In [1]:
```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import LabelEncoder, StandardScaler
import torch
import torch.nn as nn
import torch.optim
from torch.utils.data import DataLoader, TensorDataset
```

READING IN THE MODEL

In [2]:
```
df = pd.read_csv(r'/kaggle/input/yeast-dataset/yeast.xls')
df
```

Out[2]:

	mcg	gvh	alm	mit	erl	pox	vac	nuc	name
0	0.58	0.61	0.47	0.13	0.5	0.0	0.48	0.22	MIT
1	0.43	0.67	0.48	0.27	0.5	0.0	0.53	0.22	MIT
2	0.64	0.62	0.49	0.15	0.5	0.0	0.53	0.22	MIT
3	0.58	0.44	0.57	0.13	0.5	0.0	0.54	0.22	NUC
4	0.42	0.44	0.48	0.54	0.5	0.0	0.48	0.22	MIT
...	...	...	...	...	...	...	...	...	...
1479	0.81	0.62	0.43	0.17	0.5	0.0	0.53	0.22	ME2
1480	0.47	0.43	0.61	0.40	0.5	0.0	0.48	0.47	NUC
1481	0.67	0.57	0.36	0.19	0.5	0.0	0.56	0.22	ME2
1482	0.43	0.40	0.60	0.16	0.5	0.0	0.53	0.39	NUC
1483	0.65	0.54	0.54	0.13	0.5	0.0	0.53	0.22	CYT

1484 rows × 9 columns

In [3]:
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1484 entries, 0 to 1483
Data columns (total 9 columns):
 #   Column  Non-Null Count  Dtype  
---  ------  --------------  -----  
 0   mcg     1484 non-null   float64
 1   gvh     1484 non-null   float64
 2   alm     1484 non-null   float64
 3   mit     1484 non-null   float64
 4   erl     1484 non-null   float64
 5   pox     1484 non-null   float64
 6   vac     1484 non-null   float64
 7   nuc     1484 non-null   float64
 8   name    1484 non-null   object 
dtypes: float64(8), object(1)
memory usage: 104.5+ KB
```

DESCRIPTION

In [4]:
```
df.describe()
```

Out[4]:

	mcg	gvh	alm	mit	erl	pox	vac	nuc
count	1484.000000	1484.000000	1484.000000	1484.000000	1484.000000	1484.000000	1484.000000	1484.000000
mean	0.500121	0.499933	0.500034	0.261186	0.504717	0.007500	0.499885	0.276199
std	0.137299	0.123924	0.086670	0.137098	0.048351	0.075683	0.057797	0.106491
min	0.110000	0.130000	0.210000	0.000000	0.500000	0.000000	0.000000	0.000000
25%	0.410000	0.420000	0.460000	0.170000	0.500000	0.000000	0.480000	0.220000
50%	0.490000	0.490000	0.510000	0.220000	0.500000	0.000000	0.510000	0.220000
75%	0.580000	0.570000	0.550000	0.320000	0.500000	0.000000	0.530000	0.300000
max	1.000000	1.000000	1.000000	1.000000	1.000000	0.830000	0.730000	1.000000

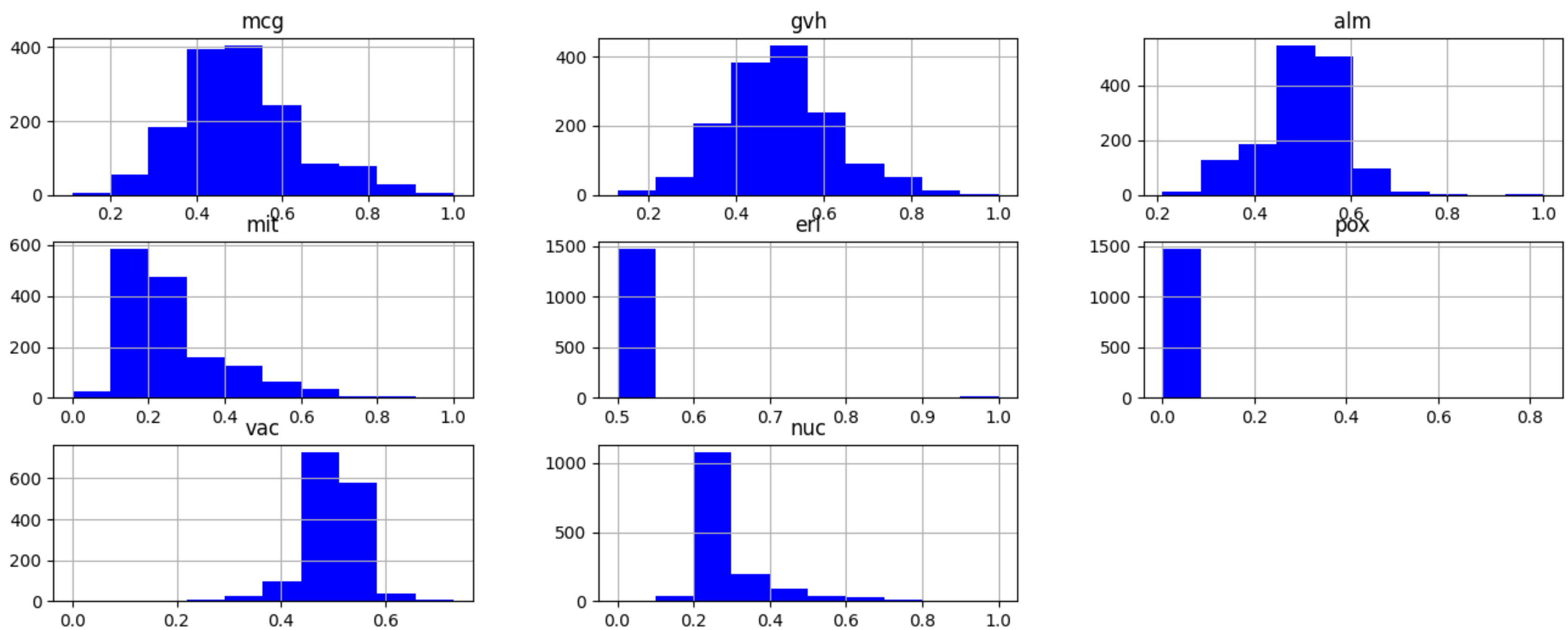
CHECKING FOR MISSING VALUES

In [5]:
```
df.isna().sum()
```

Out[5]:
```
mcg      0
gvh      0
alm      0
mit      0
erl      0
pox      0
vac      0
nuc      0
name     0
dtype: int64
```

HIST PLOT OF FEATURES

In [6]:
```
df.hist(figsize=(16, 6), color='blue');
```



RENAMING THE TARGET COLUMN

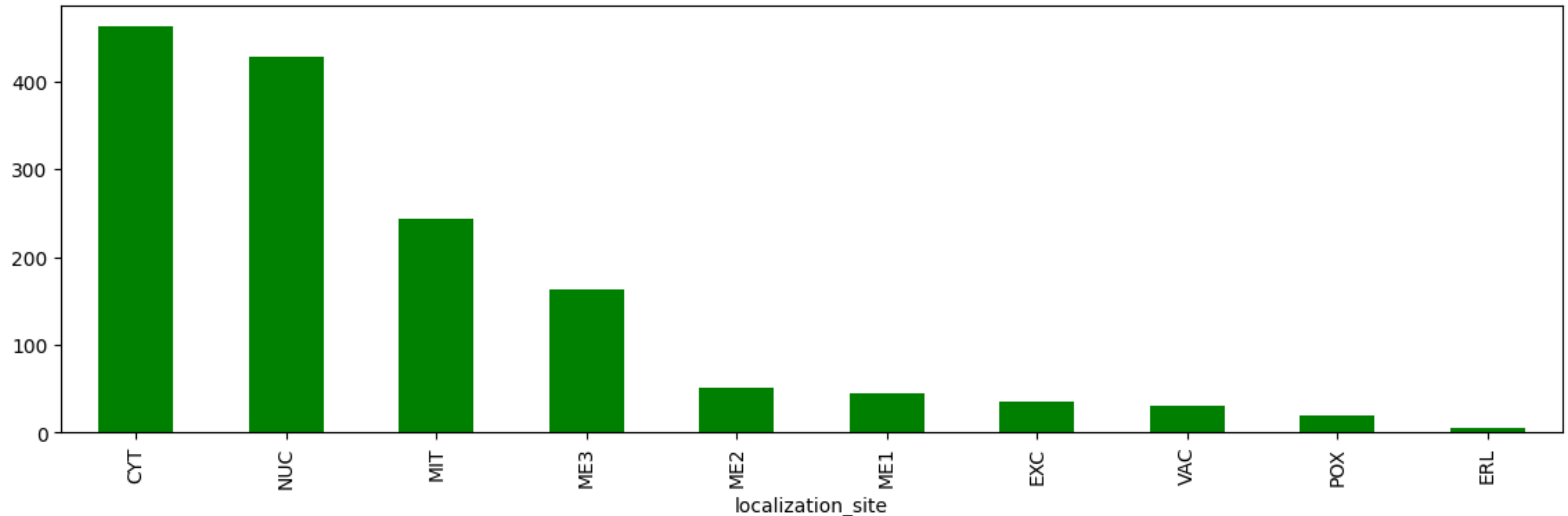
In [7]:
```
df.rename(columns = {'name':'localization_site'}, inplace=True)
```

TARGET COLUMN DESCRIPTION

In [8]:
```
print(df['localization_site'].value_counts())
df['localization_site'].value_counts().plot(kind='bar', figsize=(14, 4), color='green')
```

```
localization_site
CYT    463
NUC    429
MIT    244
ME3    163
ME2     51
ME1     44
EXC     35
VAC     30
POX     20
ERL      5
Name: count, dtype: int64
```

Out[8]: <Axes: xlabel='localization_site'>

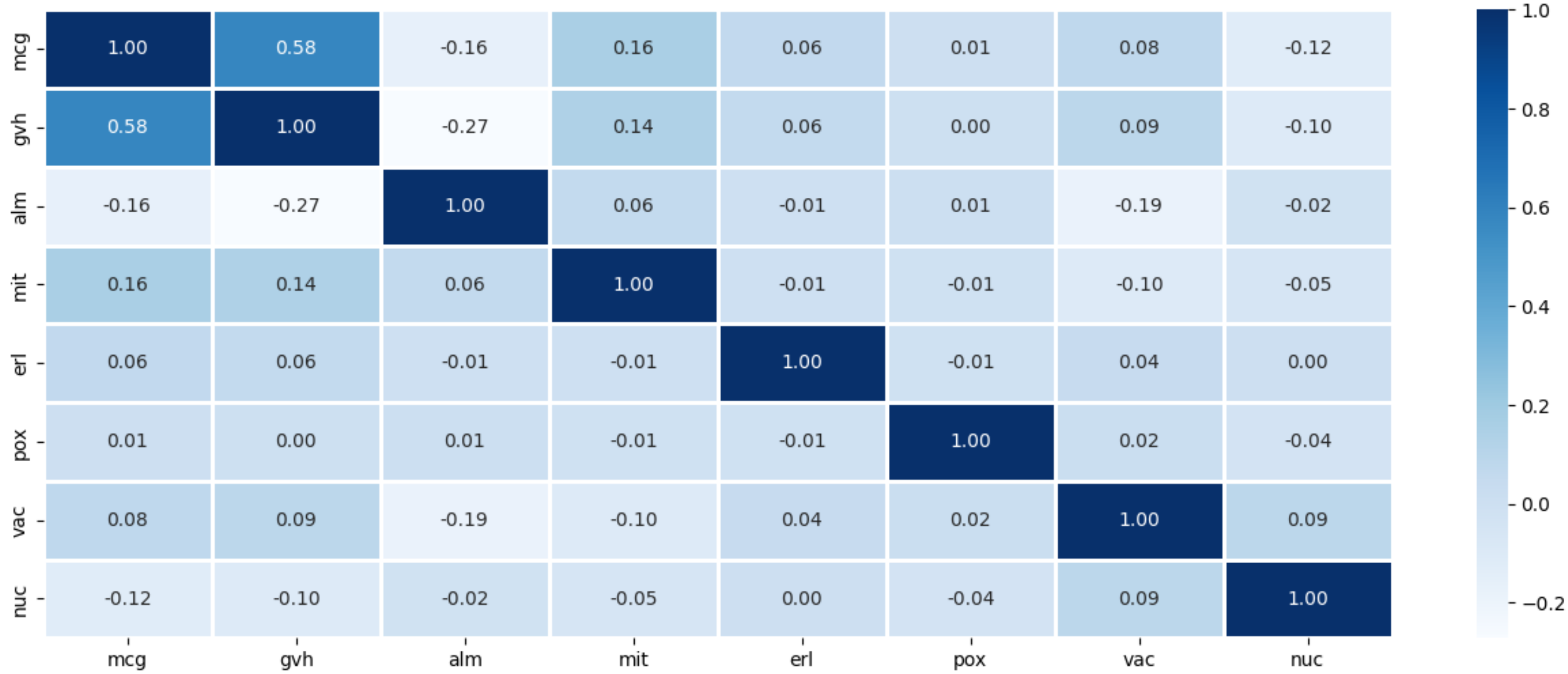


CORRELATION MATRIX

In [9]:
```
correlation = df.drop('localization_site', axis=1).corr()
plt.figure(figsize=(16, 6))
```

```
sns.heatmap(correlation, cmap='Blues', annot=True, fmt='.2f', lw=1)
```

Out[9]: <Axes: >



SPLITTING TARGET AND INPUT FEATURES

In [10]:
```
X = df.drop('localization_site', axis=1)    # INPUT FEATURES
y = df['localization_site']                # TARGET FEATURE


print("Input shape:", X.shape)
print("Target shape:", y.shape)
```

```
Input shape: (1484, 8)
Target shape: (1484,)
```

ENCODING THE TARGET COLUMN

In [11]:
```
label_encoder = LabelEncoder()       # LABEL ENCODER
y_encoded = label_encoder.fit_transform(y)  # FITTING THE TARGET COLUMN TO THE ENCODER
classes_names = label_encoder.classes_        # TARGET COLUMN CLASSES
```

SCALING THE INPUT FEATURES

In [12]:
```
scaler = StandardScaler()       # SCALER
X_scaled = scaler.fit_transform(X)  # FITTING THE INPUT FEATURES
```

SPLITTING THE TRAIN AND TEST SETS AND CONVERTING TO TENSORS

In [13]:
```
from sklearn.model_selection import train_test_split
import torch

# --------------------------------------------------------------
#  Split the dataset into training and testing sets
# --------------------------------------------------------------
# - X_scaled: your normalized or standardized feature matrix
# - y_encoded: your encoded labels (numeric form)
# - test_size=0.2 means 20% test, 80% train
# - random_state ensures reproducibility
# - stratify=y_encoded ensures class balance in both splits
X_train, X_test, y_train, y_test = train_test_split(
    X_scaled,
    y_encoded,
    test_size=0.2,
    random_state=42,
    stratify=y_encoded
)

# --------------------------------------------------------------
# Convert NumPy arrays to PyTorch tensors
# --------------------------------------------------------------
# Convert features (X) to float32 tensors — required for neural networks
X_train_tensor = torch.tensor(X_train, dtype=torch.float32)
X_test_tensor = torch.tensor(X_test, dtype=torch.float32)

# Convert labels (y) to long tensors — required by nn.CrossEntropyLoss
y_train_tensor = torch.tensor(y_train, dtype=torch.long)
y_test_tensor = torch.tensor(y_test, dtype=torch.long)
```

```
# -------------------------------------------------------------
#  Print shapes to verify data dimensions
# -------------------------------------------------------------
print("X_train shape:", X_train_tensor.shape)   # e.g., torch.Size([N_train, num_features])
print("X_test shape:", X_test_tensor.shape)     # e.g., torch.Size([N_test, num_features])
print("y_train shape:", y_train_tensor.shape)   # e.g., torch.Size([N_train])
print("y_test shape:", y_test_tensor.shape)     # e.g., torch.Size([N_test])

# -------------------------------------------------------------
# Print the number of unique classes (from LabelEncoder)
# -------------------------------------------------------------
print("Length of classes:", len(label_encoder.classes_))
```

```
X_train shape: torch.Size([1187, 8])
X_test shape: torch.Size([297, 8])
y_train shape: torch.Size([1187])
y_test shape: torch.Size([297])
Length of classes: 10
X_train shape: torch.Size([1187, 8])
X_test shape: torch.Size([297, 8])
y_train shape: torch.Size([1187])
y_test shape: torch.Size([297])
Length of classes: 10
```

BUILDING A NEURAL NETWORK

In [ ]:

```
import torch
import torch.nn as nn

# -------------------------------------------------------------
# Define a simple feedforward neural network for the Yeast dataset
# -------------------------------------------------------------
class yeast_model(nn.Module):
    def __init__(self):
        # Initialize the parent nn.Module class
        super(yeast_model, self).__init__()

        # Define the model architecture using nn.Sequential
        #  - Input layer: 8 features → 32 hidden neurons
        #  - Activation: ReLU (introduces non-linearity)
        #  - Output layer: 32 → 10 neurons (for 10 yeast classes)
```

```
        self.model = nn.Sequential(
            nn.Linear(8, 32),   # Fully connected layer (input → hidden)
            nn.ReLU(),          # Non-linear activation
            nn.Linear(32, 10)   # Fully connected layer (hidden → output)
        )

    # Define the forward pass (how data flows through the network)
    def forward(self, x):
        return self.model(x)   # Pass input through the defined layers

# ----------------------------------------------------------------
# Instantiate the model
# ----------------------------------------------------------------
model = yeast_model()

# Print model architecture summary
print(model)
```

In [15]:

```
# ----------------------------------------------------------------
# Full-Batch Gradient Descent using Adam Optimizer in PyTorch
# ----------------------------------------------------------------

import torch
import torch.nn as nn

# ----------------------------------------------------------------
# Define loss function and optimizer
# ----------------------------------------------------------------
model_ad = yeast_model()
criterion = nn.CrossEntropyLoss()                          # Multi-class classification loss
optimizer = torch.optim.Adam(model_ad.parameters(), lr=0.01)   # Adam optimizer with learning rate = 0.1

# ----------------------------------------------------------------
# Initialize metric storage
# ----------------------------------------------------------------
train_losses = []
train_accuracies = []
num_epoch = 100  # Number of training iterations (epochs)

# ----------------------------------------------------------------
# Training Loop
# ----------------------------------------------------------------
```

```python
for epoch in range(num_epoch):

    # ------------------------------------------------------------
    # Forward Pass: Compute predictions and loss
    # ------------------------------------------------------------
    logits = model_ad(X_train_tensor)             # Full-batch forward pass
    loss = criterion(logits, y_train_tensor)   # Compute cross-entropy loss

    # ------------------------------------------------------------
    # Backward Pass: Gradient computation and update
    # ------------------------------------------------------------
    optimizer.zero_grad()   # Reset accumulated gradients
    loss.backward()         # Compute new gradients
    optimizer.step()        # Update model parameters

    # ------------------------------------------------------------
    # Track metrics
    # ------------------------------------------------------------
    train_losses.append(loss.item())

    # Compute accuracy
    preds = torch.argmax(logits, dim=1)                    # Get predicted classes
    correct = (preds == y_train_tensor).sum().item()       # Count correct predictions
    accuracy = correct / len(y_train_tensor)               # Compute accuracy
    train_accuracies.append(accuracy)

    # ------------------------------------------------------------
    # Print progress every 10 epochs
    # ------------------------------------------------------------
    if (epoch + 1) % 10 == 0:
        print(f"Epoch {epoch + 1:3d} | Loss: {loss.item():.3f} | Train Acc: {accuracy * 100:.2f}%")
```

```
Epoch  10 | Loss: 1.569 | Train Acc: 47.94%
Epoch  20 | Loss: 1.237 | Train Acc: 55.60%
Epoch  30 | Loss: 1.124 | Train Acc: 58.97%
Epoch  40 | Loss: 1.063 | Train Acc: 60.91%
Epoch  50 | Loss: 1.028 | Train Acc: 62.09%
Epoch  60 | Loss: 1.005 | Train Acc: 62.85%
Epoch  70 | Loss: 0.988 | Train Acc: 63.35%
Epoch  80 | Loss: 0.973 | Train Acc: 63.52%
Epoch  90 | Loss: 0.961 | Train Acc: 63.44%
Epoch 100 | Loss: 0.949 | Train Acc: 64.20%
```

OPTIMIZATION

In [16]:
```
import torch
import torch.nn as nn

# ----------------------------------------------------------------
# Define a simple feedforward neural network for the Yeast dataset
# ----------------------------------------------------------------
class yeast_model(nn.Module):
    def __init__(self, input_dim ,hidden_layer, output_dim):
        # Initialize the parent nn.Module class
        super(yeast_model, self).__init__()

        # Define the model architecture using nn.Sequential
        #  - Input layer: 8 features → 32 hidden neurons
        #  - Activation: ReLU (introduces non-linearity)
        #  - Output layer: 32 → 10 neurons (for 10 yeast classes)
        self.model = nn.Sequential(
            nn.Linear(8, 32),   # Fully connected layer (input → hidden)
            nn.ReLU(),          # Non-linear activation
            nn.Linear(32, 10)   # Fully connected layer (hidden → output)
        )

    # Define the forward pass (how data flows through the network)
    def forward(self, x):
        return self.model(x)   # Pass input through the defined layers

input_dim = X_train_tensor.shape[1]      # 8 features
hidden_layer = 16
output_dim = len(label_encoder.classes_)

# ----------------------------------------------------------------
# Instantiate the model
# ----------------------------------------------------------------
model = yeast_model(input_dim, hidden_layer, output_dim)

# Print model architecture summary
print(model)
```

```
yeast_model(
  (model): Sequential(
    (0): Linear(in_features=8, out_features=32, bias=True)
    (1): ReLU()
    (2): Linear(in_features=32, out_features=10, bias=True)
  )
)
```

In [17]:
```python
# Combine features and labels into a single training dataset
Train_dataset = TensorDataset(X_train_tensor, y_train_tensor)

# Combine features and labels into a single test dataset
Test_dataset = TensorDataset(X_test_tensor, y_test_tensor)

# Create DataLoader for training set (batches of 32, shuffled each epoch)
train_loader = DataLoader(Train_dataset, batch_size=32, shuffle=True)

# Create DataLoader for test set (batches of 32, no shuffling)
test_loader = DataLoader(Test_dataset, batch_size=32, shuffle=False)




# Check shapes and class info
print(" Train set:", X_train_tensor.shape)
print(" Test set:", X_test_tensor.shape)
print(" Number of Classes:", len(label_encoder.classes_))
print(" Class Names:", label_encoder.classes_)
```

```
Train set: torch.Size([1187, 8])
Test set: torch.Size([297, 8])
Number of Classes: 10
Class Names: ['CYT' 'ERL' 'EXC' 'ME1' 'ME2' 'ME3' 'MIT' 'NUC' 'POX' 'VAC']
```

==

NOTE: Understanding SGD, Full-Batch, and Mini-Batch Optimizers in ML

==

1️⃣ Full-Batch Gradient Descent

▪ ***Description:***

- Uses the **entire training dataset** to compute the gradient at each step.
- The model parameters are updated **only once per epoch**.

▪ ***Advantages:***

- Produces a **stable and accurate** estimate of the gradient.
- **Guarantees convergence** for convex problems.

▪ ***Disadvantages:***

- **Computationally expensive** for large datasets.
- **Slow training** since it processes all samples before one update.

----

2 Stochastic Gradient Descent (SGD)

▪ ***Description:***

- Updates model parameters after computing the gradient on a **single sample**.
- The model updates **more frequently**, introducing randomness (noise).

▪ ***Advantages:***

- **Fast updates** → quicker learning in early epochs.
- Helps **escape local minima** due to random fluctuations.

▪ ***Disadvantages:***

- **Noisy loss curve** (fluctuates a lot).
- **Unstable convergence** without proper learning rate scheduling.

----

3 Mini-Batch Gradient Descent

▪ ***Description:***

- A **compromise** between Full-Batch and SGD.
- Divides the training data into **small batches** (e.g., 32, 64, 128 samples).
- Updates model weights after **each batch**.

▪ ***Advantages:***

- **Faster** than Full-Batch but **more stable** than SGD.
- Enables **efficient GPU computation** (vectorized operations).
- **Commonly used** in deep learning.

▪ ***Disadvantages:***

- Requires **tuning of batch size**.
- Still **slightly noisy**, though much smoother than SGD.

💡 ***Summary***

- **Full-Batch → Stable but Slow**
- **SGD → Fast but Noisy**
- **Mini-Batch → Balanced (Best for Deep Learning)**

✅ ***Most real-world neural networks use Mini-Batch Gradient Descent with adaptive optimizers like Adam, RMSProp, or SGD with Momentum.***

FULL BATCH GRADIENT DESCENT OPTMIZER

In [18]:
```
# ------------------------------------------------------------
# Full-Batch Gradient Descent (SGD) Training in PyTorch
# ------------------------------------------------------------

import torch
```

```
import torch.nn as nn

# Define optimizer and loss function
model_gd = yeast_model(input_dim, hidden_layer, output_dim)
optimizer = torch.optim.SGD(model.parameters(), lr=0.1)  # Full-batch GD
loss_fn = nn.CrossEntropyLoss()                          # Classification loss

# Track metrics
train_losses_gd = []
train_accuracy_gd = []

num_epochs = 100  # Number of full passes through the dataset

# ----------------------------------------------------------------
# Training Loop
# ----------------------------------------------------------------
for epoch in range(num_epochs):
    model.train()  # Set model to training mode (important for dropout/batchnorm)

    # ------------------------------------------------------------
    # Forward pass: compute predictions and loss
    # ------------------------------------------------------------
    logits = model(X_train_tensor)             # All samples at once (full-batch)
    loss = loss_fn(logits, y_train_tensor)

    # ------------------------------------------------------------
    # Backward pass: compute gradients and update weights
    # ------------------------------------------------------------
    optimizer.zero_grad()   #  Added parentheses
    loss.backward()
    optimizer.step()

    # ------------------------------------------------------------
    # Compute accuracy
    # ------------------------------------------------------------
    preds = torch.argmax(logits, dim=1)                # Get predicted classes
    correct = (preds == y_train_tensor).float().mean().item()  # Mean accuracy

    # ------------------------------------------------------------
    # Store metrics
    # ------------------------------------------------------------
    train_losses_gd.append(loss.item())
```

```
    train_accuracy_gd.append(correct)

    # Print progress every 10 epochs
    if (epoch + 1) % 10 == 0:
        print(f"[FULL-BATCH] Epoch {epoch + 1:3d} | Loss: {loss.item():.4f} | Accuracy: {correct * 100:.2f}%")
```

```
[FULL-BATCH] Epoch  10 | Loss: 2.0515 | Accuracy: 30.67%
[FULL-BATCH] Epoch  20 | Loss: 1.8104 | Accuracy: 35.64%
[FULL-BATCH] Epoch  30 | Loss: 1.6436 | Accuracy: 40.19%
[FULL-BATCH] Epoch  40 | Loss: 1.5242 | Accuracy: 47.35%
[FULL-BATCH] Epoch  50 | Loss: 1.4353 | Accuracy: 51.81%
[FULL-BATCH] Epoch  60 | Loss: 1.3671 | Accuracy: 53.16%
[FULL-BATCH] Epoch  70 | Loss: 1.3138 | Accuracy: 53.50%
[FULL-BATCH] Epoch  80 | Loss: 1.2717 | Accuracy: 54.59%
[FULL-BATCH] Epoch  90 | Loss: 1.2380 | Accuracy: 55.60%
[FULL-BATCH] Epoch 100 | Loss: 1.2106 | Accuracy: 56.70%
```

STOCHASTIC GRADIENT DESECNT OPTIMIZER

In [19]:
```
# STOCHASTIC GRADIENT DESCENT

# ---------------------------------------------------------------
# Set seed for reproducibility
# ---------------------------------------------------------------
torch.manual_seed(42)
import random

# ---------------------------------------------------------------
# Create a new model instance (same structure as before)
# ---------------------------------------------------------------
# Assuming yeast_model is your neural network class (e.g., YeastMLP)
model_sgd = yeast_model(input_dim, hidden_layer, output_dim)

# Define loss function and optimizer
criterion = nn.CrossEntropyLoss()                    # For multi-class classification
optimizer = torch.optim.SGD(model_sgd.parameters(), lr=0.005)  # Stochastic Gradient Descent

# ---------------------------------------------------------------
# Initialize lists to store loss and accuracy over epochs
# ---------------------------------------------------------------
train_losses_sgd = []
train_accuracy_sgd = []
```

```
# --------------------------------------------------------------
# Convert training tensors into list of (feature, label) pairs
# --------------------------------------------------------------
# This allows us to iterate sample-by-sample (true SGD)
train_samples = list(zip(X_train_tensor, y_train_tensor))

# (Optional) Track training time
# start_time = time.perf_counter()

# --------------------------------------------------------------
# Training loop - one epoch processes all samples individually
# --------------------------------------------------------------
for epoch in range(100):
    epoch_loss = 0.0
    correct = 0

    # Shuffle training samples at the start of each epoch
    torch.random.manual_seed(epoch)   # Ensures deterministic shuffling
    shuffled_samples = train_samples.copy()
    random.shuffle(shuffled_samples)

    # ----------------------------------------------------------
    # Iterate through each sample (stochastic update per sample)
    # ----------------------------------------------------------
    for x_sample, y_sample in shuffled_samples:
        # Add batch dimension since model expects 2D input: (batch_size, features)
        x_sample = x_sample.unsqueeze(0)
        y_sample = y_sample.unsqueeze(0)

        # Forward pass
        outputs = model_sgd(x_sample)
        loss = criterion(outputs, y_sample)

        # Backward pass and parameter update
        optimizer.zero_grad()   # Clear previous gradients
        loss.backward()         # Compute gradients for this sample
        optimizer.step()        # Update weights immediately

        # Track metrics
        epoch_loss += loss.item()
        _, predicted = torch.max(outputs.data, 1)
```

```
        correct += (predicted == y_sample).sum().item()

    # ------------------------------------------------------------
    # Compute average loss and accuracy for the epoch
    # ------------------------------------------------------------
    avg_loss = epoch_loss / len(train_samples)
    accuracy = correct / len(train_samples)

    train_losses_sgd.append(avg_loss)
    train_accuracy_sgd.append(accuracy)

    # Print progress every 10 epochs
    if (epoch + 1) % 10 == 0:
        print(f"[SGD] Epoch {epoch+1:>2} | Loss: {avg_loss:.4f} | Accuracy: {accuracy*100:.2f}%")

# (Optional) Print training time
# end_time = time.perf_counter()
# print(f"Training completed in {end_time - start_time:.2f} seconds")
```

```
[SGD] Epoch 10 | Loss: 1.0293 | Accuracy: 61.16%
[SGD] Epoch 20 | Loss: 0.9823 | Accuracy: 62.59%
[SGD] Epoch 30 | Loss: 0.9569 | Accuracy: 62.51%
[SGD] Epoch 40 | Loss: 0.9468 | Accuracy: 63.77%
[SGD] Epoch 50 | Loss: 0.9320 | Accuracy: 64.70%
[SGD] Epoch 60 | Loss: 0.9174 | Accuracy: 65.12%
[SGD] Epoch 70 | Loss: 0.9025 | Accuracy: 65.12%
[SGD] Epoch 80 | Loss: 0.8967 | Accuracy: 65.88%
[SGD] Epoch 90 | Loss: 0.8907 | Accuracy: 64.53%
[SGD] Epoch 100 | Loss: 0.8850 | Accuracy: 65.04%
```

MINI_BATCH STOCHASTIC GRADIENT DESCENT

In [20]:

```
# MINI BATCH SGD

# ------------------------------------------------------------
# Define hyperparameters
# ------------------------------------------------------------
batch_size = 32        # Number of samples per mini-batch
epochs = 100           # Number of full passes through the dataset
learning_rate = 0.01   # Step size for weight updates

# ------------------------------------------------------------
```

```
# Re-initialize model, loss function, and optimizer
# ----------------------------------------------------------------
model_mb = yeast_model(input_dim, hidden_layer, output_dim)
criterion = nn.CrossEntropyLoss()                              # Suitable for multi-class classification
optimizer_mb = torch.optim.SGD(model_mb.parameters(), lr=learning_rate)  # Mini-batch SGD optimizer

# ----------------------------------------------------------------
# Create DataLoader for mini-batch processing
# ----------------------------------------------------------------
# Combines input features and labels into a TensorDataset
# DataLoader automatically handles batching and shuffling
train_dataset = TensorDataset(X_train_tensor, y_train_tensor)
train_loader = DataLoader(train_dataset, batch_size=batch_size, shuffle=True)

# ----------------------------------------------------------------
# Initialize lists to store loss and accuracy for each epoch
# ----------------------------------------------------------------
train_losses_mb = []
train_accuracy_mb = []

# (Optional) Track training time
# start_time = time.perf_counter()

# ----------------------------------------------------------------
# Training Loop
# ----------------------------------------------------------------
for epoch in range(epochs):
    model_mb.train()       # Set model to training mode
    epoch_loss = 0.0       # Accumulate total loss per epoch
    correct = 0            # Count correct predictions
    total = 0              # Count total samples

    # Iterate through mini-batches
    for X_batch, y_batch in train_loader:
        # Forward pass: compute model output
        outputs = model_mb(X_batch)

        # Compute loss for the batch
        loss = criterion(outputs, y_batch)

        # Backward pass: compute gradients
        optimizer_mb.zero_grad()  # Clear existing gradients
```

```
        loss.backward()            # Compute new gradients
        optimizer_mb.step()        # Update model weights

        # Track total loss (multiply by batch size to get full sample loss)
        epoch_loss += loss.item() * X_batch.size(0)

        # Track accuracy: compare predicted vs actual labels
        _, predicted = torch.max(outputs, 1)             # Get predicted class (highest logit)
        correct += (predicted == y_batch).sum().item()   # Count correct predictions
        total += y_batch.size(0)                         # Count total samples processed

    # Compute average loss and accuracy for the epoch
    avg_loss = epoch_loss / total
    acc = correct / total

    # Store metrics for later visualization
    train_losses_mb.append(avg_loss)
    train_accuracy_mb.append(acc)

    # Print training progress
    print(f"[Mini-Batch] Epoch {epoch+1:2d}: Loss = {avg_loss:.4f} | Accuracy = {acc*100:.4f}")

# (Optional) Measure total training time
# end_time = time.perf_counter()
# print(f"Training completed in {end_time - start_time:.2f} seconds")
```

```
[Mini-Batch] Epoch  1: Loss = 2.2999 | Accuracy = 11.4575
[Mini-Batch] Epoch  2: Loss = 2.1785 | Accuracy = 29.4861
[Mini-Batch] Epoch  3: Loss = 2.0747 | Accuracy = 35.3833
[Mini-Batch] Epoch  4: Loss = 1.9854 | Accuracy = 37.0682
[Mini-Batch] Epoch  5: Loss = 1.9074 | Accuracy = 39.2586
[Mini-Batch] Epoch  6: Loss = 1.8371 | Accuracy = 39.7641
[Mini-Batch] Epoch  7: Loss = 1.7730 | Accuracy = 41.0278
[Mini-Batch] Epoch  8: Loss = 1.7142 | Accuracy = 42.1230
[Mini-Batch] Epoch  9: Loss = 1.6600 | Accuracy = 44.4819
[Mini-Batch] Epoch 10: Loss = 1.6109 | Accuracy = 46.0826
[Mini-Batch] Epoch 11: Loss = 1.5667 | Accuracy = 48.2730
[Mini-Batch] Epoch 12: Loss = 1.5258 | Accuracy = 49.5366
[Mini-Batch] Epoch 13: Loss = 1.4881 | Accuracy = 50.5476
[Mini-Batch] Epoch 14: Loss = 1.4545 | Accuracy = 52.7380
[Mini-Batch] Epoch 15: Loss = 1.4228 | Accuracy = 52.6537
[Mini-Batch] Epoch 16: Loss = 1.3940 | Accuracy = 53.4962
[Mini-Batch] Epoch 17: Loss = 1.3677 | Accuracy = 53.6647
[Mini-Batch] Epoch 18: Loss = 1.3432 | Accuracy = 54.4229
[Mini-Batch] Epoch 19: Loss = 1.3219 | Accuracy = 54.5072
[Mini-Batch] Epoch 20: Loss = 1.3023 | Accuracy = 54.6757
[Mini-Batch] Epoch 21: Loss = 1.2847 | Accuracy = 54.9284
[Mini-Batch] Epoch 22: Loss = 1.2679 | Accuracy = 55.2654
[Mini-Batch] Epoch 23: Loss = 1.2524 | Accuracy = 55.9393
[Mini-Batch] Epoch 24: Loss = 1.2385 | Accuracy = 55.5181
[Mini-Batch] Epoch 25: Loss = 1.2259 | Accuracy = 56.7818
[Mini-Batch] Epoch 26: Loss = 1.2140 | Accuracy = 56.6133
[Mini-Batch] Epoch 27: Loss = 1.2031 | Accuracy = 57.7928
[Mini-Batch] Epoch 28: Loss = 1.1932 | Accuracy = 58.1297
[Mini-Batch] Epoch 29: Loss = 1.1841 | Accuracy = 58.8037
[Mini-Batch] Epoch 30: Loss = 1.1756 | Accuracy = 59.1407
[Mini-Batch] Epoch 31: Loss = 1.1678 | Accuracy = 59.0564
[Mini-Batch] Epoch 32: Loss = 1.1608 | Accuracy = 59.1407
[Mini-Batch] Epoch 33: Loss = 1.1536 | Accuracy = 59.3934
[Mini-Batch] Epoch 34: Loss = 1.1474 | Accuracy = 59.6462
[Mini-Batch] Epoch 35: Loss = 1.1416 | Accuracy = 60.3201
[Mini-Batch] Epoch 36: Loss = 1.1359 | Accuracy = 59.5619
[Mini-Batch] Epoch 37: Loss = 1.1308 | Accuracy = 60.1516
[Mini-Batch] Epoch 38: Loss = 1.1256 | Accuracy = 60.2359
[Mini-Batch] Epoch 39: Loss = 1.1210 | Accuracy = 60.3201
[Mini-Batch] Epoch 40: Loss = 1.1167 | Accuracy = 59.9832
[Mini-Batch] Epoch 41: Loss = 1.1129 | Accuracy = 60.3201
[Mini-Batch] Epoch 42: Loss = 1.1097 | Accuracy = 60.7414
```

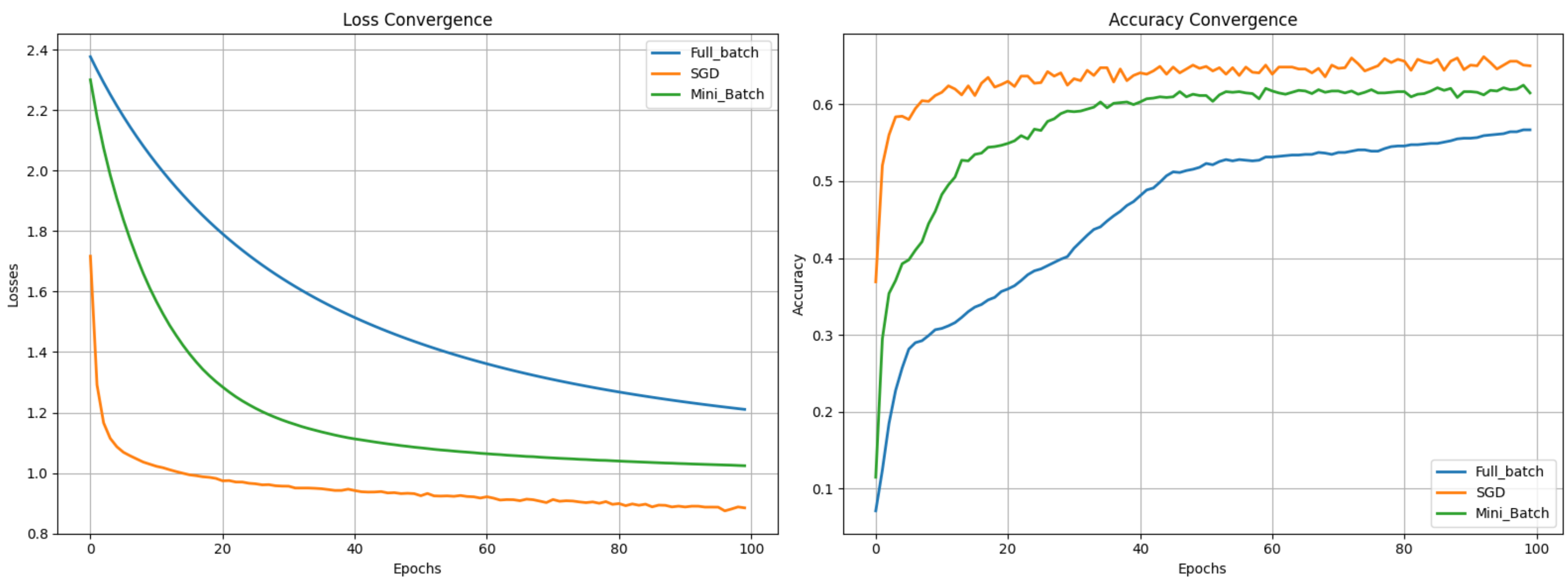
```
[Mini-Batch] Epoch 43: Loss = 1.1063 | Accuracy = 60.8256
[Mini-Batch] Epoch 44: Loss = 1.1028 | Accuracy = 60.9941
[Mini-Batch] Epoch 45: Loss = 1.0997 | Accuracy = 60.9099
[Mini-Batch] Epoch 46: Loss = 1.0966 | Accuracy = 60.9941
[Mini-Batch] Epoch 47: Loss = 1.0937 | Accuracy = 61.6681
[Mini-Batch] Epoch 48: Loss = 1.0908 | Accuracy = 60.9941
[Mini-Batch] Epoch 49: Loss = 1.0883 | Accuracy = 61.3311
[Mini-Batch] Epoch 50: Loss = 1.0856 | Accuracy = 61.1626
[Mini-Batch] Epoch 51: Loss = 1.0834 | Accuracy = 61.1626
[Mini-Batch] Epoch 52: Loss = 1.0810 | Accuracy = 60.4044
[Mini-Batch] Epoch 53: Loss = 1.0785 | Accuracy = 61.2468
[Mini-Batch] Epoch 54: Loss = 1.0764 | Accuracy = 61.6681
[Mini-Batch] Epoch 55: Loss = 1.0746 | Accuracy = 61.5838
[Mini-Batch] Epoch 56: Loss = 1.0726 | Accuracy = 61.6681
[Mini-Batch] Epoch 57: Loss = 1.0707 | Accuracy = 61.4996
[Mini-Batch] Epoch 58: Loss = 1.0691 | Accuracy = 61.4153
[Mini-Batch] Epoch 59: Loss = 1.0674 | Accuracy = 60.7414
[Mini-Batch] Epoch 60: Loss = 1.0654 | Accuracy = 62.0893
[Mini-Batch] Epoch 61: Loss = 1.0639 | Accuracy = 61.7523
[Mini-Batch] Epoch 62: Loss = 1.0623 | Accuracy = 61.4996
[Mini-Batch] Epoch 63: Loss = 1.0610 | Accuracy = 61.3311
[Mini-Batch] Epoch 64: Loss = 1.0592 | Accuracy = 61.5838
[Mini-Batch] Epoch 65: Loss = 1.0579 | Accuracy = 61.8366
[Mini-Batch] Epoch 66: Loss = 1.0565 | Accuracy = 61.7523
[Mini-Batch] Epoch 67: Loss = 1.0549 | Accuracy = 61.4153
[Mini-Batch] Epoch 68: Loss = 1.0542 | Accuracy = 61.9208
[Mini-Batch] Epoch 69: Loss = 1.0525 | Accuracy = 61.5838
[Mini-Batch] Epoch 70: Loss = 1.0512 | Accuracy = 61.7523
[Mini-Batch] Epoch 71: Loss = 1.0500 | Accuracy = 61.7523
[Mini-Batch] Epoch 72: Loss = 1.0488 | Accuracy = 61.4996
[Mini-Batch] Epoch 73: Loss = 1.0478 | Accuracy = 61.7523
[Mini-Batch] Epoch 74: Loss = 1.0468 | Accuracy = 61.3311
[Mini-Batch] Epoch 75: Loss = 1.0455 | Accuracy = 61.5838
[Mini-Batch] Epoch 76: Loss = 1.0447 | Accuracy = 61.9208
[Mini-Batch] Epoch 77: Loss = 1.0435 | Accuracy = 61.4996
[Mini-Batch] Epoch 78: Loss = 1.0424 | Accuracy = 61.4996
[Mini-Batch] Epoch 79: Loss = 1.0419 | Accuracy = 61.5838
[Mini-Batch] Epoch 80: Loss = 1.0407 | Accuracy = 61.6681
[Mini-Batch] Epoch 81: Loss = 1.0397 | Accuracy = 61.6681
[Mini-Batch] Epoch 82: Loss = 1.0386 | Accuracy = 60.9941
[Mini-Batch] Epoch 83: Loss = 1.0377 | Accuracy = 61.3311
[Mini-Batch] Epoch 84: Loss = 1.0368 | Accuracy = 61.4153
```

```
[Mini-Batch] Epoch 85: Loss = 1.0359 | Accuracy = 61.7523
[Mini-Batch] Epoch 86: Loss = 1.0350 | Accuracy = 62.1735
[Mini-Batch] Epoch 87: Loss = 1.0341 | Accuracy = 61.8366
[Mini-Batch] Epoch 88: Loss = 1.0332 | Accuracy = 62.0893
[Mini-Batch] Epoch 89: Loss = 1.0326 | Accuracy = 60.9099
[Mini-Batch] Epoch 90: Loss = 1.0316 | Accuracy = 61.6681
[Mini-Batch] Epoch 91: Loss = 1.0310 | Accuracy = 61.6681
[Mini-Batch] Epoch 92: Loss = 1.0301 | Accuracy = 61.5838
[Mini-Batch] Epoch 93: Loss = 1.0294 | Accuracy = 61.2468
[Mini-Batch] Epoch 94: Loss = 1.0287 | Accuracy = 61.8366
[Mini-Batch] Epoch 95: Loss = 1.0280 | Accuracy = 61.7523
[Mini-Batch] Epoch 96: Loss = 1.0273 | Accuracy = 62.1735
[Mini-Batch] Epoch 97: Loss = 1.0267 | Accuracy = 61.9208
[Mini-Batch] Epoch 98: Loss = 1.0261 | Accuracy = 62.0051
[Mini-Batch] Epoch 99: Loss = 1.0251 | Accuracy = 62.5105
[Mini-Batch] Epoch 100: Loss = 1.0243 | Accuracy = 61.4996
```

In [21]:

```python
# ---------------------------------------------------------------
# 📊 OPTIMIZER PERFORMANCE VISUALIZATION
# ---------------------------------------------------------------
# This section visualizes the training behavior of three optimizers:
# - Full-Batch Gradient Descent (GD)
# - Stochastic Gradient Descent (SGD)
# - Mini-Batch SGD
# The left graph shows how the loss decreases over epochs (convergence).
# The right graph shows how model accuracy improves during training.
# ---------------------------------------------------------------

epochs = len(train_losses)

plt.figure(figsize=(16, 6))

# ---------------------------------------------------------------
# 🔷 LOSS CONVERGENCE CURVES
# ---------------------------------------------------------------
plt.subplot(1, 2, 1)
plt.plot(range(epochs), train_losses_gd, label='Full_batch', lw=2)
plt.plot(range(epochs), train_losses_sgd, label='SGD', lw=2)
plt.plot(range(epochs), train_losses_mb, label='Mini_Batch', lw=2)
plt.xlabel('Epochs')
plt.ylabel('Losses')
plt.title('Loss Convergence')
```

```
plt.legend()
plt.grid(True)

# ------------------------------------------------------------
# 🔷 ACCURACY CONVERGENCE CURVES
# ------------------------------------------------------------
plt.subplot(1, 2, 2)
plt.plot(range(epochs), train_accuracy_gd, label='Full_batch', lw=2)
plt.plot(range(epochs), train_accuracy_sgd, label='SGD', lw=2)
plt.plot(range(epochs), train_accuracy_mb, label='Mini_Batch', lw=2)
plt.xlabel('Epochs')
plt.ylabel('Accuracy')
plt.title('Accuracy Convergence')
plt.legend()
plt.grid(True)

# ------------------------------------------------------------
# 🧩 LAYOUT & DISPLAY
# ------------------------------------------------------------
plt.tight_layout()
plt.show()
```




```
============================================================
```

NOTE: Interpretation of the Optimizer Comparison Graphs

==

📉 ***Loss Convergence***

- **SGD (Per Sample):** Shows the fastest initial loss drop, but the curve is **noisy and unstable**.
- **Mini-Batch SGD:** Displays a **smooth and fast descent**, offering a strong balance between **speed and stability**.
- **Full-Batch GD:** Converges **steadily but slowly**, as its updates are too infrequent for rapid learning.

📈 ***Accuracy Over Epochs***

- **SGD:** Achieves **high accuracy early**, but exhibits **fluctuations** due to noisy updates.
- **Mini-Batch SGD:** Provides **consistent and steadily improving accuracy** with fewer fluctuations.
- **Full-Batch GD:** Improves **slowly** and often reaches **lower final accuracy** than the other two optimizers.

🧠 ***Key Insight***

Mini-Batch SGD offers the **best compromise** among all optimization strategies:

- ⚙️ **Efficient GPU utilization**
- 📉 **Stable gradient updates**
- ⚡ **Faster convergence** than Full-Batch GD
- 🌊 **Smoother training** than per-sample SGD

✅ ***This is why Mini-Batch training is the standard approach in modern deep learning!***

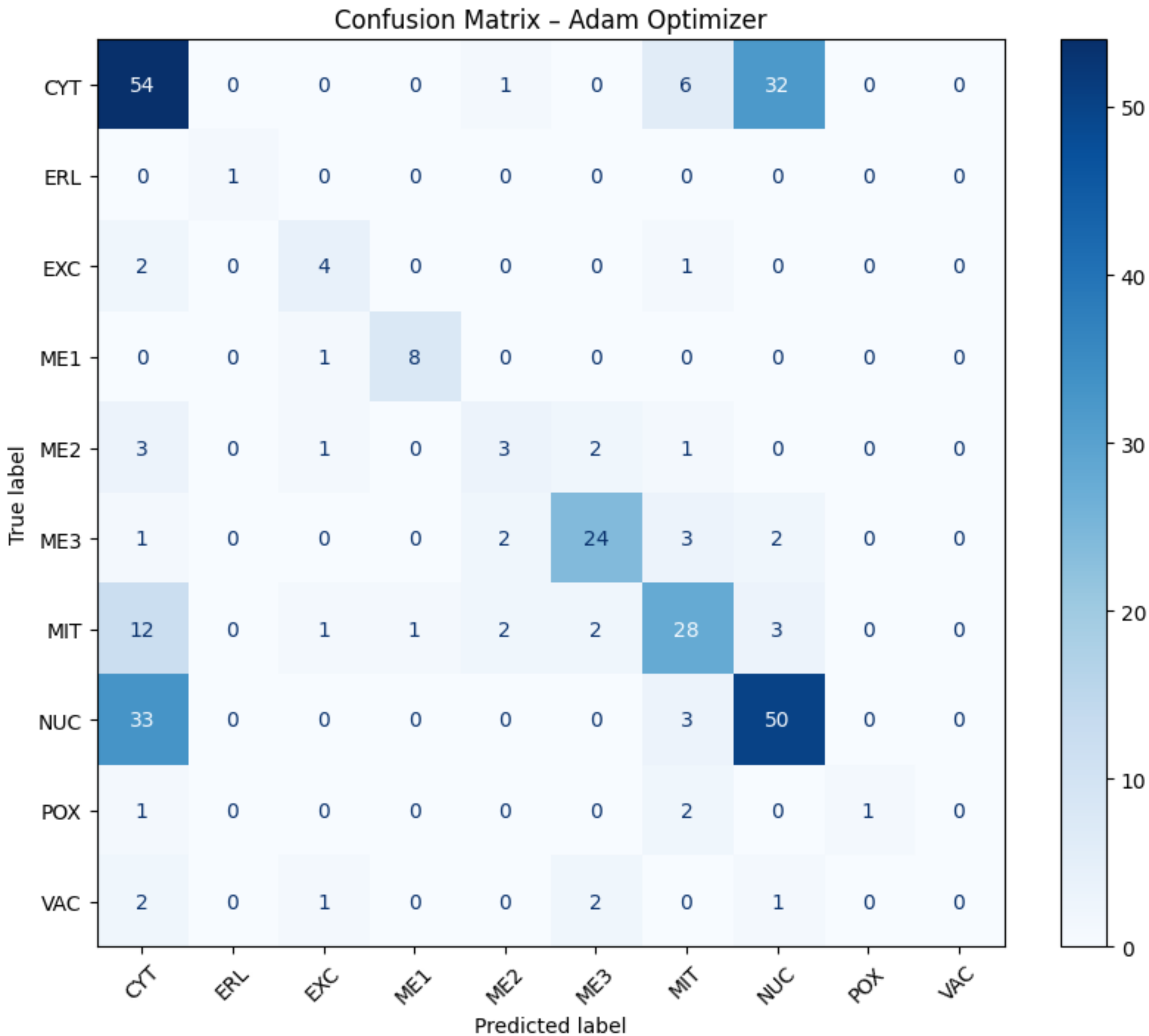
➡️ ***Next Step:*** Compare these optimizers on the **test set** using **confusion matrices** and **final accuracy metrics.***

MODEL EVALUATION ON TEST SET

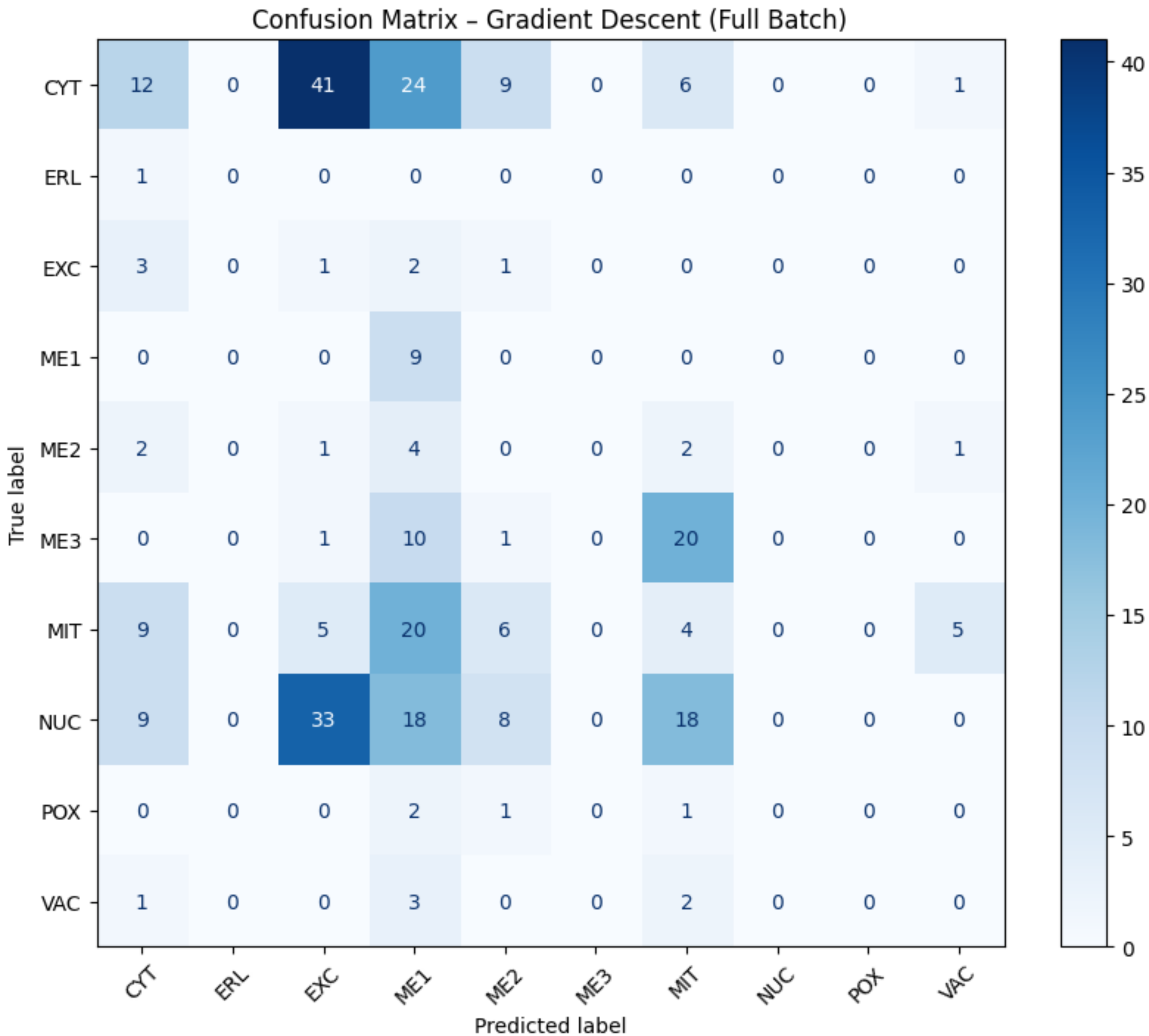
In [22]:
```
# ---------------------------------------------------------------
# 🧠 MODEL EVALUATION USING CONFUSION MATRIX & ACCURACY
# ---------------------------------------------------------------
# This section defines a helper function to evaluate trained models
# using the following metrics and visualizations:
#   - Accuracy Score (via sklearn)
#   - Confusion Matrix visualization for class performance
#
# Models evaluated:
#   1. Adam Optimizer
#   2. Full-Batch Gradient Descent (GD)
#   3. Stochastic Gradient Descent (SGD - per sample)
#   4. Mini-Batch SGD
# ---------------------------------------------------------------

from sklearn.metrics import accuracy_score, confusion_matrix, ConfusionMatrixDisplay

# ---------------------------------------------------------------
# ⚙️ EVALUATION FUNCTION
# ---------------------------------------------------------------
def evaluate_model(model, X_test, y_test, class_names, title):
    """
    Evaluate a trained PyTorch model on test data and visualize performance.
    - Displays test accuracy.
    - Shows a confusion matrix heatmap.
    """

    # Set model to evaluation mode
    model.eval()

    # Disable gradient tracking for efficiency
    with torch.no_grad():
        outputs = model(X_test)
        _, preds = torch.max(outputs, 1)  # Predicted class indices

    # Convert tensors to numpy arrays for sklearn functions
    y_true = y_test.cpu().numpy()
    y_pred = preds.cpu().numpy()
```

```
    # ------------------------------------------------------------
    # 📈 CALCULATE TEST ACCURACY
    # ------------------------------------------------------------
    acc = accuracy_score(y_true, y_pred)
    print(f"✅ Test Accuracy ({title}): {acc:.4f}")

    # ------------------------------------------------------------
    # 📊 CONFUSION MATRIX VISUALIZATION
    # ------------------------------------------------------------
    cm = confusion_matrix(y_true, y_pred)
    disp = ConfusionMatrixDisplay(confusion_matrix=cm, display_labels=class_names)

    # Display matrix
    fig, ax = plt.subplots(figsize=(10, 8))
    disp.plot(ax=ax, cmap="Blues", xticks_rotation=45)
    plt.title(f"Confusion Matrix – {title}")
    plt.show()

# ------------------------------------------------------------
# 🚀 EVALUATE ALL MODELS
# ------------------------------------------------------------
evaluate_model(model_ad, X_test_tensor, y_test_tensor, classes_names, "Adam Optimizer")
evaluate_model(model_gd, X_test_tensor, y_test_tensor, classes_names, "Gradient Descent (Full Batch)")
evaluate_model(model_sgd, X_test_tensor, y_test_tensor, classes_names, "Stochastic Gradient Descent (Per Sample)")
evaluate_model(model_mb, X_test_tensor, y_test_tensor, classes_names, "Mini-Batch SGD")
```

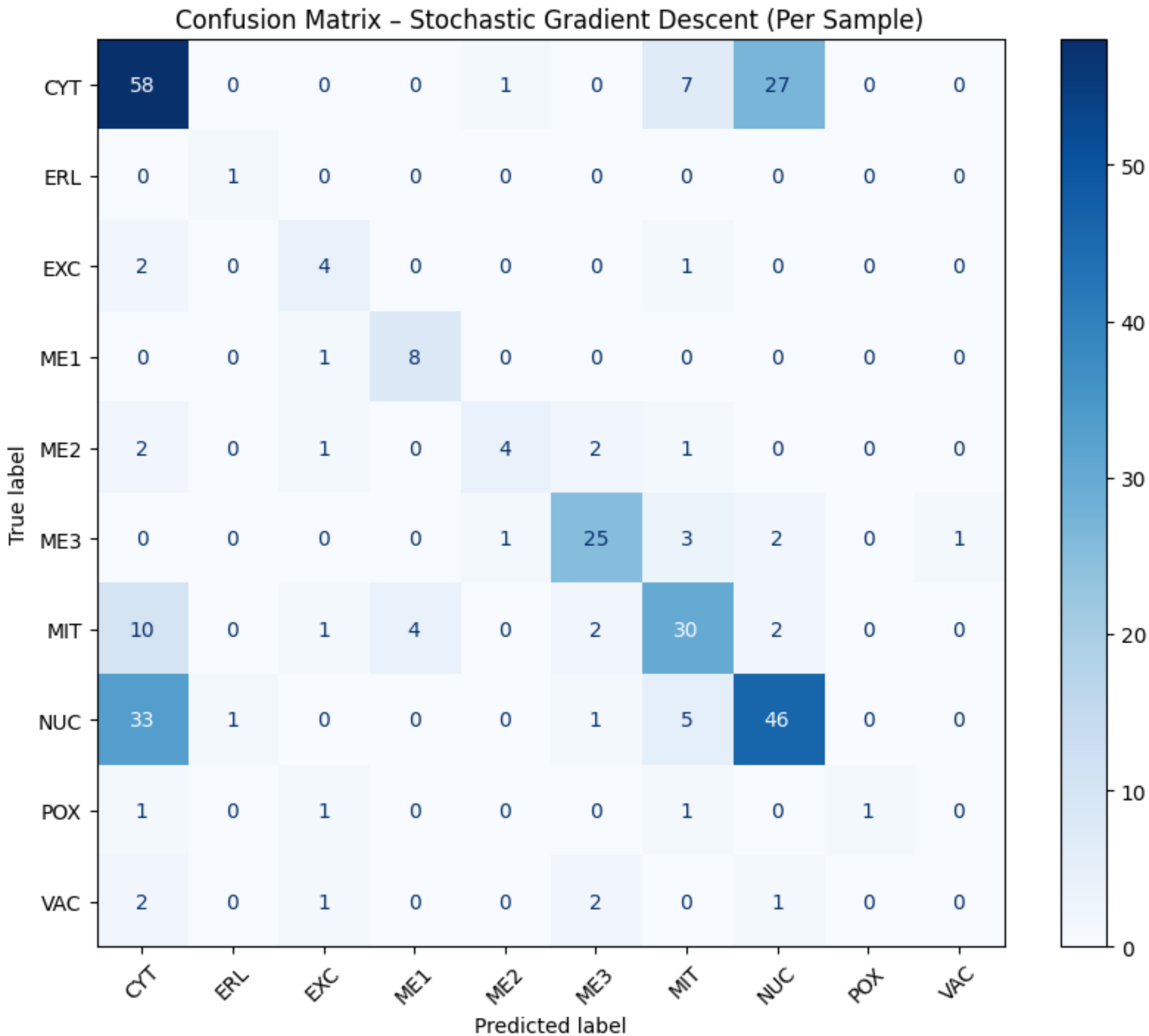
```
✅ Test Accuracy (Adam Optimizer): 0.5825
```


Confusion Matrix – Adam Optimizer
True label
Predicted label
CYT
ERL
EXC
ME1
ME2
ME3
MIT
NUC
POX
VAC
54 0 0 0 1 0 6 32 0 0
0 1 0 0 0 0 0 0 0 0
2 0 4 0 0 0 1 0 0 0
0 0 1 8 0 0 0 0 0 0
3 0 1 0 3 2 1 0 0 0
1 0 0 0 2 24 3 2 0 0
12 0 1 1 2 2 28 3 0 0
33 0 0 0 0 0 3 50 0 0
1 0 0 0 0 0 2 0 1 0
2 0 1 0 0 2 0 1 0 0
0
10
20
30
40
50

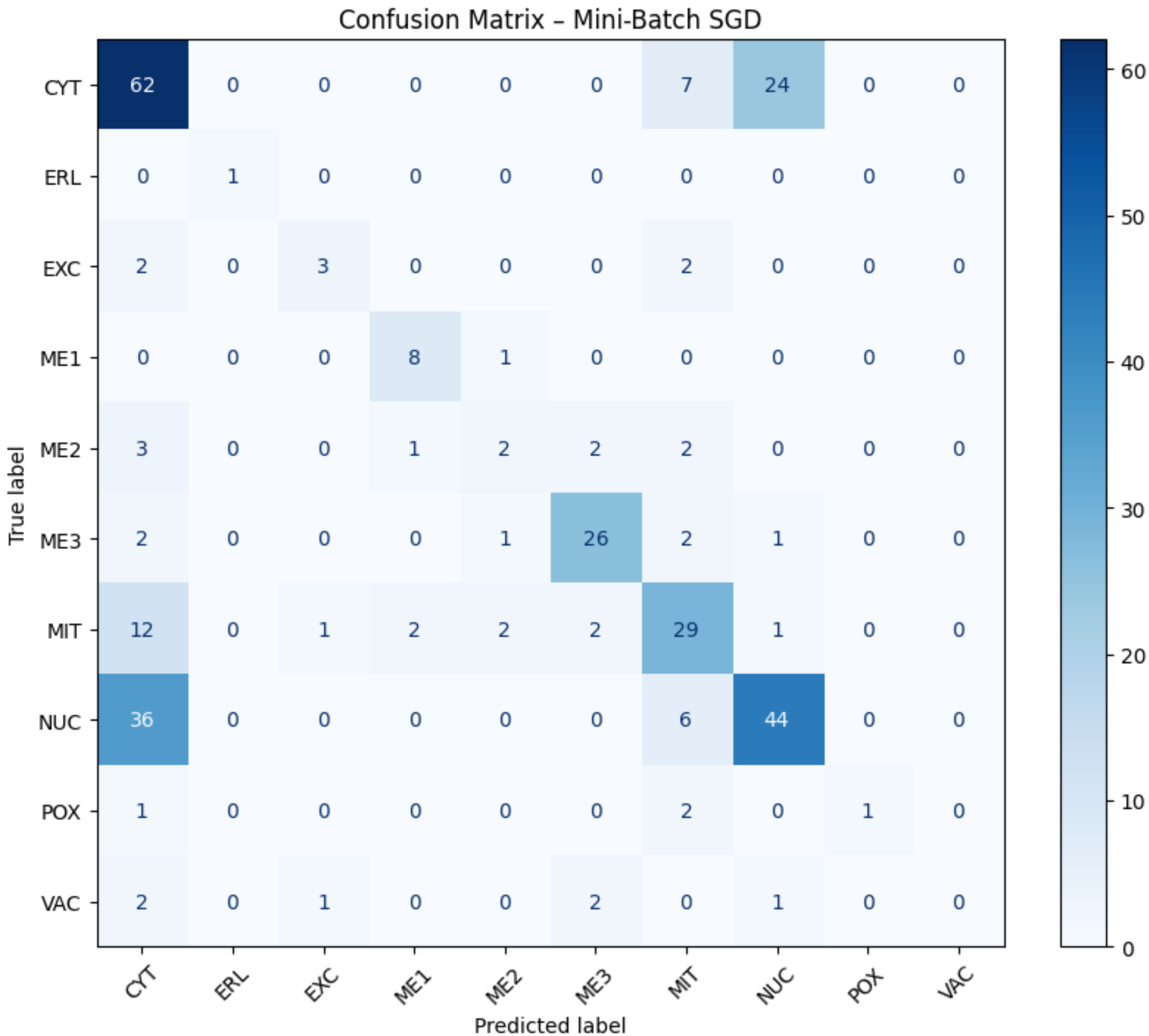
✅ Test Accuracy (Gradient Descent (Full Batch)): 0.0875


Confusion Matrix – Gradient Descent (Full Batch)
True label
Predicted label
CYT
ERL
EXC
ME1
ME2
ME3
MIT
NUC
POX
VAC

✅ Test Accuracy (Stochastic Gradient Descent (Per Sample)): 0.5960


Confusion Matrix – Stochastic Gradient Descent (Per Sample)
True label
Predicted label
CYT
ERL
EXC
ME1
ME2
ME3
MIT
NUC
POX
VAC
58 0 0 0 1 0 7 27 0 0
0 1 0 0 0 0 0 0 0 0
2 0 4 0 0 0 1 0 0 0
0 0 1 8 0 0 0 0 0 0
2 0 1 0 4 2 1 0 0 0
0 0 0 0 1 25 3 2 0 1
10 0 1 4 0 2 30 2 0 0
33 1 0 0 0 1 5 46 0 0
1 0 1 0 0 0 1 0 1 0
2 0 1 0 0 2 0 1 0 0
50
40
30
20
10
0

```
✅ Test Accuracy (Mini-Batch SGD): 0.5926
```


Confusion Matrix – Mini-Batch SGD
True label
Predicted label
CYT ERL EXC ME1 ME2 ME3 MIT NUC POX VAC
CYT 62 0 0 0 0 0 7 24 0 0
ERL 0 1 0 0 0 0 0 0 0 0
EXC 2 0 3 0 0 0 2 0 0 0
ME1 0 0 0 8 1 0 0 0 0 0
ME2 3 0 0 1 2 2 2 0 0 0
ME3 2 0 0 0 1 26 2 1 0 0
MIT 12 0 1 2 2 2 29 1 0 0
NUC 36 0 0 0 0 0 6 44 0 0
POX 1 0 0 0 0 0 2 0 1 0
VAC 2 0 1 0 0 2 0 1 0 0
0 10 20 30 40 50 60

==

NOTE: Understanding Overfitting in Machine Learning

==

📘 ***What Is Overfitting?***

Overfitting occurs when a model learns the training data too well — including its noise, randomness, and outliers — instead of learning the true underlying patterns.

When this happens:

- ✅ ***Training accuracy becomes extremely high.***
- ❌ ***Validation/Test accuracy stops improving or even worsens.***
- ❌ ***The model performs poorly on unseen (new) data.***

⚠️ ***Why Does Overfitting Happen?***

Overfitting commonly arises due to:

- ***A model that is too complex (many neurons, layers, or parameters).***
- ***Insufficient training data relative to model size.***
- ***Lack of regularization (e.g., no Dropout, no L2 penalty).***
- ***Excessive training epochs, allowing the model to memorize data noise.***

ADDING VALIDATION SET TO CHECK FOR MODEL OVERFITTING

In [23]:
```
# ==============================================================
# 📘 DATA SPLITTING – TRAIN, VALIDATION, AND TEST SETS
# ==============================================================
# ✅ Objective:
#    Split the scaled and encoded dataset into:
#    - Training (70%)
#    - Validation (15%)
```

```
#    - Testing (15%)
# ==============================================================
from sklearn.model_selection import train_test_split

# --------------------------------------------------------------
# STEP 1️⃣ - Split into Training and Temporary (Validation + Test)
# --------------------------------------------------------------
X_train, X_temp, y_train, y_temp = train_test_split(
    X_scaled,
    y_encoded,
    random_state=42,
    stratify=y_encoded,
    test_size=0.3  # 30% for validation + test
)

# --------------------------------------------------------------
# STEP 2️⃣ - Split Temporary Data into Validation and Test Sets
# --------------------------------------------------------------
X_val, X_test, y_val, y_test = train_test_split(
    X_temp,
    y_temp,
    random_state=42,
    test_size=0.5,  # Half of 30% → 15% each
    stratify=y_temp
)

# --------------------------------------------------------------
# STEP 3️⃣ - Display Dataset Shapes and Class Info
# --------------------------------------------------------------
print(f"✅ Train set: {X_train.shape}")
print(f"✅ Validation set: {X_val.shape}")
print(f"✅ Test set: {X_test.shape}")
print(f"✅ Number of Classes: {len(label_encoder.classes_)}")
print(f"✅ Class Names: {label_encoder.classes_}")
```

```
✅ Train set: (1038, 8)
✅ Validation set: (223, 8)
✅ Test set: (223, 8)
✅ Number of Classes: 10
✅ Class Names: ['CYT' 'ERL' 'EXC' 'ME1' 'ME2' 'ME3' 'MIT' 'NUC' 'POX' 'VAC']
```

In [24]:

```
# ==============================================================
```

```python
# 🎯 DATA CONVERSION – NUMPY ARRAYS TO PYTORCH TENSORS
# ==============================================================
# ✅ Objective:
#    Convert training, validation, and test sets into PyTorch tensors
#    suitable for model input and training.
# ==============================================================
import torch

# --------------------------------------------------------------
# STEP 1️⃣ – Convert Feature Matrices to Float Tensors
# --------------------------------------------------------------
X_train_tensor = torch.tensor(X_train, dtype=torch.float32)
X_val_tensor   = torch.tensor(X_val, dtype=torch.float32)
X_test_tensor  = torch.tensor(X_test, dtype=torch.float32)

# --------------------------------------------------------------
# STEP 2️⃣ – Convert Labels to Long Tensors (for Classification)
# --------------------------------------------------------------
y_train_tensor = torch.tensor(y_train, dtype=torch.long)
y_val_tensor   = torch.tensor(y_val, dtype=torch.long)
y_test_tensor  = torch.tensor(y_test, dtype=torch.long)
```

MITIGATING OVERFITTING USING DROPOUT TECHNIQUE

===

NOTE: Mitigating Overfitting Using Dropout Technique

===

1️⃣ *What Is Dropout?*

▪ ***Definition:***

Dropout is a **regularization technique** used in neural networks to **reduce overfitting** by randomly “dropping out” (i.e., deactivating) a fraction of neurons during training.

▪ ***Conceptually:***

At each training step, a random subset of neurons is ignored — they neither contribute to the forward pass nor participate in backpropagation. This prevents neurons from becoming overly dependent on specific other neurons.

----
2 *Why Dropout Helps Prevent Overfitting*

- Forces the network to **learn redundant representations**, improving robustness.
- Reduces **co-adaptation** between neurons.
- Encourages the network to **generalize better** on unseen data.
- Acts as a form of **model averaging**, since each dropout mask represents a different sub-network.

----
3 *How Dropout Works During Training vs. Inference*

- **During Training:** Randomly zeroes out a fraction of activations (e.g., 20–50%).
- **During Inference:** Dropout is **disabled** — all neurons are active, but their outputs are scaled down by the dropout rate to maintain balance.

----
4 *Typical Dropout Rates*

- **Input Layer:** 0.1 – 0.2
- **Hidden Layers:** 0.3 – 0.5
- **Output Layer:** Usually no dropout

In [36]:
```
# ------------------------------------------------------------
# Model Definition: MLP with Dropout Regularization
# ------------------------------------------------------------

import torch.nn as nn

# ------------------------------------------------------------
```

```
# Define Neural Network with Dropout to Reduce Overfitting
# ---------------------------------------------------------------
class ModelDropout(nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim, dropout_rate=0.5):
        super(ModelDropout, self).__init__()

        # -----------------------------------------------------------
        # Sequential model architecture
        # -----------------------------------------------------------
        self.net = nn.Sequential(
            nn.Linear(input_dim, hidden_dim),   # Input → Hidden Layer
            nn.ReLU(),                          # Non-linear activation
            nn.Dropout(dropout_rate),           # Dropout regularization
            nn.Linear(hidden_dim, output_dim)   # Hidden → Output Layer
        )

    # ---------------------------------------------------------------
    # Forward Pass
    # ---------------------------------------------------------------
    def forward(self, x):
        return self.net(x)

# ---------------------------------------------------------------
# Model Initialization Parameters
# ---------------------------------------------------------------
input_dim = X_train_tensor.shape[1]                      # Number of input features
hidden_dim = 32                                          # Number of hidden neurons
output_dim = len(label_encoder.classes_)                # Number of output classes
dropout_rate = 0.5                                       # Dropout rate (50%)

# ---------------------------------------------------------------
# Instantiate Model
# ---------------------------------------------------------------
model_dropout_test = ModelDropout(input_dim, hidden_dim, output_dim, dropout_rate)
print(model_dropout_test)
```

```
ModelDropout(
  (net): Sequential(
    (0): Linear(in_features=8, out_features=32, bias=True)
    (1): ReLU()
    (2): Dropout(p=0.5, inplace=False)
    (3): Linear(in_features=32, out_features=10, bias=True)
  )
)
```

In [39]:

```
# ---------------------------------------------------------------
# Training MLP Model with Dropout Regularization
# ---------------------------------------------------------------

import torch
import torch.nn as nn

# ---------------------------------------------------------------
# Define Loss Function and Optimizer
# ---------------------------------------------------------------
criterion = nn.CrossEntropyLoss()                                      # Cross-Entropy Loss for multi-class classi
optimizer = torch.optim.Adam(model_dropout_test.parameters(), lr=0.001)  # Adam optimizer with learning rate = 0.0

# ---------------------------------------------------------------
# Initialize Metric Storage
# ---------------------------------------------------------------
train_losses_dropout = []
val_losses_dropout = []
epochs = 1000  # Number of training epochs

# ---------------------------------------------------------------
# Training Loop
# ---------------------------------------------------------------
for epoch in range(epochs):

    # -----------------------------------------------------------
    # Training Phase
    # -----------------------------------------------------------
    model_dropout_test.train()                               # Enable training mode (activates dropout)
    outputs = model_dropout_test(X_train_tensor)             # Forward pass
    loss = criterion(outputs, y_train_tensor)                # Compute training loss

    optimizer.zero_grad()                                    # Reset gradients
```

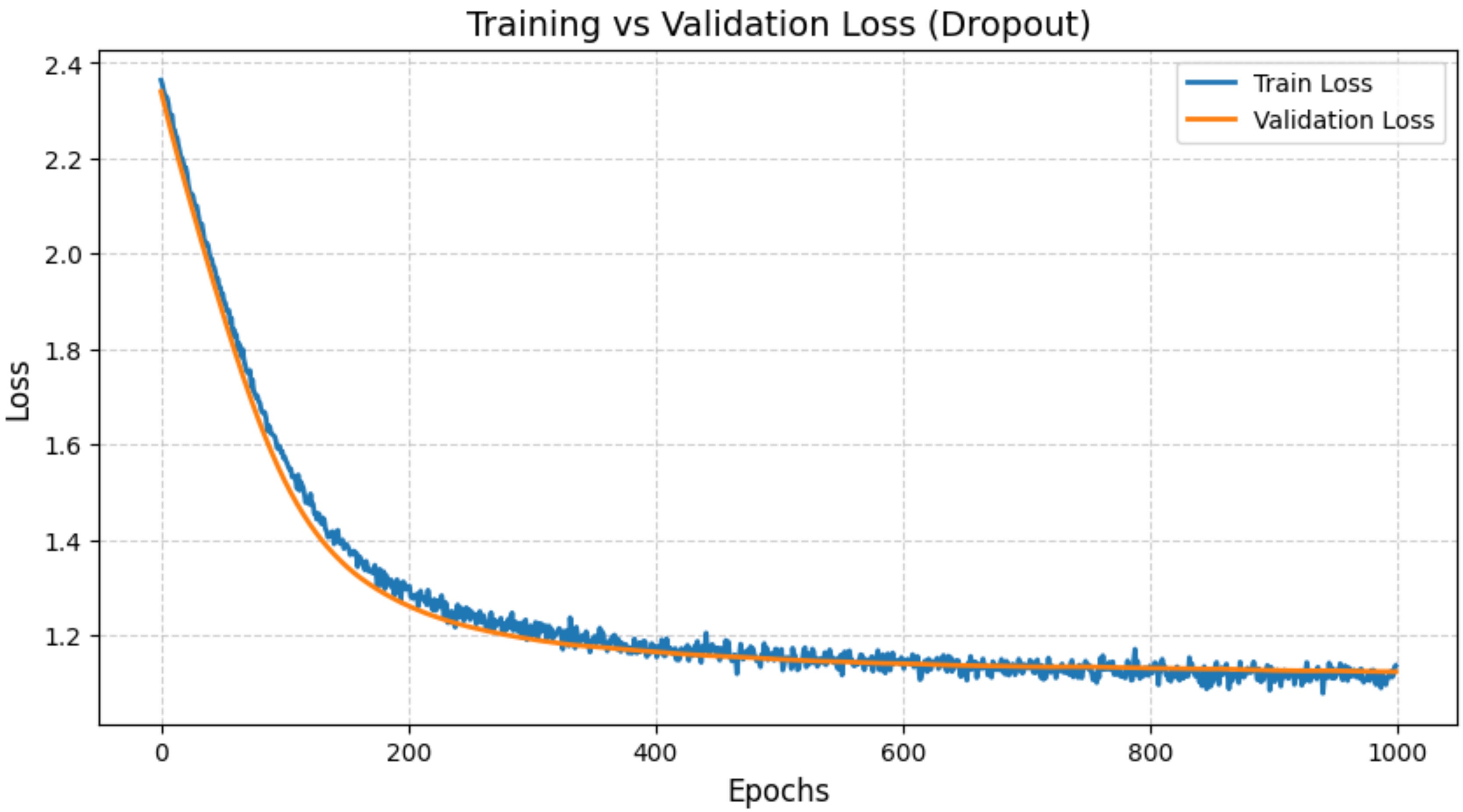
```
        loss.backward()                                                 # Backpropagation
        optimizer.step()                                                # Update model parameters
        train_losses_dropout.append(loss.item())                                # Record training loss

        # -----------------------------------------------------------
        # Validation Phase
        # -----------------------------------------------------------
        model_dropout_test.eval()                                       # Evaluation mode (disables dropout)
        with torch.no_grad():                                           # Disable gradient calculation
            val_outputs = model_dropout_test(X_val_tensor)              # Forward pass on validation data
            val_loss = criterion(val_outputs, y_val_tensor)             # Compute validation loss
            val_losses_dropout.append(val_loss.item())                          # Record validation loss

        # -----------------------------------------------------------
        # Progress Logging
        # -----------------------------------------------------------
        if (epoch + 1) % 50 == 0:
            print(f"[Dropout] Epoch {epoch + 1} | Train Loss = {loss.item():.4f} | Val Loss = {val_loss.item():.4f}")
```

```
[Dropout] Epoch 50 | Train Loss = 1.9119 | Val Loss = 1.8838
[Dropout] Epoch 100 | Train Loss = 1.5720 | Val Loss = 1.5296
[Dropout] Epoch 150 | Train Loss = 1.3886 | Val Loss = 1.3472
[Dropout] Epoch 200 | Train Loss = 1.3015 | Val Loss = 1.2634
[Dropout] Epoch 250 | Train Loss = 1.2547 | Val Loss = 1.2185
[Dropout] Epoch 300 | Train Loss = 1.2204 | Val Loss = 1.1921
[Dropout] Epoch 350 | Train Loss = 1.1930 | Val Loss = 1.1767
[Dropout] Epoch 400 | Train Loss = 1.1782 | Val Loss = 1.1656
[Dropout] Epoch 450 | Train Loss = 1.1641 | Val Loss = 1.1569
[Dropout] Epoch 500 | Train Loss = 1.1605 | Val Loss = 1.1502
[Dropout] Epoch 550 | Train Loss = 1.1544 | Val Loss = 1.1450
[Dropout] Epoch 600 | Train Loss = 1.1540 | Val Loss = 1.1407
[Dropout] Epoch 650 | Train Loss = 1.1293 | Val Loss = 1.1373
[Dropout] Epoch 700 | Train Loss = 1.1300 | Val Loss = 1.1345
[Dropout] Epoch 750 | Train Loss = 1.1320 | Val Loss = 1.1345
[Dropout] Epoch 800 | Train Loss = 1.1160 | Val Loss = 1.1315
[Dropout] Epoch 850 | Train Loss = 1.0931 | Val Loss = 1.1299
[Dropout] Epoch 900 | Train Loss = 1.1111 | Val Loss = 1.1269
[Dropout] Epoch 950 | Train Loss = 1.1099 | Val Loss = 1.1259
[Dropout] Epoch 1000 | Train Loss = 1.1368 | Val Loss = 1.1241
```

In [40]:

```
# -----------------------------------------------------------
# Visualization: Training vs Validation Loss (Dropout Regularization)
```

```python
# -------------------------------------------------------------

import matplotlib.pyplot as plt

# -------------------------------------------------------------
# Plot Loss Curves
# -------------------------------------------------------------
plt.figure(figsize=(10, 5))                                              # Set figure size
plt.plot(train_losses_dropout, label='Train Loss', linewidth=2)          # Plot training loss
plt.plot(val_losses_dropout, label='Validation Loss', linewidth=2)       # Plot validation loss

# -------------------------------------------------------------
# Graph Formatting
# -------------------------------------------------------------
plt.title("Training vs Validation Loss (Dropout)", fontsize=14)          # Title
plt.xlabel("Epochs", fontsize=12)                                        # X-axis label
plt.ylabel("Loss", fontsize=12)                                          # Y-axis label
plt.legend()                                                             # Display legend
plt.grid(True, linestyle='--', alpha=0.6)                                # Add gridlines for readability

# -------------------------------------------------------------
# Show Plot
# -------------------------------------------------------------
plt.show()
```



MITIGATING OVERFITTING WITH L2 REGULARIZATION

==

NOTE: Mitigating Overfitting Using L2 Regularization

==

----

1 What Is L2 Regularization?

▪ ***Definition:***

L2 Regularization, also known as **weight decay**, is a technique to prevent overfitting by **penalizing large weights** in the neural network.

▪ ***Conceptually:***
During training, the loss function is modified to include a term proportional to the **sum of the squares of all weights**:
Loss_total = Loss_original + λ * Σ(weights²)
where **λ** is the regularization strength.

----

2 Why L2 Helps Prevent Overfitting

- Encourages **smaller weights**, which leads to **simpler models**.
- Reduces the model's tendency to **memorize noise** in the training data.
- Improves **generalization** on unseen data.

----

3 How L2 Works During Training

- During gradient descent, each weight is **slightly shrunk** in addition to the normal update:
  - New weight = weight - learning_rate * (gradient + λ * weight)
- This penalizes large weights while keeping useful patterns.

----

4 Typical Usage

- Commonly used in **linear models, logistic regression, and neural networks**.
- In PyTorch, you can set L2 regularization with the **weight_decay** parameter in optimizers:
  `optimizer = torch.optim.Adam(model.parameters(), lr=0.001, weight_decay=1e-4)`

----

5 *Key Takeaways*

- L2 Regularization is a **simple and effective** method to reduce overfitting.
- Works by **constraining weights**, preventing overly complex models.
- Often combined with **Dropout** for stronger regularization in deep learning.

==

In [41]:
```
# ---------------------------------------------------------------
# Training MLP Model with L2 Regularization (Weight Decay)
# ---------------------------------------------------------------

import torch
import torch.nn as nn

# ---------------------------------------------------------------
# Define Neural Network with L2 Regularization
# ---------------------------------------------------------------
class YeastModelL2(nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim):
        super(YeastModelL2, self).__init__()
        self.network = nn.Sequential(
            nn.Linear(input_dim, hidden_dim),  # Input → Hidden Layer
            nn.ReLU(),                         # Activation
            nn.Linear(hidden_dim, output_dim)  # Hidden → Output Layer
        )

    # -----------------------------------------------------------
    # Forward Pass
    # -----------------------------------------------------------
    def forward(self, x):
        return self.network(x)

# ---------------------------------------------------------------
# Model, Loss Function, and Optimizer
# ---------------------------------------------------------------
model_l2 = YeastModelL2(
    input_dim=X_train_tensor.shape[1],
```

```
    hidden_dim=32,
    output_dim=len(label_encoder.classes_)
)

criterion = nn.CrossEntropyLoss()                                         # Multi-class classification loss
optimizer = torch.optim.Adam(model_l2.parameters(), lr=0.001, weight_decay=1e-4)  # Adam with L2 regularization

# ---------------------------------------------------------------
# Initialize Metric Storage
# ---------------------------------------------------------------
train_losses_l2 = []
val_losses_l2 = []
epochs = 1000

# ---------------------------------------------------------------
# Training Loop
# ---------------------------------------------------------------
for epoch in range(epochs):

    # -----------------------------------------------------------
    # Training Phase
    # -----------------------------------------------------------
    model_l2.train()                                         # Enable training mode
    outputs_l2 = model_l2(X_train_tensor)                   # Forward pass
    loss_l2 = criterion(outputs_l2, y_train_tensor)         # Compute training loss

    optimizer.zero_grad()                                    # Reset gradients
    loss_l2.backward()                                      # Backpropagation
    optimizer.step()                                        # Update model parameters
    train_losses_l2.append(loss_l2.item())                 # Record training loss

    # -----------------------------------------------------------
    # Validation Phase
    # -----------------------------------------------------------
    model_l2.eval()                                         # Evaluation mode
    with torch.no_grad():
        val_outputs_l2 = model_l2(X_val_tensor)            # Forward pass on validation set
        val_loss_l2 = criterion(val_outputs_l2, y_val_tensor)  # Compute validation loss
        val_losses_l2.append(val_loss_l2.item())          # Record validation loss

    # -----------------------------------------------------------
    # Progress Logging Every 50 Epochs
```

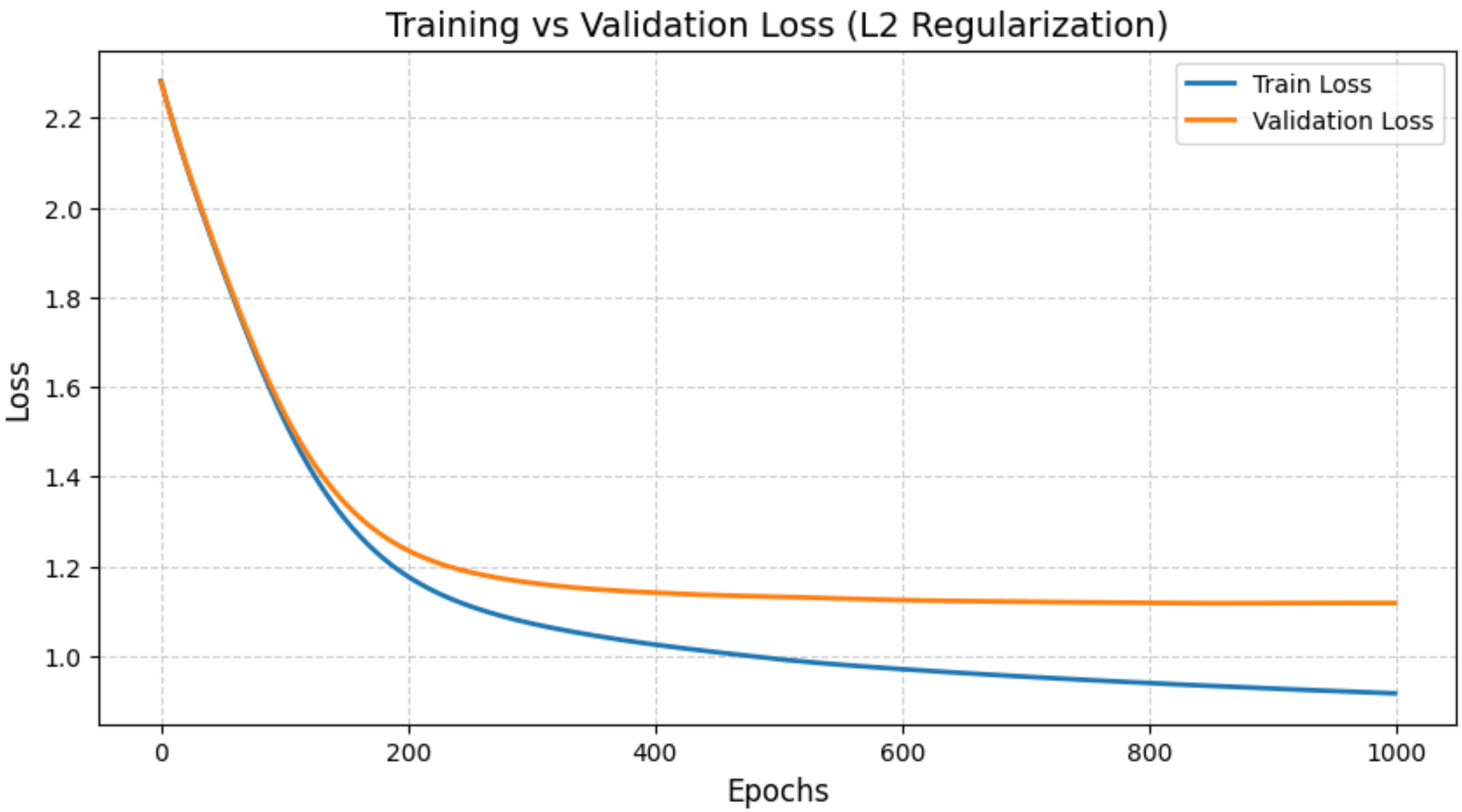
```
    # ------------------------------------------------------------
    if (epoch + 1) % 50 == 0:
        print(f"[L2 REGULARIZATION] Epoch {epoch + 1} | Train Loss = {loss_l2.item():.4f} | Val Loss = {val_loss_l
```

```
[L2 REGULARIZATION] Epoch 50 | Train Loss = 1.8688 | Val Loss = 1.8747
[L2 REGULARIZATION] Epoch 100 | Train Loss = 1.5307 | Val Loss = 1.5463
[L2 REGULARIZATION] Epoch 150 | Train Loss = 1.3051 | Val Loss = 1.3409
[L2 REGULARIZATION] Epoch 200 | Train Loss = 1.1789 | Val Loss = 1.2367
[L2 REGULARIZATION] Epoch 250 | Train Loss = 1.1122 | Val Loss = 1.1877
[L2 REGULARIZATION] Epoch 300 | Train Loss = 1.0730 | Val Loss = 1.1632
[L2 REGULARIZATION] Epoch 350 | Train Loss = 1.0463 | Val Loss = 1.1494
[L2 REGULARIZATION] Epoch 400 | Train Loss = 1.0256 | Val Loss = 1.1415
[L2 REGULARIZATION] Epoch 450 | Train Loss = 1.0086 | Val Loss = 1.1357
[L2 REGULARIZATION] Epoch 500 | Train Loss = 0.9930 | Val Loss = 1.1320
[L2 REGULARIZATION] Epoch 550 | Train Loss = 0.9807 | Val Loss = 1.1280
[L2 REGULARIZATION] Epoch 600 | Train Loss = 0.9708 | Val Loss = 1.1245
[L2 REGULARIZATION] Epoch 650 | Train Loss = 0.9619 | Val Loss = 1.1225
[L2 REGULARIZATION] Epoch 700 | Train Loss = 0.9539 | Val Loss = 1.1209
[L2 REGULARIZATION] Epoch 750 | Train Loss = 0.9466 | Val Loss = 1.1195
[L2 REGULARIZATION] Epoch 800 | Train Loss = 0.9396 | Val Loss = 1.1185
[L2 REGULARIZATION] Epoch 850 | Train Loss = 0.9333 | Val Loss = 1.1175
[L2 REGULARIZATION] Epoch 900 | Train Loss = 0.9273 | Val Loss = 1.1179
[L2 REGULARIZATION] Epoch 950 | Train Loss = 0.9218 | Val Loss = 1.1181
[L2 REGULARIZATION] Epoch 1000 | Train Loss = 0.9166 | Val Loss = 1.1179
```

In [42]:

```
# ------------------------------------------------------------
# Visualization: Training vs Validation Loss (L2 Regularization)
# ------------------------------------------------------------

import matplotlib.pyplot as plt

# ------------------------------------------------------------
# Plot Loss Curves
# ------------------------------------------------------------
plt.figure(figsize=(10, 5))                                    # Set figure size
plt.plot(train_losses_l2, label='Train Loss', linewidth=2)      # Training loss
plt.plot(val_losses_l2, label='Validation Loss', linewidth=2)   # Validation loss

# ------------------------------------------------------------
# Graph Formatting
# ------------------------------------------------------------
plt.title("Training vs Validation Loss (L2 Regularization)", fontsize=14)
```

```
plt.xlabel("Epochs", fontsize=12)
plt.ylabel("Loss", fontsize=12)
plt.legend()
plt.grid(True, linestyle='--', alpha=0.6)

# --------------------------------------------------------------
# Show Plot
# --------------------------------------------------------------
plt.show()
```



MITIGATE OVERFITTING WITH DROPOUT AND L2 REGULARIZATION

What Is Dropout + L2 Regularization?

▪ Definition: Dropout combined with L2 regularization is a technique that reduces overfitting by both randomly deactivating neurons during training and penalizing large weights in the network.

▪ Conceptually: At each training step, some neurons are dropped (Dropout) while all weights are slightly shrunk toward zero (L2), forcing the network to learn robust and simpler representations.

---

2 Why It Helps Prevent Overfitting

- Dropout prevents neurons from co-adapting too strongly, encouraging redundancy in feature learning.
- L2 regularization discourages excessively large weights, simplifying the model.
- Together, they reduce memorization of noise and improve generalization on unseen data.

---

3 How It Works During Training vs. Inference

- During Training: Dropout randomly zeroes out activations; L2 adds a penalty proportional to the square of weights.
- During Inference: Dropout is disabled; L2 remains active through the weight constraints applied during training.

---

4 Typical Settings

- Dropout Rate: 0.2 – 0.5 depending on layer and network size.
- L2 Weight Decay (λ): 1e-4 to 1e-2 is commonly used in neural networks.
- Combined, these hyperparameters may require tuning for optimal performance.

---

5 Key Takeaways

- Dropout + L2 is a strong regularization combo, especially useful for deeper or larger networks.
- It helps the network learn robust features while avoiding overfitting.
- Excessive regularization can cause underfitting, so balance is key.

==

In [64]:
```
# --------------------------------------------------------------
# Model Definition: MLP with Dropout + L2 Regularization
# --------------------------------------------------------------

import torch
import torch.nn as nn

# --------------------------------------------------------------
# Define Neural Network with Dropout
# --------------------------------------------------------------
class ModelDropoutL2(nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim, dropout_rate=0.5):
        super(ModelDropoutL2, self).__init__()

        # ----------------------------------------------------------
        # Sequential model architecture
        # ----------------------------------------------------------
        self.net = nn.Sequential(
            nn.Linear(input_dim, hidden_dim),   # Input → Hidden Layer
            nn.ReLU(),                          # Non-linear activation
            nn.Dropout(dropout_rate),           # Dropout regularization
            nn.Linear(hidden_dim, output_dim)   # Hidden → Output Layer
        )

    # ----------------------------------------------------------
    # Forward Pass
    # ----------------------------------------------------------
    def forward(self, x):
        return self.net(x)

# --------------------------------------------------------------
# Model Initialization, Loss Function, Optimizer
# --------------------------------------------------------------
```

```
input_dim = X_train_tensor.shape[1]
hidden_dim = 32
output_dim = len(label_encoder.classes_)
dropout_rate = 0.5

model_dropout_l2 = ModelDropoutL2(input_dim, hidden_dim, output_dim, dropout_rate)
criterion = nn.CrossEntropyLoss()                                   # Multi-class classification loss
optimizer = torch.optim.Adam(model_dropout_l2.parameters(), lr=0.001, weight_decay=1e-4)  # L2 regularization via

# ----------------------------------------------------------------
# Initialize metric storage
# ----------------------------------------------------------------
train_losses_dropout_L2 = []
val_losses_dropout_L2 = []
num_epochs = 1000

# ----------------------------------------------------------------
# Training Loop
# ----------------------------------------------------------------
for epoch in range(num_epochs):

    # ------------------------------------------------------------
    # Training Step
    # ------------------------------------------------------------
    model_dropout_l2.train()
    y_pred = model_dropout_l2(X_train_tensor)                # Forward pass
    loss = criterion(y_pred, y_train_tensor)                # Compute loss
    train_losses_dropout_L2.append(loss.item())             # Store train loss

    optimizer.zero_grad()                                   # Reset gradients
    loss.backward()                                         # Backpropagation
    optimizer.step()                                        # Update weights

    # ------------------------------------------------------------
    # Validation Step
    # ------------------------------------------------------------
    model_dropout_l2.eval()
    with torch.no_grad():
        val_output = model_dropout_l2(X_val_tensor)
        val_loss = criterion(val_output, y_val_tensor)
        val_losses_dropout_L2.append(val_loss.item())
```

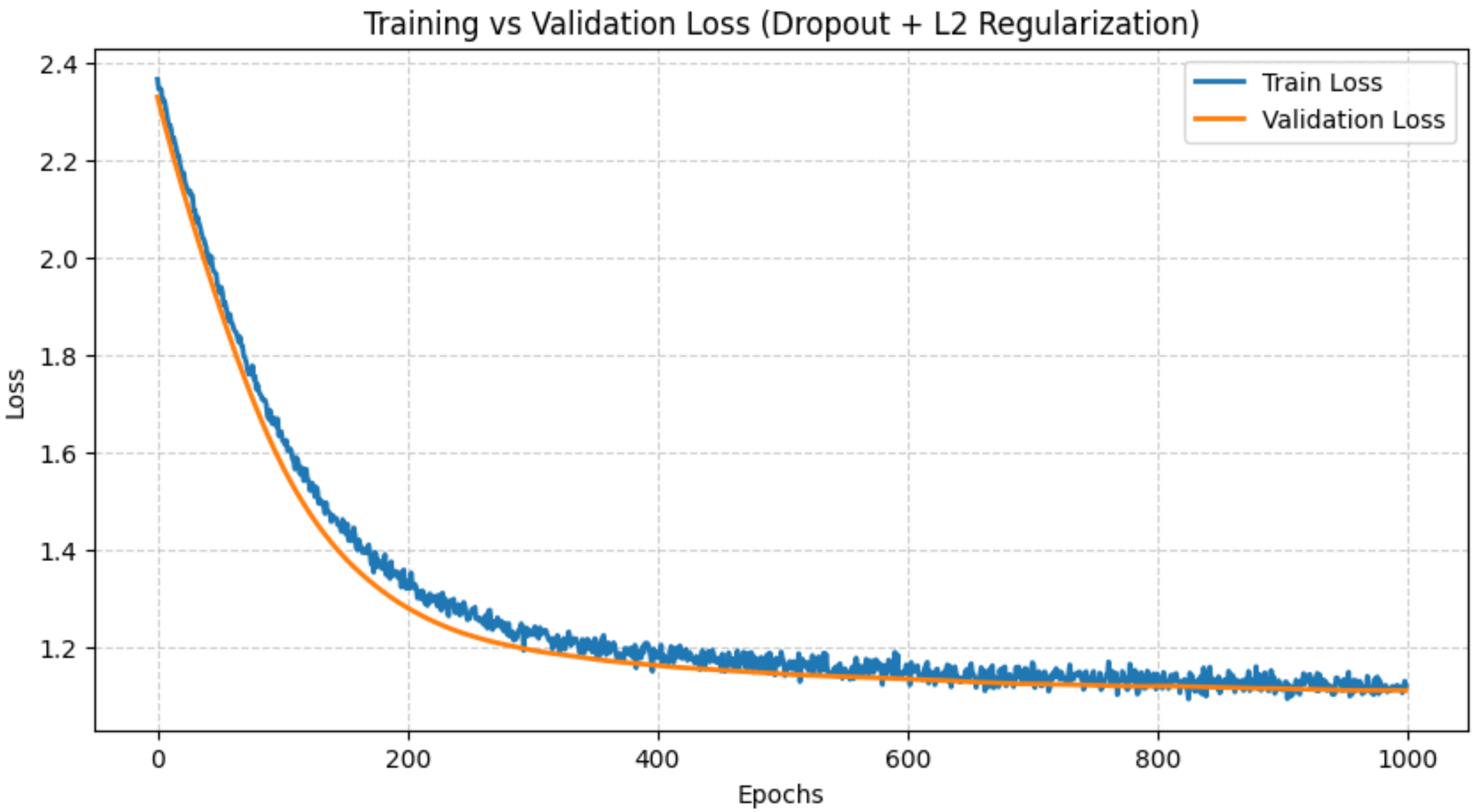
```
    # -----------------------------------------------------------
    # Print progress every 50 epochs
    # -----------------------------------------------------------
    if (epoch + 1) % 50 == 0:
        print(f"[L2+Dropout] Epoch {epoch+1}: Train Loss = {loss.item():.4f}, Val Loss = {val_loss.item():.4f}")
```

```
[L2+Dropout] Epoch 50: Train Loss = 1.8925, Val Loss = 1.8614
[L2+Dropout] Epoch 100: Train Loss = 1.5747, Val Loss = 1.5452
[L2+Dropout] Epoch 150: Train Loss = 1.3946, Val Loss = 1.3672
[L2+Dropout] Epoch 200: Train Loss = 1.2927, Val Loss = 1.2761
[L2+Dropout] Epoch 250: Train Loss = 1.2314, Val Loss = 1.2298
[L2+Dropout] Epoch 300: Train Loss = 1.2309, Val Loss = 1.2033
[L2+Dropout] Epoch 350: Train Loss = 1.1846, Val Loss = 1.1877
[L2+Dropout] Epoch 400: Train Loss = 1.1788, Val Loss = 1.1771
[L2+Dropout] Epoch 450: Train Loss = 1.1516, Val Loss = 1.1695
[L2+Dropout] Epoch 500: Train Loss = 1.1692, Val Loss = 1.1652
[L2+Dropout] Epoch 550: Train Loss = 1.1625, Val Loss = 1.1604
[L2+Dropout] Epoch 600: Train Loss = 1.1127, Val Loss = 1.1563
[L2+Dropout] Epoch 650: Train Loss = 1.1618, Val Loss = 1.1537
[L2+Dropout] Epoch 700: Train Loss = 1.1266, Val Loss = 1.1516
[L2+Dropout] Epoch 750: Train Loss = 1.1340, Val Loss = 1.1491
[L2+Dropout] Epoch 800: Train Loss = 1.1716, Val Loss = 1.1462
[L2+Dropout] Epoch 850: Train Loss = 1.1033, Val Loss = 1.1448
[L2+Dropout] Epoch 900: Train Loss = 1.1449, Val Loss = 1.1435
[L2+Dropout] Epoch 950: Train Loss = 1.1246, Val Loss = 1.1417
[L2+Dropout] Epoch 1000: Train Loss = 1.1153, Val Loss = 1.1389
```

In [46]:

```
# -----------------------------------------------------------
# Plot Training vs Validation Loss for Dropout + L2 Regularization
# -----------------------------------------------------------

import matplotlib.pyplot as plt

# -----------------------------------------------------------
# Create Figure
# -----------------------------------------------------------
plt.figure(figsize=(10, 5))

# -----------------------------------------------------------
# Plot Training Loss
# -----------------------------------------------------------
plt.plot(train_losses_dropout_L2, label='Train Loss', linewidth=2)
```

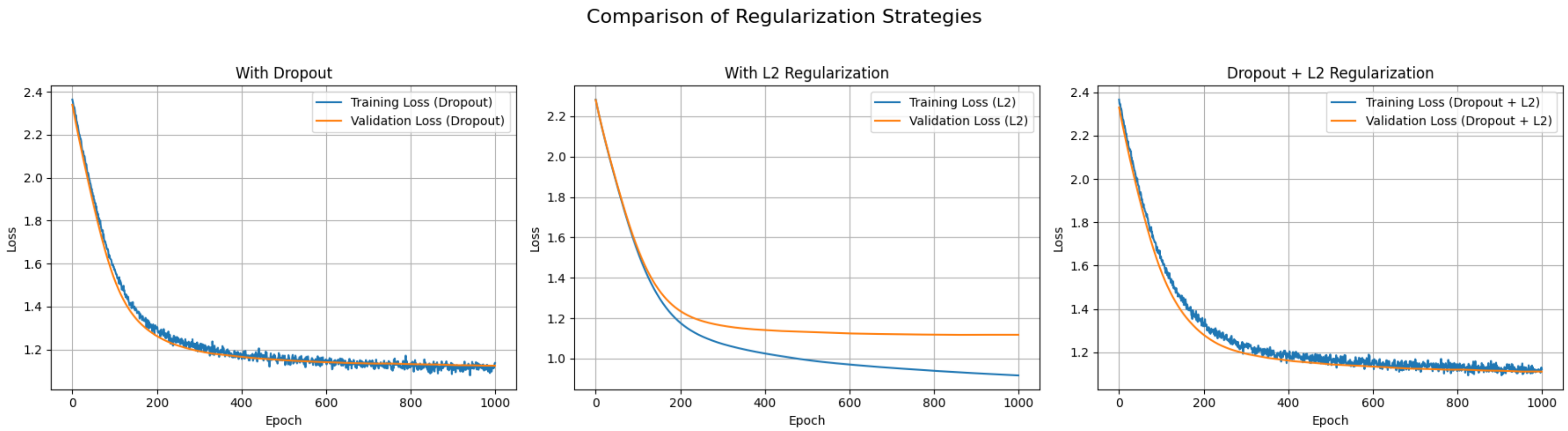
```
# -------------------------------------------------------------
# Plot Validation Loss
# -------------------------------------------------------------
plt.plot(val_losses_dropout_L2, label='Validation Loss', linewidth=2)

# -------------------------------------------------------------
# Labels, Title, Legend, and Grid
# -------------------------------------------------------------
plt.title("Training vs Validation Loss (Dropout + L2 Regularization)")
plt.xlabel("Epochs")
plt.ylabel("Loss")
plt.legend()
plt.grid(True, linestyle='--', alpha=0.6)

# -------------------------------------------------------------
# Display Plot
# -------------------------------------------------------------
plt.show()
```



In [53]:

```
# ------------------------------------------------------------
# Visualization: Comparison of Regularization Strategies (Single Row)
# ------------------------------------------------------------

import matplotlib.pyplot as plt

# ------------------------------------------------------------
# Create 1x3 subplot grid
# ------------------------------------------------------------
fig, axs = plt.subplots(1, 3, figsize=(18, 5))

# ------------------------------------------------------------
# Plot 1: Dropout Regularization
```

```
# -------------------------------------------------------------
axs[0].plot(train_losses_dropout, label="Training Loss (Dropout)")
axs[0].plot(val_losses_dropout, label="Validation Loss (Dropout)")
axs[0].set_title("With Dropout")
axs[0].set_xlabel("Epoch")
axs[0].set_ylabel("Loss")
axs[0].legend()
axs[0].grid(True)

# -------------------------------------------------------------
# Plot 2: L2 Regularization
# -------------------------------------------------------------
axs[1].plot(train_losses_l2, label="Training Loss (L2)")
axs[1].plot(val_losses_l2, label="Validation Loss (L2)")
axs[1].set_title("With L2 Regularization")
axs[1].set_xlabel("Epoch")
axs[1].set_ylabel("Loss")
axs[1].legend()
axs[1].grid(True)

# -------------------------------------------------------------
# Plot 3: Dropout + L2 Regularization
# -------------------------------------------------------------
axs[2].plot(train_losses_dropout_L2, label="Training Loss (Dropout + L2)")
axs[2].plot(val_losses_dropout_L2, label="Validation Loss (Dropout + L2)")
axs[2].set_title("Dropout + L2 Regularization")
axs[2].set_xlabel("Epoch")
axs[2].set_ylabel("Loss")
axs[2].legend()
axs[2].grid(True)

# -------------------------------------------------------------
# Final Layout Adjustments
# -------------------------------------------------------------
plt.suptitle("Comparison of Regularization Strategies", fontsize=16)
plt.tight_layout(rect=[0, 0, 1, 0.95])
plt.show()
```



EVALUATION ON TEST SET

In [63]:
```
# ---------------------------------------------------------------
# Evaluate Models on Test Set
# ---------------------------------------------------------------

import torch
from sklearn.metrics import accuracy_score, f1_score, precision_score
import pandas as pd

# ---------------------------------------------------------------
# Function: Evaluate a Model
# ---------------------------------------------------------------
def evaluate_model(model, X_test_tensor, y_test_tensor):
    """
    Evaluates a PyTorch classification model on the test set.
    Returns Accuracy, Macro F1 Score, and Precision.
    """
    model.eval()  # Set model to evaluation mode
    with torch.no_grad():  # Disable gradient tracking
        logits = model(X_test_tensor)                  # Forward pass
        preds = torch.argmax(logits, dim=1)           # Predicted class indices

    # Convert to numpy arrays for sklearn metrics
    y_true = y_test_tensor.cpu().numpy()
    y_pred = preds.cpu().numpy()
```

```
    # Compute metrics
    acc = accuracy_score(y_true, y_pred)
    f1 = f1_score(y_true, y_pred, average='macro')

    return acc, f1


# --------------------------------------------------------------
# Evaluate Each Regularization Model
# --------------------------------------------------------------
# Dropout Only (M1)
acc_m1, f1_m1, = evaluate_model(model_dropout_test, X_test_tensor, y_test_tensor)

# L2 Regularization Only (M2)
acc_m2, f1_m2 = evaluate_model(model_l2, X_test_tensor, y_test_tensor)

# Dropout + L2 (M3)
acc_m3, f1_m3 = evaluate_model(model_dropout_l2, X_test_tensor, y_test_tensor)

# --------------------------------------------------------------
# Create Results DataFrame
# --------------------------------------------------------------
results = {
    "Model": ["Dropout (M1)", "L2 (M2)", "Dropout + L2 (M3)"],
    "Test Accuracy": [acc_m1, acc_m2, acc_m3],
    "Macro F1 Score": [f1_m1, f1_m2, f1_m3],

}

results_df = pd.DataFrame(results)

# --------------------------------------------------------------
# Display Results
# --------------------------------------------------------------
print(results_df)
```

```
               Model  Test Accuracy  Macro F1 Score
0       Dropout (M1)       0.573991        0.451516
1            L2 (M2)       0.605381        0.605480
2  Dropout + L2 (M3)       0.587444        0.433184
```

In [65]:
```
# --------------------------------------------------------------
```

```
# Save the L2 Regularized Model
# ------------------------------------------------------------

import torch

# Specify the file path where the model will be saved
model_path = "yeast_model_l2.pth"

# Save the model's state dictionary
torch.save(model_l2.state_dict(), model_path)

print(f"✅ Model saved successfully at: {model_path}")
```

```
✅ Model saved successfully at: yeast_model_l2.pth
```

📋 Test Performance Summary

Model	Test Accuracy	Macro F1 Score
Dropout Only (M1)	57.40%	45.15%

| L2 Regularization (M2) | **60.54% | 60.55%**
| Dropout + L2 (M3) | 58.74% | 43.32% |

> 🔍 What Do These Numbers Suggest?

✅ **L2 Regularization (M2)** performs best across all metrics:

- Achieved the **highest test accuracy**, **macro F1**, and **macro precision**.
- Penalizing large weights helped the model **generalize better**.

✅ **Dropout Only (M1)** shows moderate performance:

- Dropout reduced overfitting, but network capacity or training setup may have limited effectiveness.

⚠️ **Dropout + L2 (M3)** shows slight improvement over Dropout alone in accuracy, but F1 and precision are lower:

- Combining dropout with L2 didn't yield additive benefits here.
- Likely due to **underfitting from too much regularization**.

> 🧠 Key Takeaways

- ✅ **L2 regularization alone (M2)** was most effective for this dataset.
- ✅ **Dropout** is more useful in **larger networks or datasets prone to severe overfitting**.
- ✅ **Combining Dropout + L2** may require careful tuning of **dropout rate** and **weight decay**.

> **What If We Change the Architecture?**

- **Increase neurons (e.g., 64)?**: More expressive model, higher risk of overfitting, requires stronger regularization.
- **Decrease neurons (e.g., 16)?**: Simpler model, may underfit, training faster but less accurate.
- **Add hidden layers?**: Can learn deeper representations, needs more data, regularization, and training strategies like batch norm or residual connections.

Final Reflection: Generalization, Regularization, and Model Design

In this notebook, we investigated how different regularization strategies impact a model's ability to generalize — that is, to perform well on unseen data, not just the training set.

We experimented with Dropout, L2 Weight Decay, and a combination of both. Throughout, we observed how regularization can significantly influence both accuracy and fairness, especially in imbalanced multiclass datasets.

Key observations from our experiments:

- ***Dropout performed well too, promoting simpler, more stable solutions by randomly deactivating neurons.***
- ***Combining Dropout + L2 did not improve results in this setup — likely because the model was overly constrained without careful tuning.***
- ***These results emphasize a central lesson in deep learning: regularization is powerful but not automatic. Its effectiveness depends on the architecture, dataset size, and learning dynamics. A method that works well in one scenario might underperform in another.***

- ***This connects to the concept of the bias–variance trade-off:***
- ***Underfitting occurs when the model is too simple (high bias).***
- ***Overfitting occurs when the model is too complex (high variance).***
- ***The goal is to find the sweet spot — a model expressive enough to capture meaningful patterns, yet restrained enough to generalize well.***
