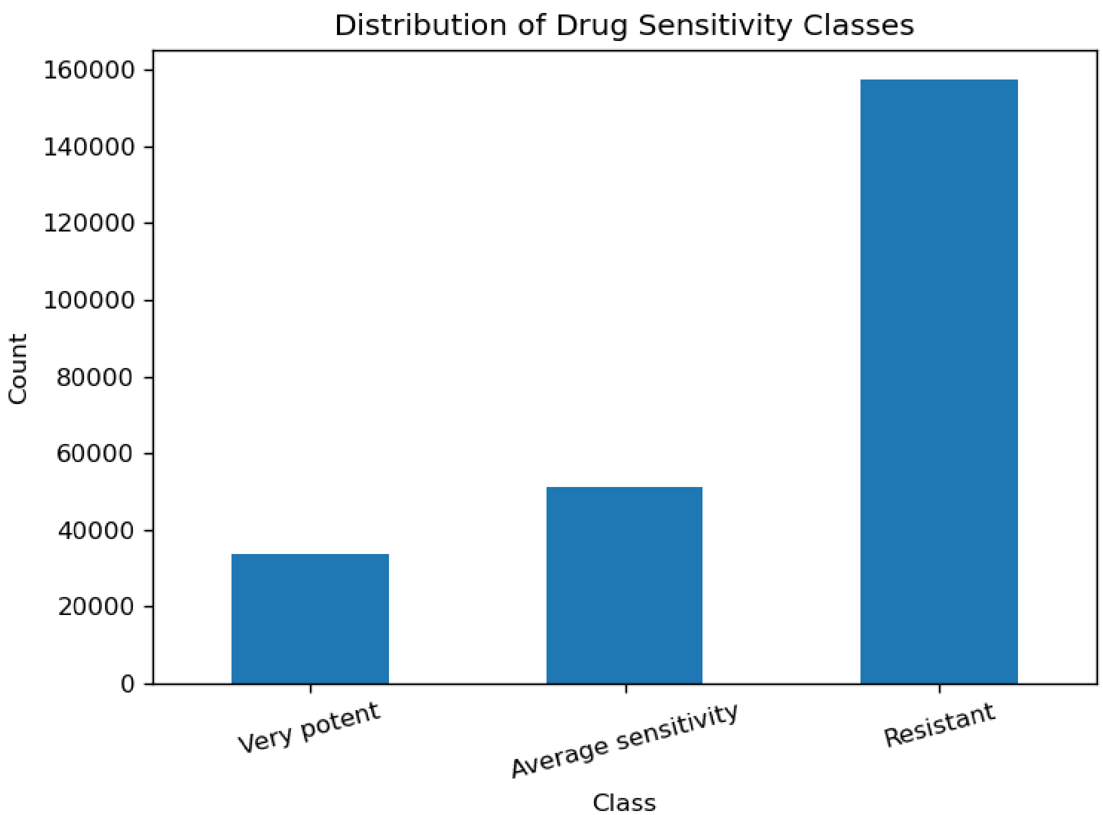
[9]:
```
df = pd.read_csv("GDSC_DATASET.csv")
print("Raw shape:", df.shape)
df.head()

LOW, HIGH = 0.0, np.log(10.0)

def label_ic50(x):
    if x < LOW:
        return "Very potent"
```

```
    elif x <= HIGH:
        return "Average sensitivity"
    else:
        return "Resistant"

df = df.dropna(subset=["LN_IC50"]).copy()
df["TargetClass"] = df["LN_IC50"].apply(label_ic50)

df["TargetClass"].value_counts()
```

```
Raw shape: (242035, 19)
```

[9]:
```
TargetClass
Resistant              157188
Average sensitivity     51171
Very potent             33676
Name: count, dtype: int64
```

[10]:
```
ax = df["TargetClass"].value_counts().reindex(
    ["Very potent","Average sensitivity","Resistant"]
).plot(kind="bar")
ax.set_title("Distribution of Drug Sensitivity Classes")
ax.set_xlabel("Class")
ax.set_ylabel("Count")
plt.xticks(rotation=15)
plt.tight_layout()
plt.show()
```



[5]:
```
X_num.dtypes

X_num.apply(lambda col: pd.to_numeric(col, errors="coerce")).isna().sum()
```

[5]:
```
AUC                      0
Z_SCORE                  0
CNA                 242035
Gene Expression     242035
Methylation         242035
dtype: int64
```

[11]:
```
num_feats = [c for c in ["AUC", "Z_SCORE"] if c in df.columns]

cat_feats = [
    "GDSC Tissue descriptor 1",
    "TARGET_PATHWAY",
    "Microsatellite instability Status (MSI)",
    "Screen Medium",
    "Growth Properties",
    "CNA",
    "Gene Expression",
```

```python
    "Methylation"
]

cat_feats = [c for c in cat_feats if c in df.columns]

print("Numeric features:", num_feats)
print("Categorical features:", cat_feats)
```

```
Numeric features: ['AUC', 'Z_SCORE']
Categorical features: ['GDSC Tissue descriptor 1', 'TARGET_PATHWAY',
'Microsatellite instability Status (MSI)', 'Screen Medium', 'Growth Properties',
'CNA', 'Gene Expression', 'Methylation']
```

[12]:
```python
X_num = df[num_feats].copy()
X_cat = df[cat_feats].copy()
y = df["TargetClass"].copy()

print("X_num shape:", X_num.shape)
print("X_cat shape:", X_cat.shape)
print("y shape:", y.shape)
```

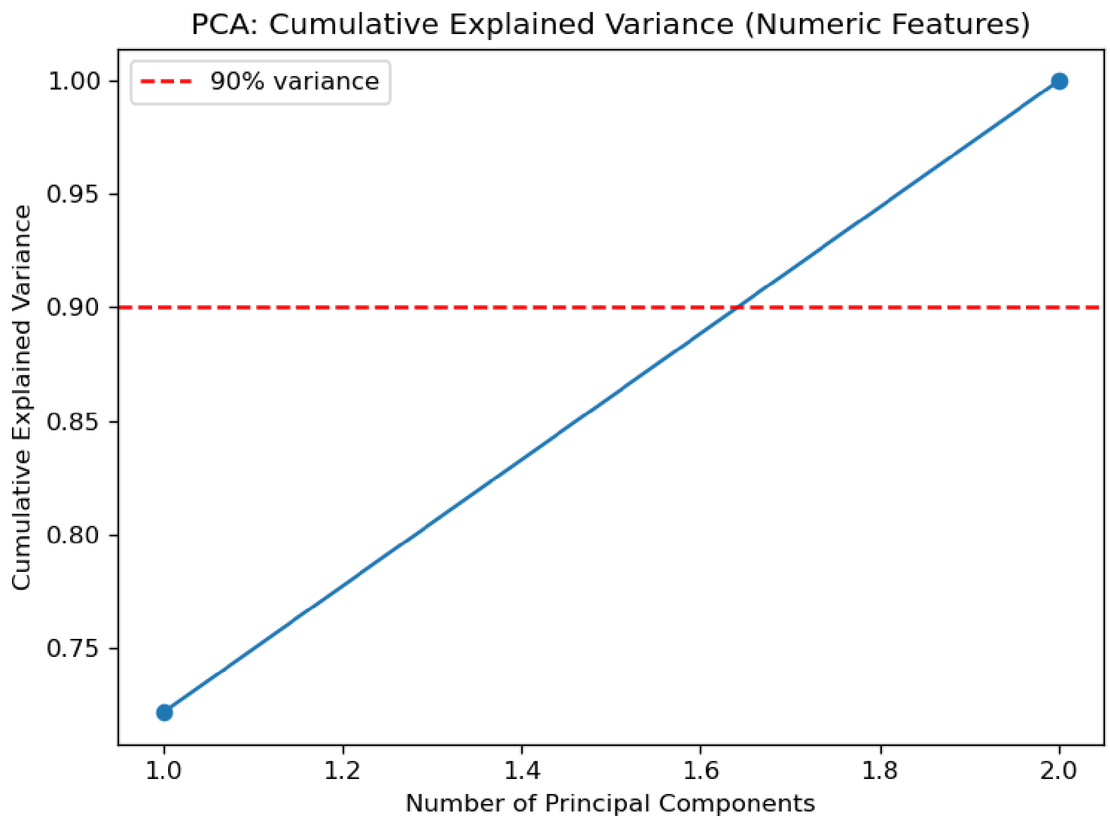
```
X_num shape: (242035, 2)
X_cat shape: (242035, 8)
y shape: (242035,)
```

[15]:
```python
X_num_clean = X_num.apply(lambda col: pd.to_numeric(col, errors="coerce"))

num_imputer = SimpleImputer(strategy="median")
X_num_imputed = num_imputer.fit_transform(X_num_clean)

scaler = StandardScaler()
X_num_scaled = scaler.fit_transform(X_num_imputed)

print("Numeric scaled shape:", X_num_scaled.shape)

cat_imputer = SimpleImputer(strategy="most_frequent")
X_cat_imputed = cat_imputer.fit_transform(X_cat)


ohe = OneHotEncoder(handle_unknown="ignore", sparse_output=False)
X_cat_encoded = ohe.fit_transform(X_cat_imputed)

print("Categorical encoded shape:", X_cat_encoded.shape)
```

```
Numeric scaled shape: (242035, 2)
Categorical encoded shape: (242035, 56)
```

[16]:

```
pca_full = PCA()
pca_full.fit(X_num_scaled)

explained_var_ratio = pca_full.explained_variance_ratio_
cum_explained = np.cumsum(explained_var_ratio)

plt.figure()
plt.plot(range(1, len(cum_explained)+1), cum_explained, marker="o")
plt.axhline(0.9, color="red", linestyle="--", label="90% variance")
plt.xlabel("Number of Principal Components")
plt.ylabel("Cumulative Explained Variance")
plt.title("PCA: Cumulative Explained Variance (Numeric Features)")
plt.legend()
plt.tight_layout()
plt.show()
```



[17]:

```
n_components = 2

pca = PCA(n_components=n_components)
X_num_pca = pca.fit_transform(X_num_scaled)
```

```python
print("Original numeric shape:", X_num_scaled.shape)
print("After PCA numeric shape:", X_num_pca.shape)
print("Explained variance of chosen components:", pca.explained_variance_ratio_)
print("Total variance explained:", pca.explained_variance_ratio_.sum())
```

```
Original numeric shape: (242035, 2)
After PCA numeric shape: (242035, 2)
Explained variance of chosen components: [0.72129403 0.27870597]
Total variance explained: 1.0
```

[18]:
```python
X_all = np.hstack([X_num_pca, X_cat_encoded])
print("Final feature matrix shape:", X_all.shape)
```

```
Final feature matrix shape: (242035, 58)
```

[19]:
```python
X_train, X_test, y_train_text, y_test_text = train_test_split(
    X_all, y, test_size=0.2, random_state=42, stratify=y
)

print("Train size:", X_train.shape[0])
print("Test size:", X_test.shape[0])
print("Train class counts:\n", y_train_text.value_counts())
print("\nTest class counts:\n", y_test_text.value_counts())

label_to_int = {"Very potent": 0, "Average sensitivity": 1, "Resistant": 2}
int_to_label = {v: k for k, v in label_to_int.items()}

y_train_int = y_train_text.map(label_to_int).values
y_test_int  = y_test_text.map(label_to_int).values

y_train_oh = to_categorical(y_train_int, num_classes=3)
y_test_oh  = to_categorical(y_test_int, num_classes=3)

print("y_train_int shape:", y_train_int.shape)
print("y_train_oh shape:", y_train_oh.shape)
```

```
Train size: 193628
Test size: 48407
Train class counts:
 TargetClass
Resistant              125750
Average sensitivity     40937
Very potent             26941
Name: count, dtype: int64

Test class counts:
 TargetClass
Resistant              31438
```

```
Average sensitivity    10234
Very potent             6735
Name: count, dtype: int64
y_train_int shape: (193628,)
y_train_oh shape: (193628, 3)
```

[20]:
```
input_dim = X_train.shape[1]

model = Sequential([
    Dense(64, activation="relu", input_shape=(input_dim,)),
    Dropout(0.3),
    Dense(32, activation="relu"),
    Dropout(0.2),
    Dense(3, activation="softmax")
])

model.compile(
    loss="categorical_crossentropy",
    optimizer="adam",
    metrics=["accuracy"]
)

model.summary()

history = model.fit(
    X_train, y_train_oh,
    validation_split=0.2,
    epochs=20,
    batch_size=256,
    verbose=1
)
```

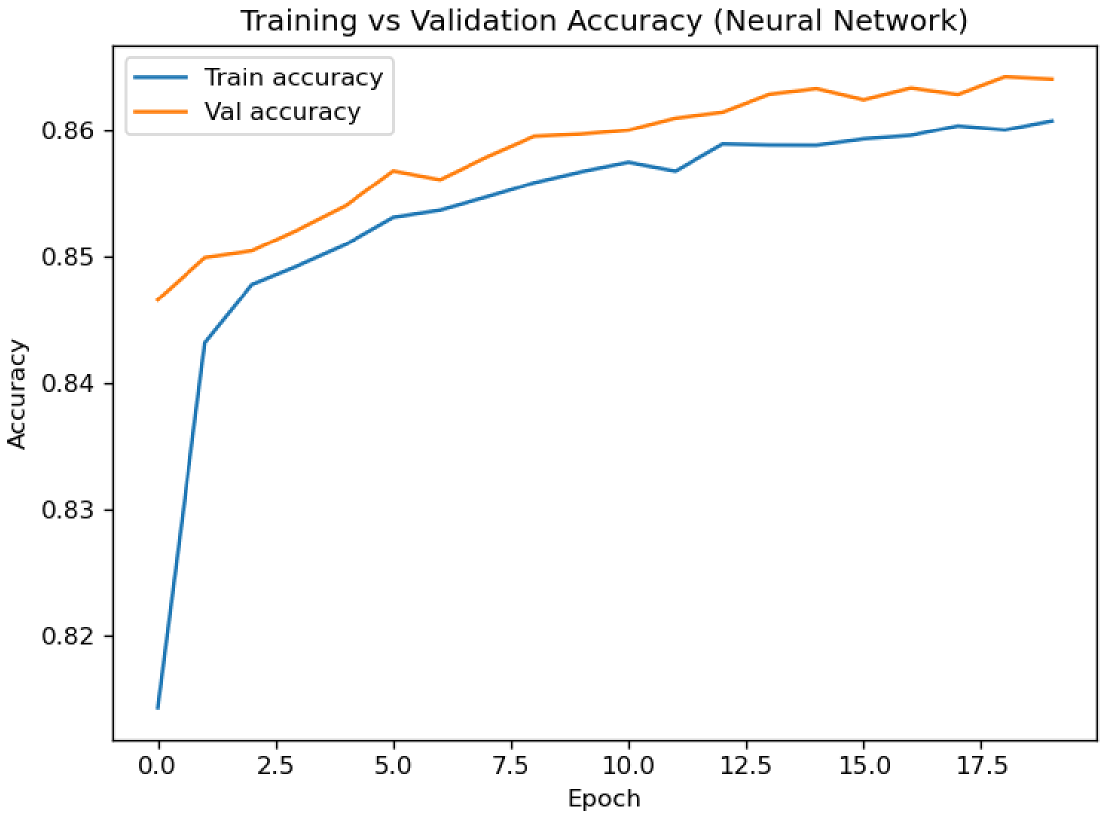
```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense (Dense)               (None, 64)                3776

 dropout (Dropout)           (None, 64)                0

 dense_1 (Dense)             (None, 32)                2080

 dropout_1 (Dropout)         (None, 32)                0

 dense_2 (Dense)             (None, 3)                 99

=================================================================
Total params: 5,955
```

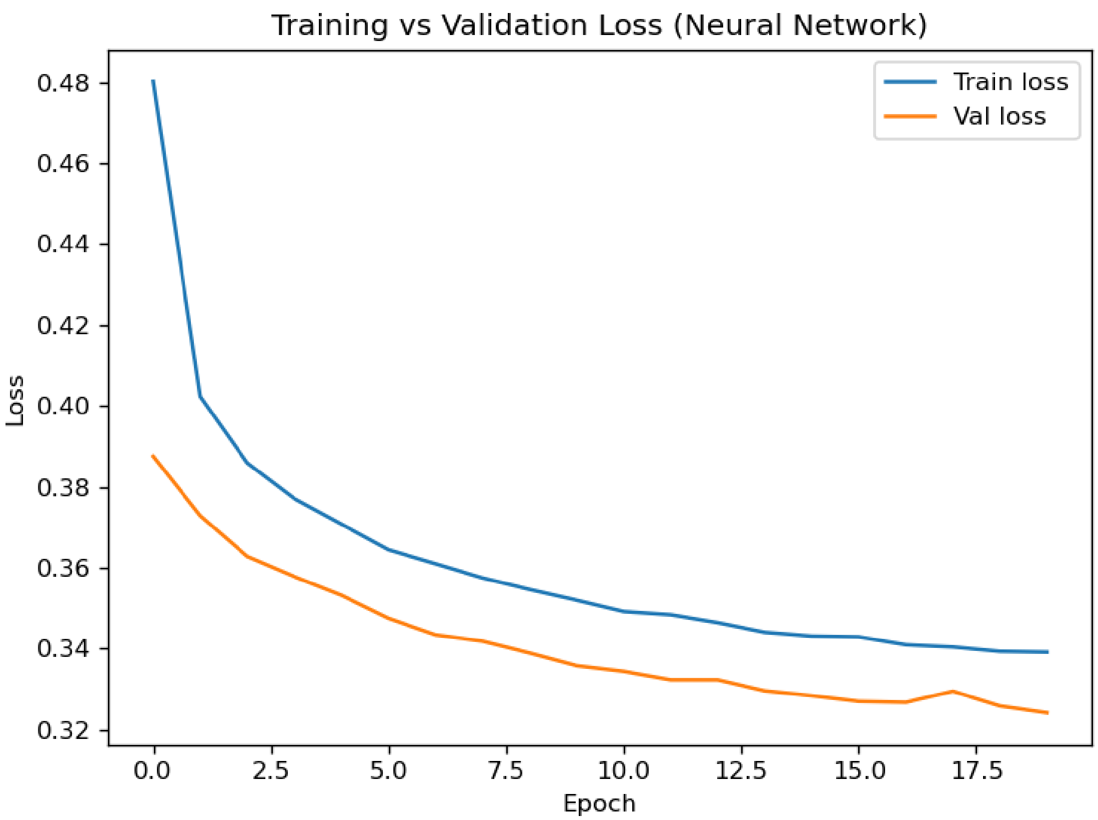
```
Trainable params: 5,955
Non-trainable params: 0
_________________________________________________________________
2025-12-07 23:59:43.533800: I tensorflow/core/platform/cpu_feature_guard.cc:193]
This TensorFlow binary is optimized with oneAPI Deep Neural Network Library
(oneDNN) to use the following CPU instructions in performance-critical
operations:  SSE4.1 SSE4.2 AVX AVX2 AVX512F FMA
To enable them in other operations, rebuild TensorFlow with the appropriate
compiler flags.
2025-12-07 23:59:43.538504: I
tensorflow/core/common_runtime/process_util.cc:146] Creating new thread pool
with default inter op setting: 2. Tune using inter_op_parallelism_threads for
best performance.

Epoch 1/20
606/606 [==============================] - 7s 10ms/step - loss: 0.4802 -
accuracy: 0.8143 - val_loss: 0.3875 - val_accuracy: 0.8466
Epoch 2/20
606/606 [==============================] - 4s 6ms/step - loss: 0.4023 -
accuracy: 0.8432 - val_loss: 0.3728 - val_accuracy: 0.8499
Epoch 3/20
606/606 [==============================] - 5s 8ms/step - loss: 0.3859 -
accuracy: 0.8478 - val_loss: 0.3628 - val_accuracy: 0.8505
Epoch 4/20
606/606 [==============================] - 5s 8ms/step - loss: 0.3771 -
accuracy: 0.8493 - val_loss: 0.3578 - val_accuracy: 0.8522
Epoch 5/20
606/606 [==============================] - 13s 21ms/step - loss: 0.3707 -
accuracy: 0.8510 - val_loss: 0.3532 - val_accuracy: 0.8541
Epoch 6/20
606/606 [==============================] - 6s 10ms/step - loss: 0.3644 -
accuracy: 0.8531 - val_loss: 0.3475 - val_accuracy: 0.8568
Epoch 7/20
606/606 [==============================] - 5s 9ms/step - loss: 0.3609 -
accuracy: 0.8537 - val_loss: 0.3434 - val_accuracy: 0.8561
Epoch 8/20
606/606 [==============================] - 6s 9ms/step - loss: 0.3574 -
accuracy: 0.8547 - val_loss: 0.3418 - val_accuracy: 0.8579
Epoch 9/20
606/606 [==============================] - 6s 9ms/step - loss: 0.3546 -
accuracy: 0.8559 - val_loss: 0.3389 - val_accuracy: 0.8595
Epoch 10/20
606/606 [==============================] - 6s 10ms/step - loss: 0.3519 -
accuracy: 0.8567 - val_loss: 0.3358 - val_accuracy: 0.8597
Epoch 11/20
606/606 [==============================] - 5s 7ms/step - loss: 0.3491 -
accuracy: 0.8575 - val_loss: 0.3344 - val_accuracy: 0.8600
Epoch 12/20
```

```
606/606 [==============================] - 4s 6ms/step - loss: 0.3483 -
accuracy: 0.8568 - val_loss: 0.3323 - val_accuracy: 0.8610
Epoch 13/20
606/606 [==============================] - 4s 6ms/step - loss: 0.3464 -
accuracy: 0.8589 - val_loss: 0.3323 - val_accuracy: 0.8614
Epoch 14/20
606/606 [==============================] - 4s 6ms/step - loss: 0.3440 -
accuracy: 0.8588 - val_loss: 0.3295 - val_accuracy: 0.8629
Epoch 15/20
606/606 [==============================] - 5s 9ms/step - loss: 0.3431 -
accuracy: 0.8588 - val_loss: 0.3283 - val_accuracy: 0.8633
Epoch 16/20
606/606 [==============================] - 9s 14ms/step - loss: 0.3429 -
accuracy: 0.8593 - val_loss: 0.3269 - val_accuracy: 0.8624
Epoch 17/20
606/606 [==============================] - 4s 6ms/step - loss: 0.3409 -
accuracy: 0.8596 - val_loss: 0.3267 - val_accuracy: 0.8633
Epoch 18/20
606/606 [==============================] - 4s 6ms/step - loss: 0.3404 -
accuracy: 0.8604 - val_loss: 0.3294 - val_accuracy: 0.8628
Epoch 19/20
606/606 [==============================] - 4s 7ms/step - loss: 0.3393 -
accuracy: 0.8600 - val_loss: 0.3258 - val_accuracy: 0.8642
Epoch 20/20
606/606 [==============================] - 4s 6ms/step - loss: 0.3391 -
accuracy: 0.8608 - val_loss: 0.3241 - val_accuracy: 0.8640
```

[21]:

```python
plt.figure()
plt.plot(history.history["accuracy"], label="Train accuracy")
plt.plot(history.history["val_accuracy"], label="Val accuracy")
plt.xlabel("Epoch")
plt.ylabel("Accuracy")
plt.title("Training vs Validation Accuracy (Neural Network)")
plt.legend()
plt.tight_layout()
plt.show()

plt.figure()
plt.plot(history.history["loss"], label="Train loss")
plt.plot(history.history["val_loss"], label="Val loss")
plt.xlabel("Epoch")
plt.ylabel("Loss")
plt.title("Training vs Validation Loss (Neural Network)")
plt.legend()
plt.tight_layout()
plt.show()
```


Training vs Validation Accuracy (Neural Network)
Train accuracy
Val accuracy
Accuracy
0.86
0.85
0.84
0.83
0.82
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Epoch



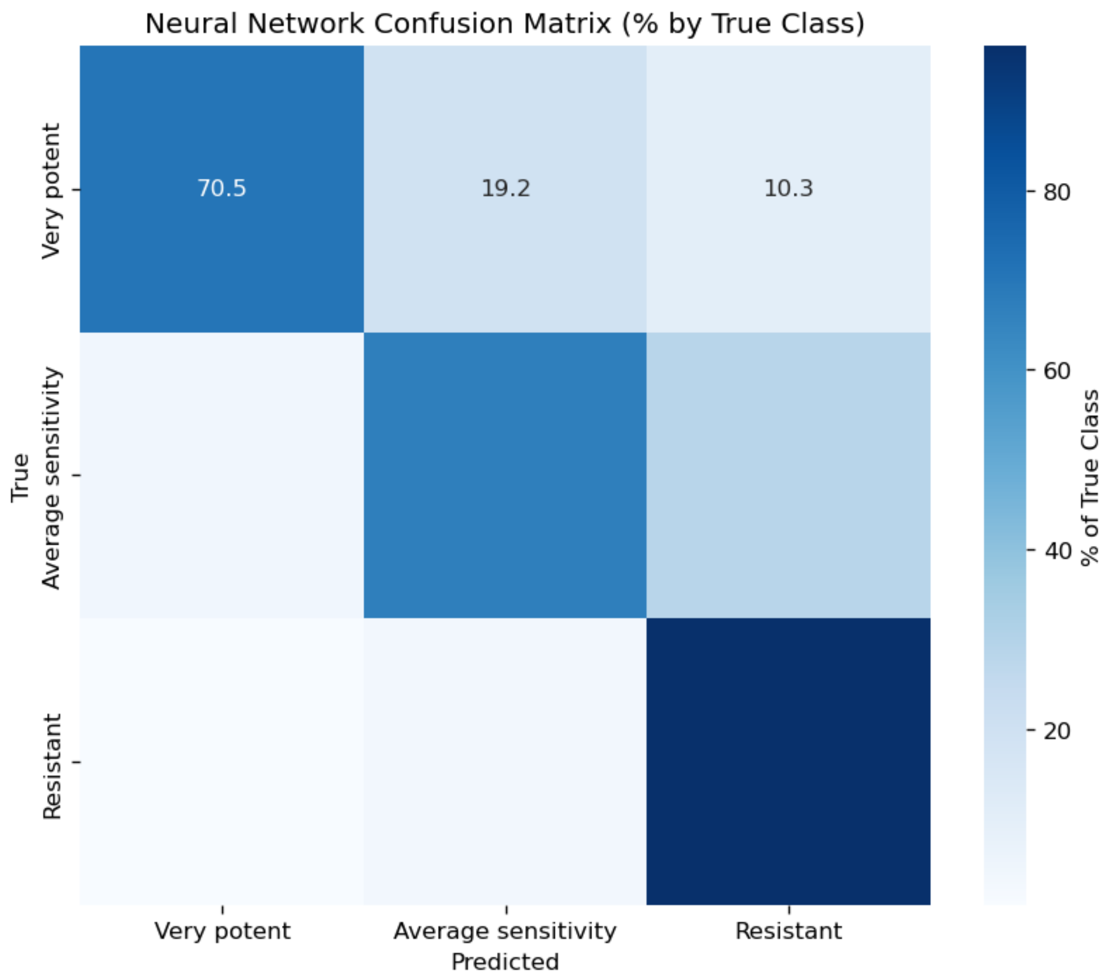
[22]:
```python
test_loss, test_acc = model.evaluate(X_test, y_test_oh, verbose=0)
print(f"Test accuracy: {test_acc:.3f}")
print(f"Test loss: {test_loss:.3f}")

y_pred_proba = model.predict(X_test)
y_pred_int = np.argmax(y_pred_proba, axis=1)
y_pred_labels = pd.Series(y_pred_int).map(int_to_label)

print("Classification report (Neural Network):")
print(classification_report(y_test_text, y_pred_labels, digits=3))
```

```
Test accuracy: 0.864
Test loss: 0.323
1513/1513 [==============================] - 10s 7ms/step
Classification report (Neural Network):
                     precision    recall  f1-score   support

Average sensitivity      0.744     0.672     0.706     10234
          Resistant      0.893     0.961     0.926     31438
        Very potent      0.891     0.705     0.788      6735
```

```
     accuracy                           0.864     48407
    macro avg       0.843     0.779     0.806     48407
 weighted avg       0.861     0.864     0.860     48407
```

[23]:

```python
labels_order = ["Very potent","Average sensitivity","Resistant"]

cm = confusion_matrix(y_test_text, y_pred_labels, labels=labels_order)
cm_df = pd.DataFrame(cm, index=labels_order, columns=labels_order)
cm_perc = cm_df.div(cm_df.sum(axis=1), axis=0) * 100

plt.figure(figsize=(7,6))
sns.heatmap(cm_perc, annot=True, fmt=".1f", cmap="Blues",
            xticklabels=labels_order, yticklabels=labels_order,
            cbar_kws={'label': '% of True Class'})
plt.title("Neural Network Confusion Matrix (% by True Class)")
plt.xlabel("Predicted")
plt.ylabel("True")
plt.tight_layout()
plt.show()
```


Neural Network Confusion Matrix (% by True Class)
True
Very potent
Average sensitivity
Resistant
70.5
19.2
10.3
Predicted
Very potent
Average sensitivity
Resistant
% of True Class
80
60
40
20

```
[ ]:
```