PyTorch Basics: Deep Learning & Data Analysis

Over the next few weeks we will learn the basics of Deep Learning using pytorch

Do the coding exercises below, add comments and markdown explanations, and upload the resulting notebook together with the collab corresponding to mini project 2.

This notebook covers:

1. Problem setup & data splits (train/val/test)
2. PyTorch tensors, datasets, and dataloaders
3. Models: linear regression, MLP for classification, CNN
4. Losses, regularization (L2/weight decay & dropout), and metrics
5. Optimization: gradient descent w/ `torch.optim`
6. Experiment tracking: random seeds, reproducibility, and plotting learning curves

> This notebook uses only standard libraries available in Colab: `torch` , `numpy` , `matplotlib` , and the `sklearn` library for toy data.

In [ ]:
```
#@title Imports & reproducibility helpers
import math, random, os, time
import numpy as np
import torch
from torch import nn
from torch.utils.data import Dataset, DataLoader, random_split
from typing import Tuple, Dict, Any

try:
    from sklearn.datasets import make_moons, make_circles
    _HAS_SKLEARN = True
except Exception as e:
    print("scikit-learn not found; synthetic dataset generators will fall back to torch-onl
y.")
    _HAS_SKLEARN = False

import matplotlib.pyplot as plt

def set_seed(seed: int = 123):
    random.seed(seed)
    np.random.seed(seed)
    torch.manual_seed(seed)
    torch.cuda.manual_seed_all(seed)
    torch.backends.cudnn.deterministic = True
    torch.backends.cudnn.benchmark = False

DEVICE = "cuda" if torch.cuda.is_available() else "cpu"
set_seed(7)
DEVICE
```

Out[ ]:
```
'cuda'
```

🧩🧩🧩

-1) Tensors

Tensors in pytorch are very similar to numpy arrays

1. 🧩 How do we construct a tensor?

Say we want to construct the following tensor using torch functions:

```
tensor([[0, 3, 6],
        [1, 4, 7],
        [2, 5, 8]])
```

1. 🧩 What's the size of this tensor?

```
In [ ]: #@title Answer 1
        my_tensor = torch.tensor([[0, 1, 2],
                                  [3, 4, 5],
                                  [6, 7, 8]])

        print(my_tensor)
```

```
tensor([[0, 1, 2],
        [3, 4, 5],
        [6, 7, 8]])
```

```
In [ ]: #@title Answer 2
        my_tensor.shape
```

```
Out[ ]: torch.Size([3, 3])
```

```
In [ ]: #@title Pytorch has many useful functions for creating, indexing and operating with tensor
        # Parameters
        sequence = torch.arange(5)   # [0, 1, 2, 3, 4]
        repeats = 3                  # number of times to repeat

        # Construct the repeated tensor
        x = sequence.repeat(repeats)

        print(sequence), print(x)
```

```
tensor([0, 1, 2, 3, 4])
tensor([0, 1, 2, 3, 4, 0, 1, 2, 3, 4, 0, 1, 2, 3, 4])
```

```
Out[ ]: (None, None)
```

```
In [ ]: #@title 🧩 Print a tensor of size (5,3), where all the values have one fixed size
        torch.full((5,3), -2.0)
```

```
Out[ ]: tensor([[-2., -2., -2.],
                [-2., -2., -2.],
                [-2., -2., -2.],
                [-2., -2., -2.],
                [-2., -2., -2.]])
```

🧩 Construct* the following tensor:

```python tensor([[0, 1, 2, 3, 4], [0, 1, 2, 3, 4], [0, 1, 2, 3, 4]])
```

At some point in my code, I need to write an equation that uses 2 * pi. I get an error allerting me that my code returns a float where a tensor is expected. What is the type of

```
type(2*torch.py)
```

and how do I turn into a tensor?

```
In [ ]: #@title 🧩 Use pytorch functions to generate this matrix

        n = 4
        A = torch.eye(n)                             # diagonal of 1s
        A += torch.diag(torch.full((n-1,), -2.), diagonal=-1)  # sub-diagonal
        A += torch.diag(torch.full((n-1,), -2.), diagonal=1)   # super-diagonal

        print(A)
```

```
tensor([[ 1., -2.,  0.,  0.],
        [-2.,  1., -2.,  0.],
        [ 0., -2.,  1., -2.],
        [ 0.,  0., -2.,  1.]])
```

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0) Broadcasting, Indexing, and Distributions in PyTorch

Goal: Practice *broadcasting*, *masking*, and *distributions* in PyTorch through short guided exercises.

Run each code cell, fill in the `# TODO` parts, and test your answers.

```
In [ ]: import torch
        import torch.distributions as dist
        import matplotlib.pyplot as plt
        torch.manual_seed(0)

Out[ ]: <torch._C.Generator at 0x7cef26ed7770>
```

Broadcasting and Fancy Indexing

Broadcasting and indexing make PyTorch efficient and expressive.

🧩 Exercise 0.1

Construct a tensor `X` where `X[i,j] = 2*i + j` using broadcasting.

Example Output:

```
tensor([[0, 1, 2, 3],
        [2, 3, 4, 5],
        [4, 5, 6, 7]])
```

In [ ]:
```python
# TODO: Construct X using broadcasting
# i = torch.arange(...).view(-1, 1)
# j = torch.arange(...).view(1, -1)
# X = ...

i = torch.arange(3).view(-1, 1)
j = torch.arange(4).view(1, -1)
X = 2*i + j

print(X)
```

```
tensor([[0, 1, 2, 3],
        [2, 3, 4, 5],
        [4, 5, 6, 7]])
```

Exercise 0.2

Compute a **distance matrix** `D` where `D[i,j]` is the Euclidean distance between `X[i]` and `X[j]` .

Use broadcasting (no loops).

In [ ]:
```python
X = torch.arange(12, dtype=float).reshape(6, 2)
# TODO: Compute pairwise distances using broadcasting
# D = ...
D = (X.unsqueeze(1) - X.unsqueeze(0)).norm(dim=-1)

print (D)
```

```
tensor([[ 0.0000,  2.8284,  5.6569,  8.4853, 11.3137, 14.1421],
        [ 2.8284,  0.0000,  2.8284,  5.6569,  8.4853, 11.3137],
        [ 5.6569,  2.8284,  0.0000,  2.8284,  5.6569,  8.4853],
        [ 8.4853,  5.6569,  2.8284,  0.0000,  2.8284,  5.6569],
        [11.3137,  8.4853,  5.6569,  2.8284,  0.0000,  2.8284],
        [14.1421, 11.3137,  8.4853,  5.6569,  2.8284,  0.0000]],
       dtype=torch.float64)
```

Exercise 0.3

Extract the submatrix of rows `[1,4]` and columns `[0,2,3]` of
`A = torch.arange(36).reshape(6, 6)`

Expected Output:

```
tensor([[ 6,  8,  9],
        [24, 26, 27]])
```

In [ ]:
```python
A = torch.arange(36).reshape(6, 6)
# TODO: Extract submatrix using indexing
# rows = torch.tensor([...])
# cols = torch.tensor([...])
# subA = ...
rows = torch.tensor([1,4])
cols = torch.tensor([0,2,3])
subA = A[rows][:,cols]

print(subA)
```

```
tensor([[ 6,  8,  9],
        [24, 26, 27]])
```

Exercise 0.4

Create a **boolean mask** `M` where `M[i,j]` is True iff `A[i,j]` is divisible by 5 or 7.

```
In [ ]: A = torch.arange(36).reshape(6, 6)
        # TODO: Create boolean mask
        # M = ...
        # print(M.sum())

        M = (A % 5 == 0) | (A % 7 == 0)
        print(M.sum())
```

```
tensor(12)
```

Exercise 0.5

Using the mask `M`, add 10 to elements of `A` that are divisible by 5 or 7 (in-place).

```
In [ ]: # TODO: Update A in-place
        # A[M] += 10
        # print(A)

        A[M] += 10
        print(A)
```

```
tensor([[10,  1,  2,  3,  4, 15],
        [ 6, 17,  8,  9, 20, 11],
        [12, 13, 24, 25, 16, 17],
        [18, 19, 30, 31, 22, 23],
        [24, 35, 26, 27, 38, 29],
        [40, 31, 32, 33, 34, 45]])
```

Distributions

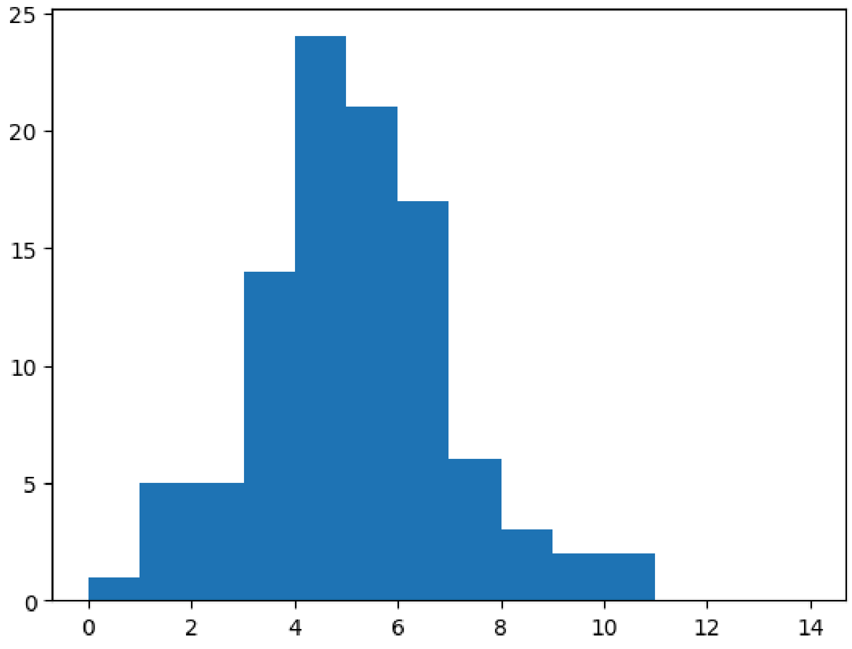
`torch.distributions` provides a clean API for probability distributions and supports broadcasting.

Exercise 0.6

Draw **100 samples** from a Poisson distribution with rate λ = 4.5.

In [ ]:
```
# TODO: Draw samples and plot histogram
# samples = dist.Poisson(4.5).sample((100,))
# plt.hist(samples.numpy(), bins=range(0,15))
# plt.show()

samples = dist.Poisson(4.5).sample((100,))
plt.hist(samples.numpy(), bins=range(0,15))
plt.show()
```



Exercise 0.7

Construct a matrix `P` where
`P[i,j] = exp(−λ[i]) ∗ λ[i]^j / j!`
for λ = `torch.arange(1.,6.)` and j = `torch.arange(5.)`.

In [ ]:
```
lam = torch.arange(1.,6.).view(-1,1)
j = torch.arange(5.).view(1,-1)
# TODO: Compute P using broadcasting and torch.lgamma
# factorial = torch.exp(torch.lgamma(j+1))
# P = ...

factorial = torch.exp(torch.lgamma(j+1))
P = torch.exp(-lam) * lam**j / factorial
print(P)
```

```
tensor([[0.3679, 0.3679, 0.1839, 0.0613, 0.0153],
        [0.1353, 0.2707, 0.2707, 0.1804, 0.0902],
        [0.0498, 0.1494, 0.2240, 0.2240, 0.1680],
        [0.0183, 0.0733, 0.1465, 0.1954, 0.1954],
        [0.0067, 0.0337, 0.0842, 0.1404, 0.1755]])
```

Exercise 0.8

Evaluate the **log-probability** of `[0.5, 2.0, 5.0]`
under a Gamma distribution with shape=3.0, rate=2.0.

```
In [ ]: # TODO: Evaluate log probability
        # g = dist.Gamma(concentration=3.0, rate=2.0)
        # logp = g.log_prob(torch.tensor([0.5, 2.0, 5.0]))
        # print(logp)

        g = dist.Gamma(concentration=3.0, rate=2.0)
        logp = g.log_prob(torch.tensor([0.5, 2.0, 5.0]))
        print(logp)
```

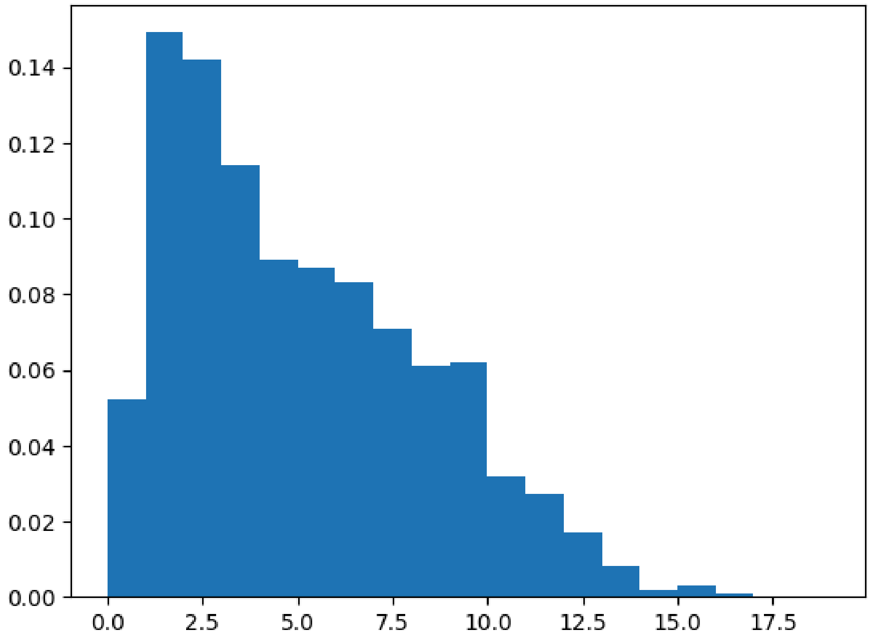
```
tensor([-1.0000, -1.2274, -5.3948])
```

Problem 0.9

Draw **1000 samples** from a mixture of two Poisson distributions
with rates 2 and 7, equal weights (0.5, 0.5).
Plot a normalized histogram.

```
In [ ]: # TODO: Draw samples from mixture
        # z = torch.bernoulli(torch.full((1000,), 0.5))
        # lam = torch.where(z.bool(), torch.tensor(7.), torch.tensor(2.))
        # samples = dist.Poisson(lam).sample()
        # plt.hist(samples.numpy(), bins=range(0,20), density=True)
        # plt.show()

        z = torch.bernoulli(torch.full((1000,), 0.5))
        lam = torch.where(z.bool(), torch.tensor(7.), torch.tensor(2.))
        samples = dist.Poisson(lam).sample()
        plt.hist(samples.numpy(), bins=range(0,20), density=True)
        plt.show()
```



Normal Distributions

Problem 0.10

Use `dist.Normal` to draw a batch of shape `(200, 3)` of independent standard normal random variables.

```
In [ ]: # TODO: Draw standard normal samples
        # normals = dist.Normal(0, 1).sample((200,3))
        # print(normals.shape)

        normals = dist.Normal(0, 1).sample((200,3))
        print(normals.shape)
```

```
torch.Size([200, 3])
```

🧩 Problem 0.11

Use `dist.Normal` to draw a batch of shape `(4, 4)`
with means given by `mu` and variance 1.0.

```
In [ ]: mu = torch.tensor([[ 0,  1,  2,  3],
                           [ 4,  5,  6,  7],
                           [ 8,  9, 10, 11],
                           [12, 13, 14, 15]], dtype=torch.float32)
        # TODO: Draw samples
        # samples = dist.Normal(mu, 1.0).sample()
        # print(samples.shape)

        samples = dist.Normal(mu, 1.0).sample()
        print(samples.shape)
```

```
torch.Size([4, 4])
```

✅ Notes / Extensions

- Vary λ and j shapes to visualize broadcasting.
- Plot distance matrices `plt.imshow(D)` to see patterns.
- Compare the Poisson mixture histogram with theoretical PMFs.
- Explore `dist.MixtureSameFamily` for more complex mixtures.

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1) Data: from arrays to `Dataset`/`DataLoader` + train/val/test split

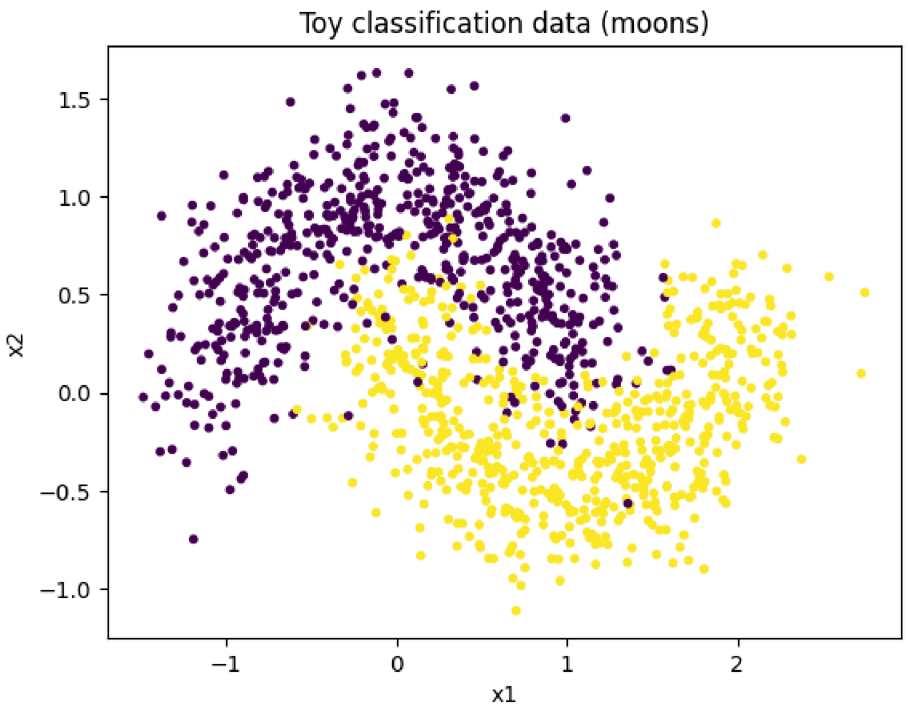
Key ideas

- Always separate data into **train / validation / test** (e.g., 70/15/15).
- Wrap arrays in a custom `Dataset` to keep the training loop clean.
- Use a `DataLoader` for batching, shuffling, and parallel loading.

We'll start with toy 2D datasets for classification (moons and circles) and a simple 1D regression problem.

In [ ]:
```python
#@title Toy datasets (classification: moons/circles) + (regression: y = ax + b + noise)
def make_toy_classification(n_samples=1000, kind="moons", noise=0.2, seed=0):
    set_seed(seed)
    if _HAS_SKLEARN:
        if kind == "moons":
            X, y = make_moons(n_samples=n_samples, noise=noise)
        elif kind == "circles":
            X, y = make_circles(n_samples=n_samples, factor=0.4, noise=noise)
        else:
            raise ValueError("kind must be 'moons' or 'circles'")
        X = X.astype(np.float32); y = y.astype(np.int64)
    else:
        # Torch-only fallback: two Gaussian blobs
        c1 = torch.randn(n_samples//2, 2) * (1+noise) + torch.tensor([0.0, 0.0])
        c2 = torch.randn(n_samples//2, 2) * (1+noise) + torch.tensor([2.5, 2.5])
        X = torch.cat([c1, c2], dim=0).numpy().astype(np.float32)
        y = torch.cat([torch.zeros(len(c1)), torch.ones(len(c2))]).numpy().astype(np.int64)
    return X, y

def make_toy_regression(n_samples=600, a=2.0, b=-1.0, noise_std=0.3, seed=0):
    set_seed(seed)
    x = np.random.uniform(-2.0, 2.0, size=(n_samples, 1)).astype(np.float32)
    y = (a * x + b + np.random.normal(0, noise_std, size=x.shape)).astype(np.float32)
    return x, y

class NumpyDataset(Dataset):
    def __init__(self, X: np.ndarray, y: np.ndarray):
        self.X = torch.from_numpy(X)
        self.y = torch.from_numpy(y)
    def __len__(self):
        return len(self.X)
    def __getitem__(self, idx):
        return self.X[idx], self.y[idx]

def train_val_test_split(ds: Dataset, ratios=(0.7, 0.15, 0.15), seed=42):
    assert abs(sum(ratios) - 1.0) < 1e-6, "Ratios must sum to 1"
    n = len(ds)
    n_train = int(ratios[0] * n)
    n_val = int(ratios[1] * n)
    n_test = n - n_train - n_val
    set_seed(seed)
    return random_split(ds, [n_train, n_val, n_test])
```

In [ ]:
```python
#@title Visualize a toy classification dataset
Xc, yc = make_toy_classification(n_samples=1200, kind="moons", noise=0.25, seed=1)
ds_cls = NumpyDataset(Xc, yc)
train_ds, val_ds, test_ds = train_val_test_split(ds_cls, (0.7, 0.15, 0.15), seed=1)

plt.figure()
plt.scatter(Xc[:,0], Xc[:,1], c=yc, s=10)
plt.title("Toy classification data (moons)")
plt.xlabel("x1"); plt.ylabel("x2")
plt.show()

len(train_ds), len(val_ds), len(test_ds)
```



Out[ ]:
```
(840, 180, 180)
```

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2) Linear Regression in PyTorch (MSE loss)

We'll fit a line to noisy data: (y \approx ax + b).
This section introduces:

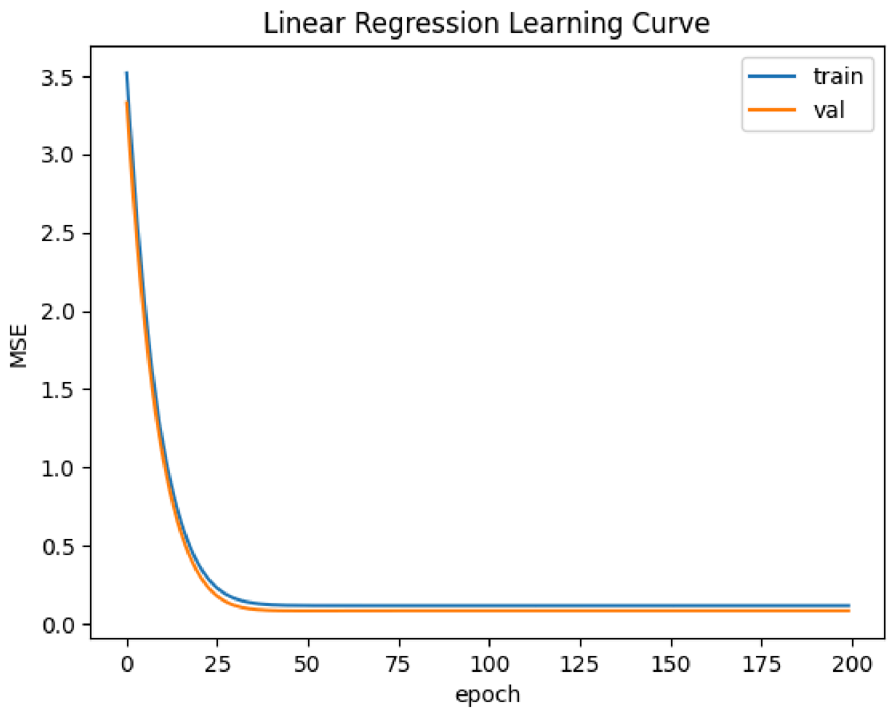
- `nn.Module` for models
- Mean Squared Error (MSE) loss
- `optim.SGD` and `optim.Adam`

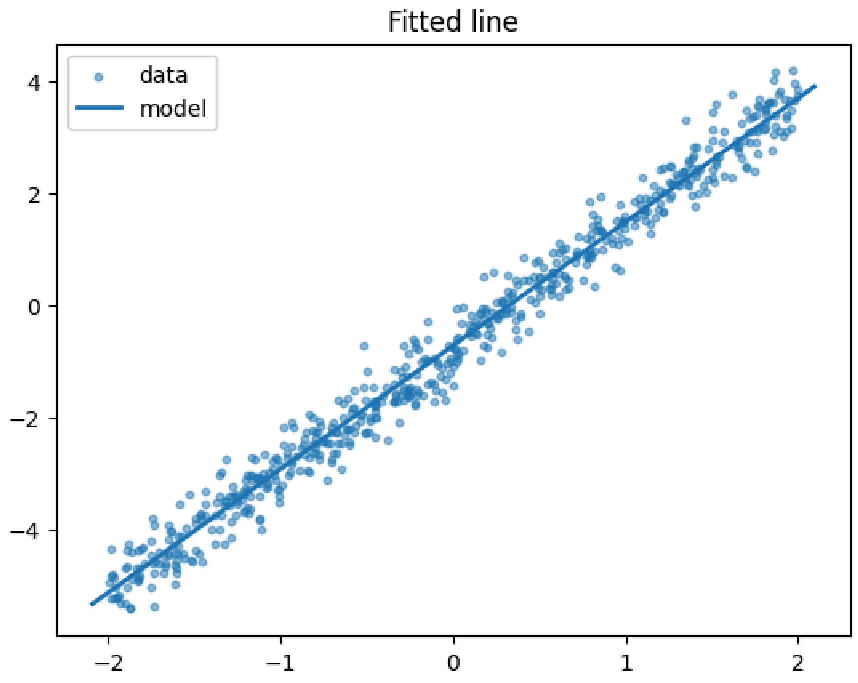
In [ ]:
```
#@title Linear regression dataset & model
Xr, yr = make_toy_regression(n_samples=600, a=2.2, b=-0.7, noise_std=0.35, seed=2)
ds_reg = NumpyDataset(Xr, yr)

train_r, val_r, test_r = train_val_test_split(ds_reg, (0.7, 0.15, 0.15), seed=2)
train_loader_r = DataLoader(train_r, batch_size=64, shuffle=True)
val_loader_r   = DataLoader(val_r, batch_size=128, shuffle=False)
test_loader_r  = DataLoader(test_r, batch_size=128, shuffle=False)

class LinearRegressor(nn.Module):
    def __init__(self):
        super().__init__()
        self.linear = nn.Linear(1, 1)
    def forward(self, x):
        return self.linear(x)

model = LinearRegressor().to(DEVICE)
criterion = nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=1e-2, weight_decay=0.0)  # weight_decay
= L2
```

In [ ]:
```
#@title Training & evaluation utilities
def train_epoch(model, loader, criterion, optimizer):
    model.train()
    total_loss = 0.0
    for xb, yb in loader:
        xb, yb = xb.to(DEVICE), yb.to(DEVICE)
        optimizer.zero_grad()
        preds = model(xb)
        loss = criterion(preds, yb)
        loss.backward()
        optimizer.step()
        total_loss += loss.item() * xb.size(0)
    return total_loss / len(loader.dataset)

@torch.no_grad()
def evaluate(model, loader, criterion):
    model.eval()
    total_loss = 0.0
    for xb, yb in loader:
        xb, yb = xb.to(DEVICE), yb.to(DEVICE)
        preds = model(xb)
        loss = criterion(preds, yb)
        total_loss += loss.item() * xb.size(0)
    return total_loss / len(loader.dataset)
```

In [ ]:
```
#@title Fit linear model & plot learning curve
train_hist, val_hist = [], []
epochs = 200
best_val = float("inf")
best_state = None

for epoch in range(1, epochs+1):
    tr = train_epoch(model, train_loader_r, criterion, optimizer)
    va = evaluate(model, val_loader_r, criterion)
    train_hist.append(tr); val_hist.append(va)
    if va < best_val:
        best_val = va; best_state = {k: v.cpu().clone() for k, v in model.state_dict().items
()}
    if epoch % 50 == 0:
        print(f"Epoch {epoch:03d} | train: {tr:.4f} | val: {va:.4f}")

# restore best
model.load_state_dict(best_state)

plt.figure()
plt.plot(train_hist, label="train")
plt.plot(val_hist, label="val")
plt.xlabel("epoch"); plt.ylabel("MSE")
plt.title("Linear Regression Learning Curve")
plt.legend(); plt.show()

# Visualize fit
@torch.no_grad()
def predict(x):
    return model(torch.from_numpy(x).to(DEVICE)).cpu().numpy()

xs = np.linspace(Xr.min()-0.1, Xr.max()+0.1, 200).reshape(-1,1).astype(np.float32)
ys = predict(xs)

plt.figure()
plt.scatter(Xr, yr, s=10, alpha=0.5, label="data")
plt.plot(xs, ys, linewidth=2, label="model")
plt.legend(); plt.title("Fitted line"); plt.show()
```

```
Epoch 050 | train: 0.1175 | val: 0.0840
Epoch 100 | train: 0.1170 | val: 0.0847
Epoch 150 | train: 0.1170 | val: 0.0847
Epoch 200 | train: 0.1170 | val: 0.0848
```





Exercise A

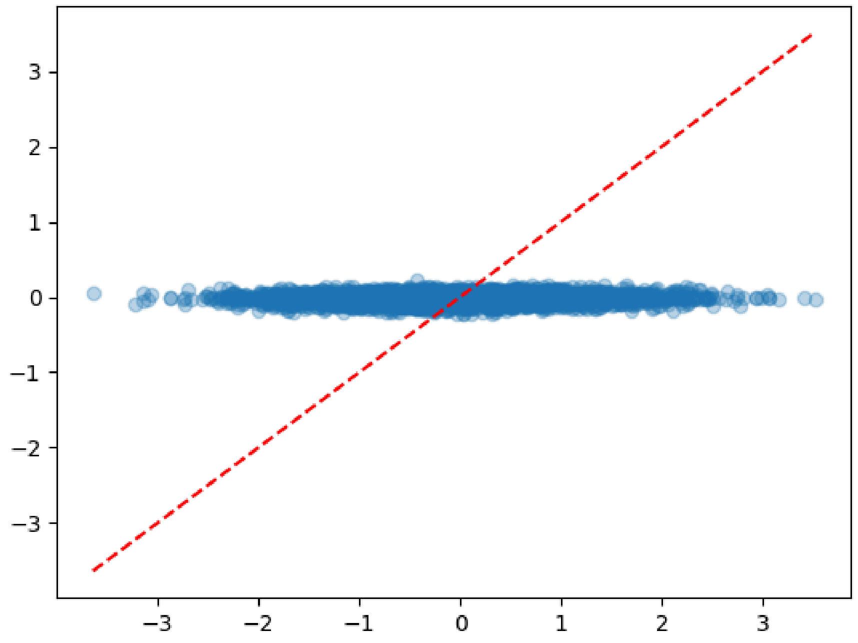
Create a synthetic data where the regressor x is an (n,2) dimensional tensor and the target y is a (n,4) dimensional tensor. Does the LinearRegressor model

```
class LinearRegressor(nn.Module):
    def __init__(self):
        super().__init__()
        self.linear = nn.Linear(1, 1)
    def forward(self, x):
        return self.linear(x)
```

work? Why or why not? How can you modify the class to make it work? Once you fit the model, visualize the result.

Answer: No! Because The model won't work because nn.Linear(1, 1) expects input dim 1 and output dim 1, but x is (n,2) and y is (n,4). After plots, it can say that there's no relationship between x and y. And model fails to learn.

```
In [ ]: #Create
n = 1000
x = torch.randn(n, 2)
y = torch.randn(n, 4)

model = nn.Linear(2, 4).to(DEVICE)
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)

for _ in range(200):
    loss = ((model(x.to(DEVICE)) - y.to(DEVICE))**2).mean()
    optimizer.zero_grad(); loss.backward(); optimizer.step()

with torch.no_grad():
    y_pred = model(x.to(DEVICE)).cpu()
plt.scatter(y.flatten(), y_pred.flatten(), alpha=0.3)
plt.plot([y.min(), y.max()], [y.min(), y.max()], 'r--')
plt.show()
```



Exercise B

The function train_val_test_split does the job, but it does not seem very elegant. Using

```
from torch.utils.data import random_split
```

create a 60-20-20 split of your data and train a model using that.

```
In [ ]: from torch.utils.data import TensorDataset, DataLoader, random_split

        ds = TensorDataset(x, y)
        train_ds, val_ds, test_ds = random_split(ds, [0.6, 0.2, 0.2])
        train_loader = DataLoader(train_ds, batch_size=64, shuffle=True)

        model = nn.Linear(2, 4).to(DEVICE)
        opt = torch.optim.Adam(model.parameters())

        for _ in range(200):
            for xb, yb in train_loader:
                opt.zero_grad(); ((model(xb.to(DEVICE)) - yb.to(DEVICE))**2).mean().backward(); opt.
        step()
```

Exercise C

Write your own Mean Squared Error

PyTorch provides a built-in criterion:

~~~~
criterion = nn.MSELoss()

But it’s important to understand what happens under the hood.
Let’s implement our own version — call it nn.MeanSquaredOops — that behaves like nn.MSELoss. It s
hould work as a callable class:

```python
criterion = MeanSquaredOops()
loss = criterion(y_pred, y_true)


```python
# YOUR WORK: Implement MeanSquaredOops to mimic nn.MSELoss

import torch
import torch.nn as nn

class MeanSquaredOops(nn.Module):
    def __init__(self):
        super().__init__()
    def forward(self, y_pred, y_true):
        return ((y_pred - y_true)**2).mean()
        # compute the mean of squared differences
        raise NotImplementedError("Implement the MSE formula here!")

# Test it
criterion = nn.MSELoss()
oops = MeanSquaredOops()

y_pred = torch.tensor([2.5, 0.0, 2.1])
y_true = torch.tensor([3.0, -0.5, 2.0])

print("PyTorch MSELoss:", criterion(y_pred, y_true).item())
print("Your MeanSquaredOops:", oops(y_pred, y_true).item())
~~~~

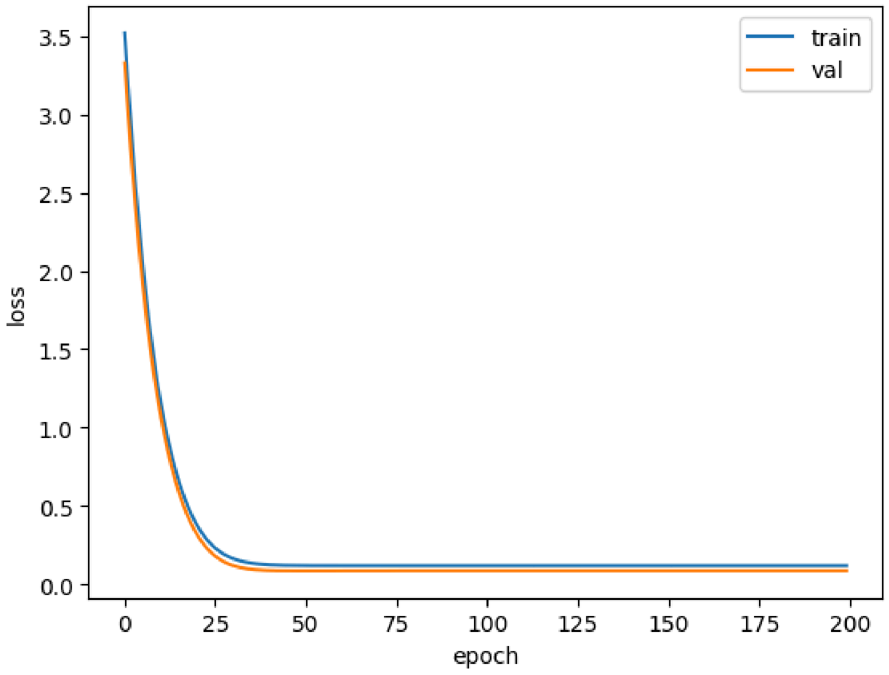
Write a function to visualize the loss function curves on: training, testing and evaluation datasets. How do they look like?

In [ ]:

```python
class MeanSquaredOops(nn.Module):
    def __init__(self):
        super().__init__()
    def forward(self, y_pred, y_true):
        return ((y_pred - y_true)**2).mean()

# Test it
criterion = nn.MSELoss()
oops = MeanSquaredOops()

y_pred = torch.tensor([2.5, 0.0, 2.1])
y_true = torch.tensor([3.0, -0.5, 2.0])

print("PyTorch MSELoss:", criterion(y_pred, y_true).item())
print("Your MeanSquaredOops:", oops(y_pred, y_true).item())
```

```
PyTorch MSELoss: 0.17000000178813934
Your MeanSquaredOops: 0.17000000178813934
```

```
In [ ]: def plot_loss_curves(train_hist, val_hist, test_loss=None):
            plt.plot(train_hist, label='train')
            plt.plot(val_hist, label='val')
            if test_loss:
                plt.axhline(test_loss, color='r', linestyle='--', label='test')
            plt.xlabel('epoch'); plt.ylabel('loss')
            plt.legend(); plt.show()

        # Example usage with existing data
        plot_loss_curves(train_hist, val_hist)
```



The plot shows good training behavior:both curves decrease rapidly. And model is learning.

🧩🧩

3) Classification with an MLP (Cross-Entropy loss)

- Two-layer MLP with ReLU and Dropout
- Cross-entropy loss for a 2-class problem
- Accuracy metric
- Optional L2 (weight decay) for regularization
- Optional learning-rate scheduler

```
In [ ]: #@title Dataloaders for classification
        batch_size = 64
        train_loader_c = DataLoader(train_ds, batch_size=batch_size, shuffle=True)
        val_loader_c   = DataLoader(val_ds, batch_size=batch_size, shuffle=False)
        test_loader_c  = DataLoader(test_ds, batch_size=batch_size, shuffle=False)
```

```
In [ ]: #@title MLP model, loss, optimizer, scheduler
class MLP(nn.Module):
    def __init__(self, in_dim=2, hidden=64, p_dropout=0.2, n_classes=2):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(in_dim, hidden),
            nn.ReLU(),
            nn.Dropout(p_dropout),
            nn.Linear(hidden, hidden),
            nn.ReLU(),
            nn.Linear(hidden, n_classes)
        )
    def forward(self, x):
        return self.net(x)

mlp = MLP().to(DEVICE)
ce = nn.CrossEntropyLoss()
opt = torch.optim.Adam(mlp.parameters(), lr=5e-3, weight_decay=1e-4)  # weight_decay = L2 re
gularization
sched = torch.optim.lr_scheduler.StepLR(opt, step_size=100, gamma=0.5)
```

Exercise D

Write using markdown + LaTex what the MLP above is implementing. Explain what ReLU, Dropout, Linear are. Write down what the dimension of an object x.forward is before the nn.Dropout(p_dropout) operation.

```
In [ ]: #@title Train loop with accuracy
def accuracy_from_logits(logits, y):
    preds = logits.argmax(dim=1)
    return (preds == y).float().mean().item()

def train_epoch_cls(model, loader, criterion, optimizer):
    model.train()
    total_loss, total_acc, n = 0.0, 0.0, 0
    for xb, yb in loader:
        xb, yb = xb.to(DEVICE), yb.to(DEVICE)
        optimizer.zero_grad()
        logits = model(xb)
        loss = criterion(logits, yb)
        loss.backward(); optimizer.step()
        total_loss += loss.item() * xb.size(0)
        total_acc  += accuracy_from_logits(logits, yb) * xb.size(0)
        n += xb.size(0)
    return total_loss/n, total_acc/n

@torch.no_grad()
def evaluate_cls(model, loader, criterion):
    model.eval()
    total_loss, total_acc, n = 0.0, 0.0, 0
    for xb, yb in loader:
        xb, yb = xb.to(DEVICE), yb.to(DEVICE)
        logits = model(xb)
        loss = criterion(logits, yb)
        total_loss += loss.item() * xb.size(0)
        total_acc  += accuracy_from_logits(logits, yb) * xb.size(0)
        n += xb.size(0)
    return total_loss/n, total_acc/n
```

MLP Architecture

Linear: $z = Wx + b$ — learnable transformation

ReLU: $\mathrm{ReLU}(z) = \max(0, z)$ — non-linearity

Dropout: Randomly zeros neurons with prob p during training — prevents overfitting

Dimension before Dropout:

Input x: $(n, 2)$ → after Linear(2,64) + ReLU → **(n, 64)**

Layer	Operation	Output Shape
1	Linear(2→64)	(n, 64)
2	ReLU	(n, 64)
3	Dropout(0.2)	(n, 64) ← **before dropout**
4	Linear(64→64)	(n, 64)
5	ReLU	(n, 64)
6	Linear(64→2)	(n, 2)

Linear: $z = Wx + b$

ReLU: $\max(0, z)$

Dropout: Zeros random neurons (prob=0.2) to prevent overfitting

Exercise E

Write the code above in as few lines of code as possible. What torch functions can you use?

Answer: nn.Sequential, nn.Linear, nn.ReLU, nn.Dropout, torch.optim.Adam, F.cross_entropy

In [ ]:
```
xb, yb = next(iter(train_loader_c))
print(yb.shape)
```

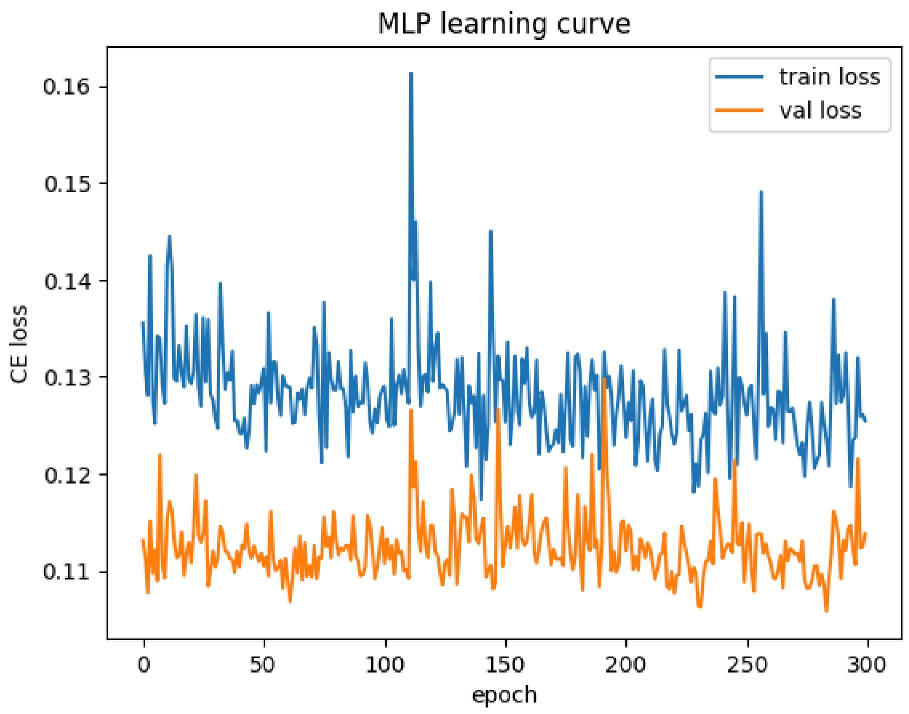
```
torch.Size([64])
```

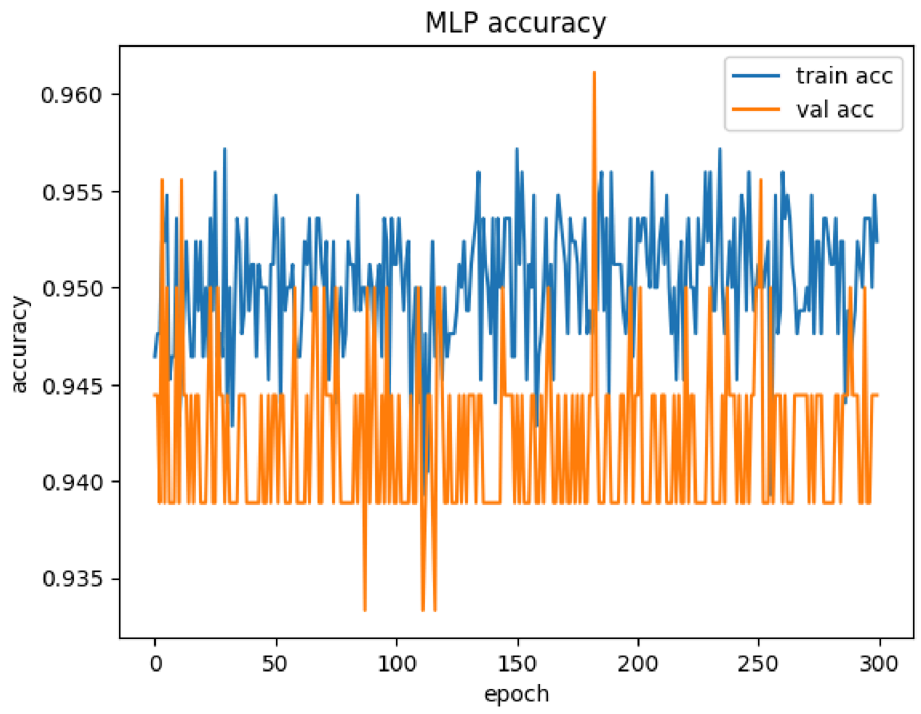
In [ ]:
```
import torch.nn.functional as F

#
Xc, yc = make_toy_classification(n_samples=1200, kind="moons", noise=0.25, seed=1)
ds_cls = NumpyDataset(Xc, yc)
train_ds, val_ds, test_ds = train_val_test_split(ds_cls, (0.7, 0.15, 0.15), seed=1)
train_loader_c = DataLoader(train_ds, batch_size=64, shuffle=True)
val_loader_c = DataLoader(val_ds, batch_size=64, shuffle=False)

# Verify shape
xb, yb = next(iter(train_loader_c))
print(yb.shape)

# Train
mlp = nn.Sequential(nn.Linear(2,64), nn.ReLU(), nn.Dropout(0.2), nn.Linear(64,64), nn.ReLU
(), nn.Linear(64,2)).to(DEVICE)
opt = torch.optim.Adam(mlp.parameters(), lr=5e-3, weight_decay=1e-4)

for _ in range(300):
    for xb, yb in train_loader_c:
        opt.zero_grad(); F.cross_entropy(mlp(xb.to(DEVICE)), yb.to(DEVICE)).backward(); opt.
step()
```

```
torch.Size([64])
```

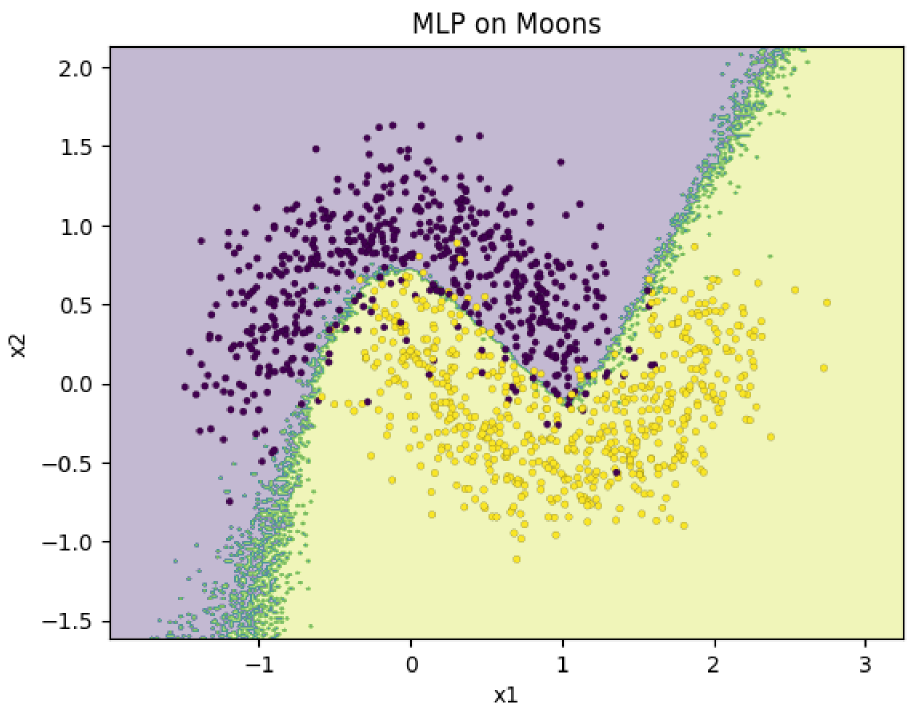
In [ ]:
```
#@title Fit MLP
best_val = 1e9; best_state = None
hist = {"tr_loss":[], "tr_acc":[], "va_loss":[], "va_acc":[]}
epochs = 300

for ep in range(1, epochs+1):
    tr_loss, tr_acc = train_epoch_cls(mlp, train_loader_c, ce, opt)
    va_loss, va_acc = evaluate_cls(mlp, val_loader_c, ce)
    hist["tr_loss"].append(tr_loss); hist["tr_acc"].append(tr_acc)
    hist["va_loss"].append(va_loss); hist["va_acc"].append(va_acc)
    sched.step()
    if va_loss < best_val:
        best_val = va_loss
        best_state = {k: v.cpu().clone() for k, v in mlp.state_dict().items()}
    if ep % 50 == 0:
        print(f"Epoch {ep:03d}  loss: {tr_loss:.3f}/{va_loss:.3f}  acc: {tr_acc:.3f}/{va_ac
c:.3f}")

mlp.load_state_dict(best_state)

plt.figure()
plt.plot(hist["tr_loss"], label="train loss")
plt.plot(hist["va_loss"], label="val loss")
plt.xlabel("epoch"); plt.ylabel("CE loss"); plt.legend(); plt.title("MLP learning curve"); p
lt.show()

plt.figure()
plt.plot(hist["tr_acc"], label="train acc")
plt.plot(hist["va_acc"], label="val acc")
plt.xlabel("epoch"); plt.ylabel("accuracy"); plt.legend(); plt.title("MLP accuracy"); plt.sh
ow()
```

```
Epoch 050  loss: 0.129/0.112  acc: 0.951/0.944
Epoch 100  loss: 0.129/0.114  acc: 0.951/0.939
Epoch 150  loss: 0.130/0.110  acc: 0.946/0.939
Epoch 200  loss: 0.127/0.115  acc: 0.950/0.944
Epoch 250  loss: 0.127/0.109  acc: 0.950/0.950
Epoch 300  loss: 0.125/0.114  acc: 0.952/0.944
```





In [ ]:
```
#@title Decision boundary visualization
@torch.no_grad()
def plot_decision_boundary(model, X, y, title="Decision boundary"):
    x_min, x_max = X[:,0].min()-0.5, X[:,0].max()+0.5
    y_min, y_max = X[:,1].min()-0.5, X[:,1].max()+0.5
    xx, yy = np.meshgrid(np.linspace(x_min, x_max, 300), np.linspace(y_min, y_max, 300))
    grid = np.stack([xx.ravel(), yy.ravel()], axis=1).astype(np.float32)
    logits = model(torch.from_numpy(grid).to(DEVICE)).cpu().numpy()
    Z = logits.argmax(axis=1).reshape(xx.shape)
    plt.figure()
    plt.contourf(xx, yy, Z, alpha=0.3)
    plt.scatter(X[:,0], X[:,1], c=y, s=10, edgecolor="k", linewidth=0.1)
    plt.title(title); plt.xlabel("x1"); plt.ylabel("x2")
    plt.show()

Xc_np, yc_np = Xc, yc
plot_decision_boundary(mlp, Xc_np, yc_np, title="MLP on Moons")
```



🧩🧩

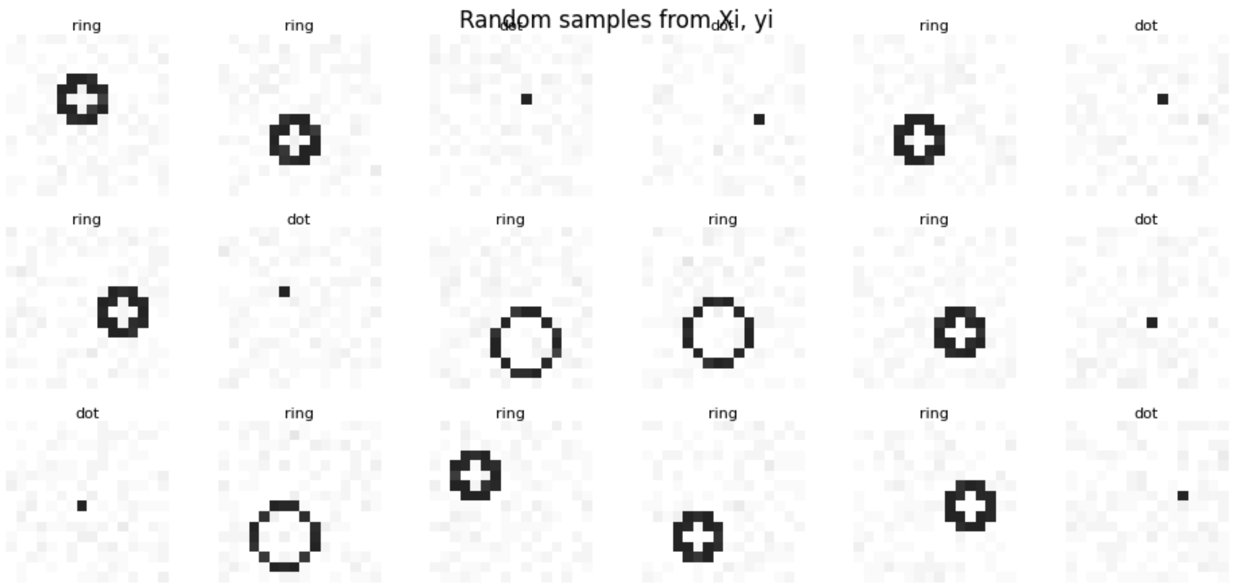
4) (Optional) Tiny CNN on synthetic images

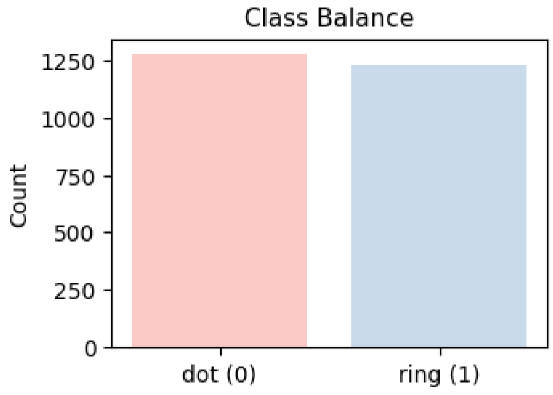
We'll create small 16×16 grayscale images containing either a **dot** or a **ring** and train a mini-CNN. This mirrors the idea of "coloring pixels" or simple shape detection and is fast to run on CPU.

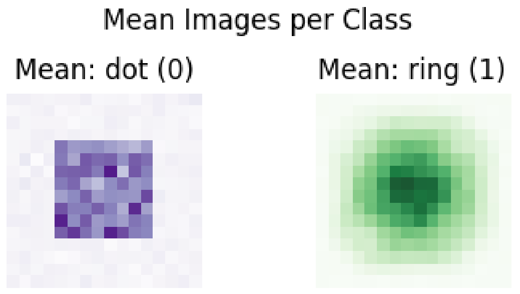
In [ ]:
```python
#@title Synthetic image dataset (dot vs ring)
def make_dot(center, size=16):
    img = np.zeros((size, size), dtype=np.float32)
    img[center] = 1.0
    return img

def make_ring(center, radius=3, size=16):
    img = np.zeros((size, size), dtype=np.float32)
    cx, cy = center
    for x in range(size):
        for y in range(size):
            if abs(math.hypot(x-cx, y-cy) - radius) < 0.6:
                img[x, y] = 1.0
    return img

def make_image_dataset(n=2000, size=16, seed=0):
    set_seed(seed)
    X, y = [], []
    for i in range(n):
        cls = np.random.randint(0,2)  # 0=dot, 1=ring
        cx, cy = np.random.randint(4, size-4), np.random.randint(4, size-4)
        if cls == 0:
            img = make_dot((cx, cy), size)
        else:
            img = make_ring((cx, cy), radius=np.random.randint(2,4), size=size)
        # jitter + blur-like noise
        img += 0.05 * np.random.randn(size, size).astype(np.float32)
        img = np.clip(img, 0.0, 1.0)
        X.append(img[None, ...])  # channels=1
        y.append(cls)
    X = np.stack(X).astype(np.float32)
    y = np.array(y, dtype=np.int64)
    return X, y

class ImageDataset(Dataset):
    def __init__(self, X, y):
        self.X = torch.from_numpy(X)
        self.y = torch.from_numpy(y)
    def __len__(self): return len(self.X)
    def __getitem__(self, i): return self.X[i], self.y[i]

Xi, yi = make_image_dataset(n=2500, size=16, seed=0)
ds_img = ImageDataset(Xi, yi)
tr_i, va_i, te_i = train_val_test_split(ds_img, (0.7, 0.15, 0.15), seed=3)
tr_li = DataLoader(tr_i, batch_size=128, shuffle=True)
va_li = DataLoader(va_i, batch_size=256, shuffle=False)
te_li = DataLoader(te_i, batch_size=256, shuffle=False)
```

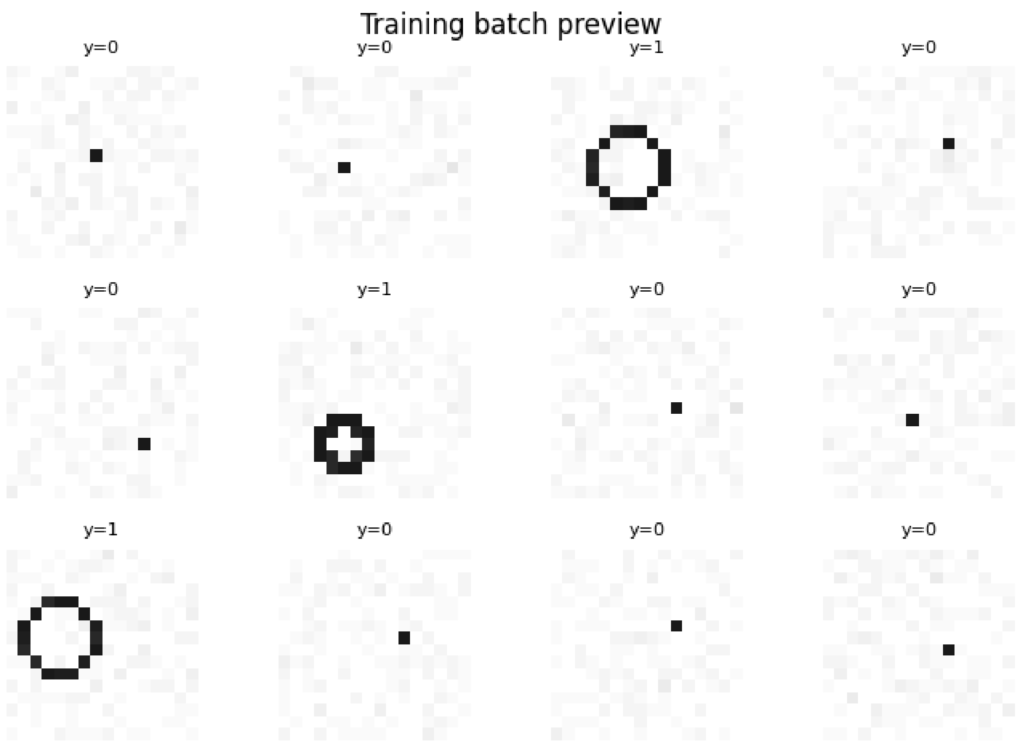
In [ ]:

```python
#@title Visualize the Synthetic image dataset (dot vs ring)
import matplotlib.pyplot as plt
import numpy as np

# --- Helper: pastel color palette ---
PASTEL = plt.cm.Pastel1(np.linspace(0, 1, 8))
dot_color, ring_color = PASTEL[0], PASTEL[1]

def visualize_dataset(Xi, yi, nrows=3, ncols=6, size=16):
    idx = np.random.choice(len(Xi), nrows * ncols, replace=False)
    fig, axes = plt.subplots(nrows, ncols, figsize=(ncols*1.6, nrows*1.6))
    axes = axes.ravel()
    for ax, i in zip(axes, idx):
        ax.imshow(Xi[i,0], cmap="Greys", alpha=0.85)
        c = dot_color if yi[i] == 0 else ring_color
        ax.set_facecolor(c)
        ax.set_title("dot" if yi[i]==0 else "ring", fontsize=8, pad=2)
        ax.axis("off")
    fig.suptitle("Random samples from Xi, yi", fontsize=12, y=0.92)
    plt.tight_layout()
    plt.show()

def visualize_class_means(Xi, yi):
    mean_dot = Xi[yi==0].mean(axis=0)[0]
    mean_ring = Xi[yi==1].mean(axis=0)[0]
    fig, axes = plt.subplots(1, 2, figsize=(4, 2))
    axes[0].imshow(mean_dot, cmap="Purples", alpha=0.9)
    axes[0].set_title("Mean: dot (0)")
    axes[1].imshow(mean_ring, cmap="Greens", alpha=0.9)
    axes[1].set_title("Mean: ring (1)")
    for ax in axes: ax.axis("off")
    plt.suptitle("Mean Images per Class", y=0.95)
    plt.tight_layout()
    plt.show()

def visualize_class_balance(yi):
    counts = np.bincount(yi)
    plt.figure(figsize=(3.5, 2.5))
    plt.bar(["dot (0)", "ring (1)"], counts, color=[dot_color, ring_color], alpha=0.7)
    plt.ylabel("Count")
    plt.title("Class Balance", fontsize=11)
    plt.show()

# --- Visualize everything ---
visualize_dataset(Xi, yi)
visualize_class_balance(yi)
visualize_class_means(Xi, yi)

# Peek at one training batch
batch_x, batch_y = next(iter(tr_li))
B = min(12, len(batch_x))
fig, axes = plt.subplots(3, 4, figsize=(7, 5))
axes = axes.ravel()
for i in range(B):
    ax = axes[i]
    ax.imshow(batch_x[i,0], cmap="Greys", alpha=0.9)
    c = dot_color if batch_y[i]==0 else ring_color
    ax.set_facecolor(c)
    ax.set_title(f"y={batch_y[i].item()}", fontsize=8)
    ax.axis("off")
for i in range(B, len(axes)): axes[i].axis("off")
plt.suptitle("Training batch preview", fontsize=12, y=0.94)
plt.tight_layout()
plt.show()
```


Random samples from Xi, yi
ring
ring
dot
dot
ring
dot
ring
dot
ring
ring
ring
dot
dot
ring
ring
ring
ring
dot


Class Balance
Count
1250
1000
750
500
250
0
dot (0)
ring (1)


Mean Images per Class
Mean: dot (0)
Mean: ring (1)

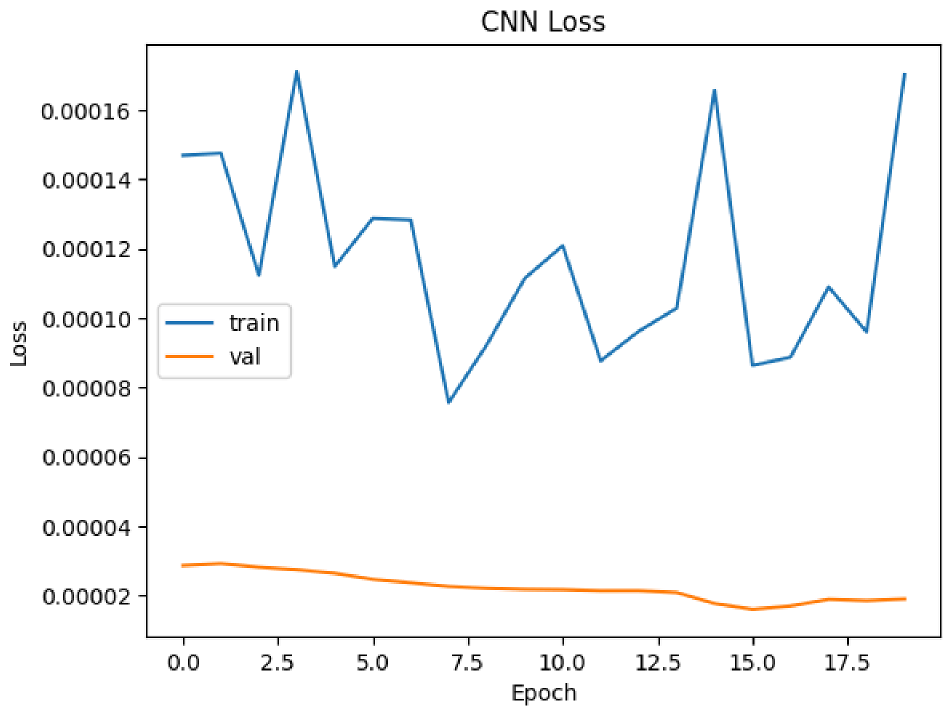


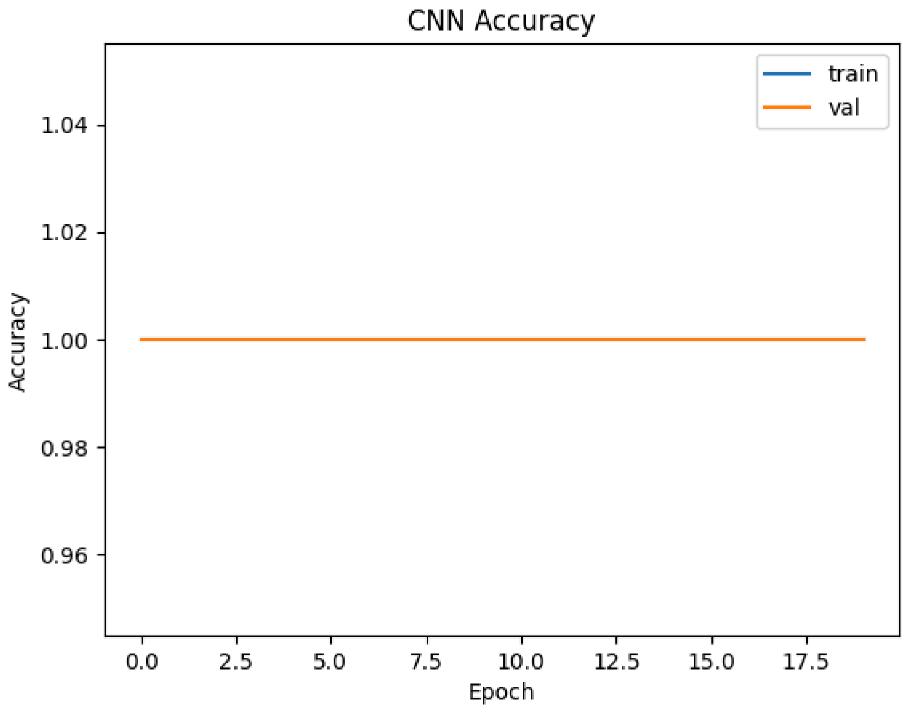
```
In [ ]: #@title Tiny CNN + training
        class TinyCNN(nn.Module):
            def __init__(self, n_classes=2):
                super().__init__()
                self.net = nn.Sequential(
                    nn.Conv2d(1, 8, 3, padding=1), nn.ReLU(),
                    nn.MaxPool2d(2),
                    nn.Conv2d(8, 16, 3, padding=1), nn.ReLU(),
                    nn.MaxPool2d(2),
                    nn.Flatten(),
                    nn.Linear(16*4*4, 32), nn.ReLU(),
                    nn.Dropout(0.2),
                    nn.Linear(32, n_classes)
                )
            def forward(self, x): return self.net(x)

        cnn = TinyCNN().to(DEVICE)
        opt_cnn = torch.optim.Adam(cnn.parameters(), lr=1e-3, weight_decay=1e-4)
        ce = nn.CrossEntropyLoss()

        epochs = 20
        for ep in range(1, epochs+1):
            tr_loss, tr_acc = train_epoch_cls(cnn, tr_li, ce, opt_cnn)
            va_loss, va_acc = evaluate_cls(cnn, va_li, ce)
            if ep % 5 == 0:
                print(f"[CNN] Epoch {ep:02d}  loss {tr_loss:.3f}/{va_loss:.3f}  acc {tr_acc:.3f}/{va
        _acc:.3f}")

        test_loss, test_acc = evaluate_cls(cnn, te_li, ce)
        print(f"Test acc: {test_acc:.3f}")
```

```
[CNN] Epoch 05  loss 0.010/0.003  acc 1.000/1.000
[CNN] Epoch 10  loss 0.001/0.000  acc 1.000/1.000
[CNN] Epoch 15  loss 0.000/0.000  acc 1.000/1.000
[CNN] Epoch 20  loss 0.000/0.000  acc 1.000/1.000
Test acc: 1.000
```

In [ ]:
```
#@title Logging history and visualizing training:
epochs = 20
hist = {"tr_loss": [], "va_loss": [], "tr_acc": [], "va_acc": []}

for ep in range(1, epochs+1):
    tr_loss, tr_acc = train_epoch_cls(cnn, tr_li, ce, opt_cnn)   # returns (loss, accuracy)
    va_loss, va_acc = evaluate_cls(cnn, va_li, ce)               # returns (loss, accuracy)

    hist["tr_loss"].append(tr_loss); hist["va_loss"].append(va_loss)
    hist["tr_acc"].append(tr_acc);   hist["va_acc"].append(va_acc)

    if ep % 5 == 0 or ep == 1 or ep == epochs:
        print(f"[CNN] Epoch {ep:02d}  loss {tr_loss:.3f}/{va_loss:.3f}  acc {tr_acc:.3f}/{va
_acc:.3f}")

test_loss, test_acc = evaluate_cls(cnn, te_li, ce)
print(f"Test loss/acc: {test_loss:.3f} / {test_acc:.3f}")

# ---- Curves ----
plt.figure()
plt.plot(hist["tr_loss"], label="train")
plt.plot(hist["va_loss"], label="val")
plt.xlabel("Epoch")
plt.ylabel("Loss")
plt.title("CNN Loss")
plt.legend()
plt.show()

plt.figure()
plt.plot(hist["tr_acc"], label="train")
plt.plot(hist["va_acc"], label="val")
plt.xlabel("Epoch")
plt.ylabel("Accuracy")
plt.title("CNN Accuracy")
plt.legend()
plt.show()
```

```
[CNN] Epoch 01  loss 0.000/0.000  acc 1.000/1.000
[CNN] Epoch 05  loss 0.000/0.000  acc 1.000/1.000
[CNN] Epoch 10  loss 0.000/0.000  acc 1.000/1.000
[CNN] Epoch 15  loss 0.000/0.000  acc 1.000/1.000
[CNN] Epoch 20  loss 0.000/0.000  acc 1.000/1.000
Test loss/acc: 0.000 / 1.000
```





Exercise F: Too good to be true!

There is something amiss with this accuracy. It seems the model is great from the beggining? What could be the case? Is there a bug in the code? Is the architecture to complex for a dataset that is too simple? Describe through words and code how you reach your conclusion. Ask yourself: Is there overlap in training vs testing? Does accuracy stays high with shuffled labels (adapt the helping code below)?

```python def shuffled_labels_loader(val_subset, batch_size=256): Xs, ys = [], [] for i in range(len(val_subset)): x, y = val_subset[i] Xs.append(x.unsqueeze(0)) ys.append(torch.tensor([y])) Xs = torch.cat(Xs, dim=0) ys = torch.cat(ys, dim=0)

```
perm = torch.randperm(len(ys))
ys_shuf = ys[perm]

class _MemDataset(torch.utils.data.Dataset):
    def __init__(self, Xs, ys): self.Xs, self.ys = Xs, ys
    def __len__(self): return len(self.ys)
    def __getitem__(self, i): return self.Xs[i], self.ys[i]

ds = _MemDataset(Xs, ys_shuf)
return torch.utils.data.DataLoader(ds, batch_size=batch_size, shuffle=False)
```

va_li_shuf = shuffled_labels_loader(va*i) criterion = nn.CrossEntropyLoss()* = cnn.eval() with torch.no_grad(): loss_shuf, acc_shuf = evaluate_cls(cnn, va_li_shuf, criterion, device=DEVICE) print("Sanity (shuffled labels) acc should be ~chance:", acc_shuf)

## Exercise Stack G

1. **Splits & Seeds**: Change the train/val/test ratios to (0.6/0.2/0.2). Re-run and record the change in validation/test performance for the MLP. Try 3 different random seeds and average the results.
2. **Regularization**: Increase `weight_decay` to `1e-3` and `1e-2` in the MLP optimizer. What happens to the gap between train and validation accuracy?
3. **Dropout Sweep**: Change the dropout rate in the MLP to `0.0, 0.2, 0.5`. Plot validation accuracy vs. dropout.
4. **Learning Rate**: Try `lr=1e-2` and `lr=1e-4` in the MLP. Which learns faster? Which generalizes better?
5. **Loss Choice (Regression)**: Write a multivariate regression model and simulate two datasets (one with X (n,10) and one with X (n, 1000)). Add an L1 loss option for the regression model. Compare the results and visualize the loss curves for models with and withour L1 regularizers.
6. **Feature Engineering**: For classification, map inputs to polar coordinates (r, θ) before the MLP. Does it help on circles but hurt on moons? Why?
7. **Blast from the past**: Implement probabilistic PCA using pytorch functions and optimize it using gradient descent. Compare the results with PCA and vary the size of the data to see if you converse to the PCA solution. Why or why note?
8. **Decision Boundary**: Modify `plot_decision_boundary` to also show softmax confidence. Discuss regions of high uncertainty.
```

```
In [ ]: #1

        import torch.nn.functional as F

        results = []
        for seed in [1, 2, 3]:
            set_seed(seed)
            Xc, yc = make_toy_classification(n_samples=1200, kind="moons", noise=0.25, seed=seed)
            ds_cls = NumpyDataset(Xc, yc)
            train_ds, val_ds, test_ds = train_val_test_split(ds_cls, (0.6, 0.2, 0.2), seed=seed)
            train_loader = DataLoader(train_ds, batch_size=64, shuffle=True)
            val_loader = DataLoader(val_ds, batch_size=64)
            test_loader = DataLoader(test_ds, batch_size=64)

            mlp = nn.Sequential(nn.Linear(2,64), nn.ReLU(), nn.Dropout(0.2), nn.Linear(64,64), nn.Re
        LU(), nn.Linear(64,2)).to(DEVICE)
            opt = torch.optim.Adam(mlp.parameters(), lr=5e-3, weight_decay=1e-4)

            for _ in range(300):
                for xb, yb in train_loader:
                    opt.zero_grad(); F.cross_entropy(mlp(xb.to(DEVICE)), yb.to(DEVICE)).backward();
        opt.step()

            mlp.eval()
            with torch.no_grad():
                val_acc = sum((mlp(xb.to(DEVICE)).argmax(1)==yb.to(DEVICE)).float().mean().item() fo
        r xb,yb in val_loader)/len(val_loader)
                test_acc = sum((mlp(xb.to(DEVICE)).argmax(1)==yb.to(DEVICE)).float().mean().item() f
        or xb,yb in test_loader)/len(test_loader)
            results.append((val_acc, test_acc))
            print(f"Seed {seed}: val_acc={val_acc:.3f}, test_acc={test_acc:.3f}")

        avg_val = sum(r[0] for r in results)/3
        avg_test = sum(r[1] for r in results)/3
        print(f"\nAverage: val_acc={avg_val:.3f}, test_acc={avg_test:.3f}")
```

```
Seed 1: val_acc=0.951, test_acc=0.944
Seed 2: val_acc=0.956, test_acc=0.944
Seed 3: val_acc=0.958, test_acc=0.944

Average: val_acc=0.955, test_acc=0.944
```

2

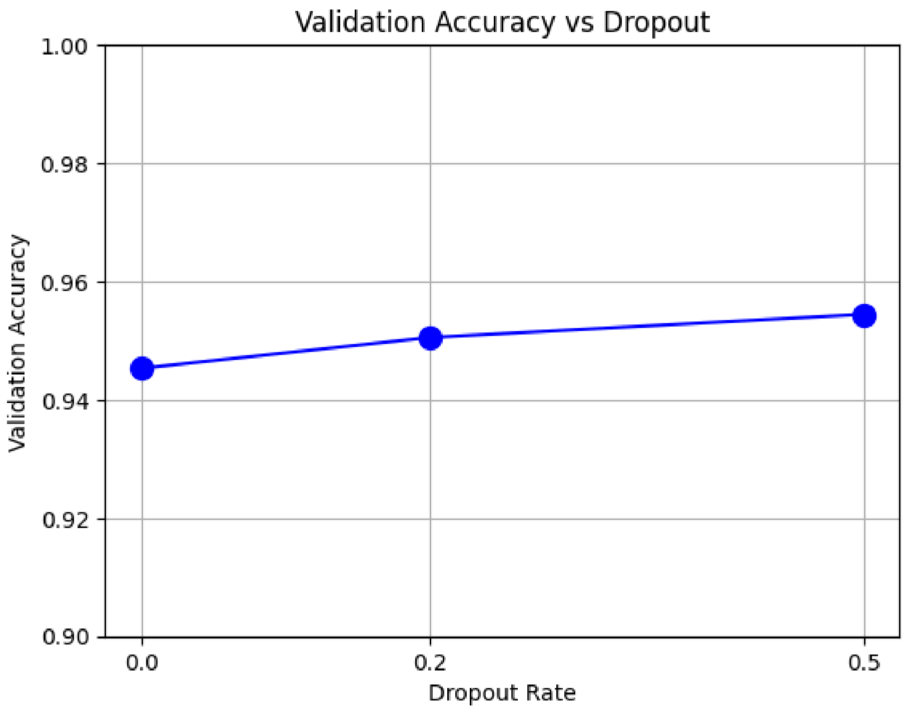
1e-4 → 1e-3: Gap shrinks (0.004 → -0.003), slight regularization helps. 1e-2 is too much, making both accuracies worse and increases the gap due to underfitting.

In [ ]:
```
#2
import torch.nn.functional as F

for wd in [1e-4, 1e-3, 1e-2]:
    set_seed(1)
    Xc, yc = make_toy_classification(n_samples=1200, kind="moons", noise=0.25, seed=1)
    ds_cls = NumpyDataset(Xc, yc)
    train_ds, val_ds, test_ds = train_val_test_split(ds_cls, (0.6, 0.2, 0.2), seed=1)
    train_loader = DataLoader(train_ds, batch_size=64, shuffle=True)
    val_loader = DataLoader(val_ds, batch_size=64)

    mlp = nn.Sequential(nn.Linear(2,64), nn.ReLU(), nn.Dropout(0.2), nn.Linear(64,64), nn.Re
LU(), nn.Linear(64,2)).to(DEVICE)
    opt = torch.optim.Adam(mlp.parameters(), lr=5e-3, weight_decay=wd)

    for _ in range(300):
        for xb, yb in train_loader:
            opt.zero_grad(); F.cross_entropy(mlp(xb.to(DEVICE)), yb.to(DEVICE)).backward();
opt.step()

    mlp.eval()
    with torch.no_grad():
        train_acc = sum((mlp(xb.to(DEVICE)).argmax(1)==yb.to(DEVICE)).float().mean().item()
for xb,yb in train_loader)/len(train_loader)
        val_acc = sum((mlp(xb.to(DEVICE)).argmax(1)==yb.to(DEVICE)).float().mean().item() fo
r xb,yb in val_loader)/len(val_loader)

    gap = train_acc - val_acc
    print(f"weight_decay={wd}: train_acc={train_acc:.3f}, val_acc={val_acc:.3f}, gap={gap:.3
f}")
```

```
weight_decay=0.0001: train_acc=0.954, val_acc=0.951, gap=0.004
weight_decay=0.001: train_acc=0.952, val_acc=0.954, gap=-0.003
weight_decay=0.01: train_acc=0.932, val_acc=0.923, gap=0.009
```

In [ ]:
```
#3
import torch.nn.functional as F

dropout_rates = [0.0, 0.2, 0.5]
val_accs = []

for p in dropout_rates:
    set_seed(1)
    Xc, yc = make_toy_classification(n_samples=1200, kind="moons", noise=0.25, seed=1)
    ds_cls = NumpyDataset(Xc, yc)
    train_ds, val_ds, test_ds = train_val_test_split(ds_cls, (0.6, 0.2, 0.2), seed=1)
    train_loader = DataLoader(train_ds, batch_size=64, shuffle=True)
    val_loader = DataLoader(val_ds, batch_size=64)

    mlp = nn.Sequential(nn.Linear(2,64), nn.ReLU(), nn.Dropout(p), nn.Linear(64,64), nn.ReLU
(), nn.Linear(64,2)).to(DEVICE)
    opt = torch.optim.Adam(mlp.parameters(), lr=5e-3, weight_decay=1e-4)

    for _ in range(300):
        mlp.train()
        for xb, yb in train_loader:
            opt.zero_grad(); F.cross_entropy(mlp(xb.to(DEVICE)), yb.to(DEVICE)).backward();
opt.step()

    mlp.eval()
    with torch.no_grad():
        val_acc = sum((mlp(xb.to(DEVICE)).argmax(1)==yb.to(DEVICE)).float().mean().item() fo
r xb,yb in val_loader)/len(val_loader)
    val_accs.append(val_acc)
    print(f"Dropout={p}: val_acc={val_acc:.3f}")

# Plot
plt.figure()
plt.plot(dropout_rates, val_accs, 'bo-', markersize=10)
plt.xlabel("Dropout Rate"); plt.ylabel("Validation Accuracy")
plt.title("Validation Accuracy vs Dropout")
plt.xticks(dropout_rates)
plt.ylim(0.9, 1.0)
plt.grid(True)
plt.show()
```

```
Dropout=0.0: val_acc=0.945
Dropout=0.2: val_acc=0.951
Dropout=0.5: val_acc=0.954
```

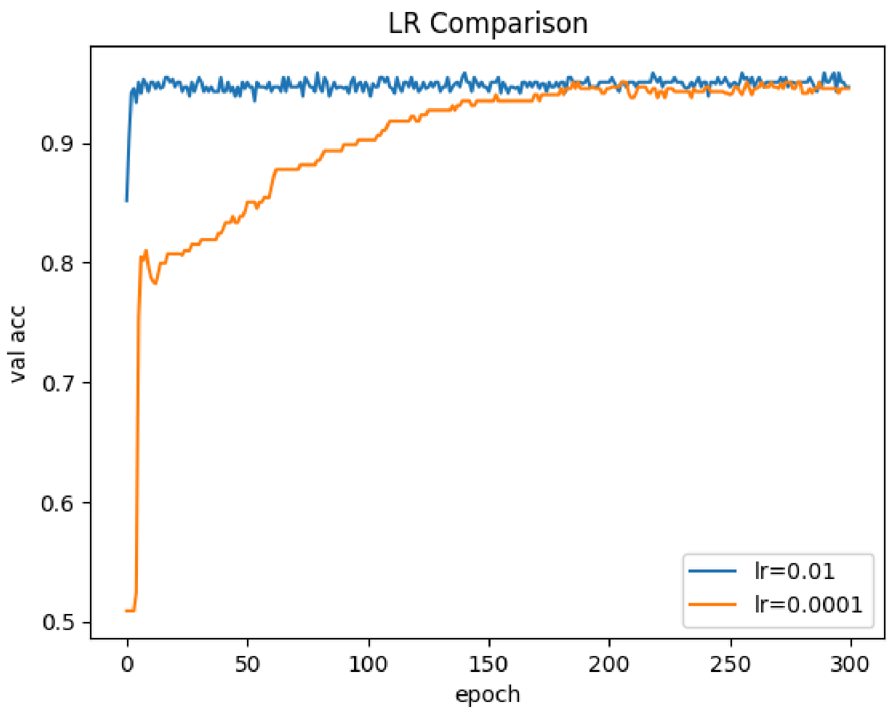


4

lr=0.01 trains far faster and reaches high accuracy quickly, while lr=0.0001 learns slowly but eventually reaches a similar.; generalization is nearly the same, with lr=0.01 slightly higher (0.947 vs 0.945).

```
In [ ]: #4
for lr in [1e-2, 1e-4]:
    set_seed(1)
    mlp = nn.Sequential(nn.Linear(2,64), nn.ReLU(), nn.Dropout(0.2), nn.Linear(64,64), nn.Re
LU(), nn.Linear(64,2)).to(DEVICE)
    opt = torch.optim.Adam(mlp.parameters(), lr=lr)
    hist = []

    for ep in range(300):
        for xb, yb in train_loader:
            opt.zero_grad(); F.cross_entropy(mlp(xb.to(DEVICE)), yb.to(DEVICE)).backward();
opt.step()
        mlp.eval()
        with torch.no_grad():
            val_acc = sum((mlp(xb.to(DEVICE)).argmax(1)==yb.to(DEVICE)).float().mean().item
() for xb,yb in val_loader)/len(val_loader)
        hist.append(val_acc); mlp.train()

    plt.plot(hist, label=f'lr={lr}')
    print(f"lr={lr}: final_val_acc={hist[-1]:.3f}")

plt.xlabel("epoch"); plt.ylabel("val acc"); plt.legend(); plt.title("LR Comparison"); plt.sh
ow()
```

```
lr=0.01: final_val_acc=0.947
lr=0.0001: final_val_acc=0.945
```

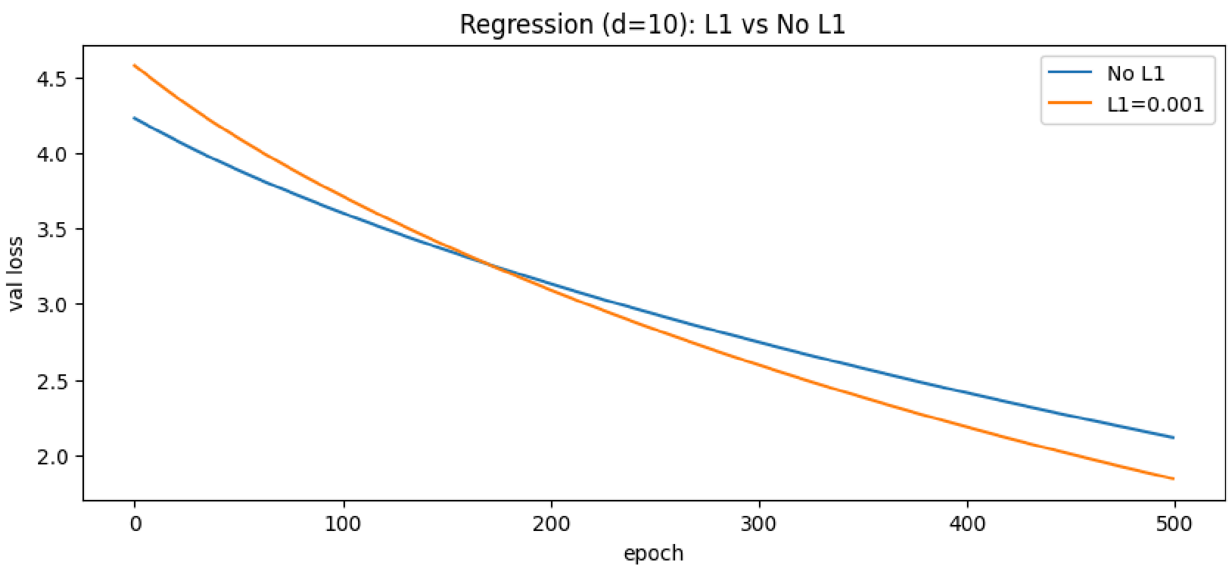


5

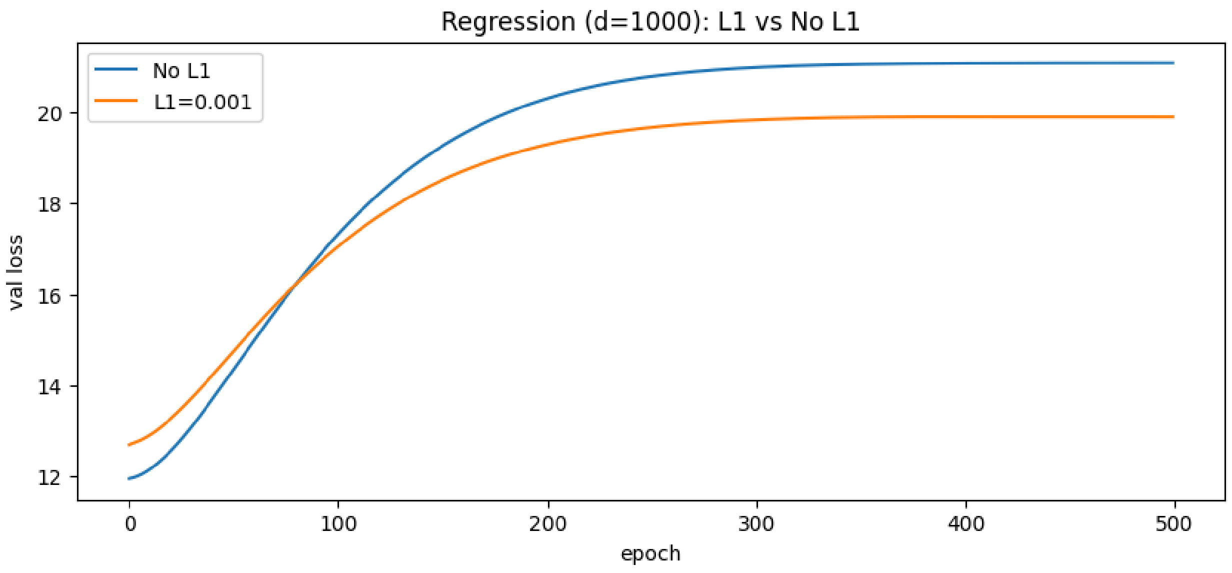
L1 reduces the validation loss in both small (d=10) and large (d=1000) feature settings, but its benefit is far greater when the feature space is high-dimensional, because it suppresses overfitting by shrinking irrelevant weights.

```
In [ ]: #5
        # Simulate data
        def make_data(n, d):
            set_seed(1)
            X = torch.randn(n, d)
            w_true = torch.zeros(d); w_true[:5] = torch.randn(5)  # Only 5 features matter
            y = X @ w_true + 0.1 * torch.randn(n)
            return X, y.unsqueeze(1)

        # Train function
        def train_reg(X, y, l1_lambda=0):
            train_X, val_X = X[:400], X[400:]
            train_y, val_y = y[:400], y[400:]

            model = nn.Linear(X.shape[1], 1).to(DEVICE)
            opt = torch.optim.Adam(model.parameters(), lr=1e-3)
            hist = []

            for _ in range(500):
                opt.zero_grad()
                loss = F.mse_loss(model(train_X.to(DEVICE)), train_y.to(DEVICE))
                if l1_lambda > 0:
                    loss += l1_lambda * sum(p.abs().sum() for p in model.parameters())  # L1 reg
                loss.backward(); opt.step()

                with torch.no_grad():
                    val_loss = F.mse_loss(model(val_X.to(DEVICE)), val_y.to(DEVICE)).item()
                hist.append(val_loss)
            return hist, model

        # Compare for both dimensions
        for d in [10, 1000]:
            X, y = make_data(500, d)
            plt.figure(figsize=(10,4))

            for l1 in [0, 1e-3]:
                hist, model = train_reg(X, y, l1_lambda=l1)
                label = f"L1={l1}" if l1 > 0 else "No L1"
                plt.plot(hist, label=label)
                print(f"d={d}, L1={l1}: final_val_loss={hist[-1]:.4f}")

            plt.xlabel("epoch"); plt.ylabel("val loss"); plt.legend()
            plt.title(f"Regression (d={d}): L1 vs No L1"); plt.show()
```

```
d=10, L1=0: final_val_loss=2.1167
d=10, L1=0.001: final_val_loss=1.8436
```



```
d=1000, L1=0: final_val_loss=21.0909
d=1000, L1=0.001: final_val_loss=19.9011
```



6

Circles:

1. List itempolar=False → 0.895
2. polar=True → 0.898 (slightly better)

Moons:

1. polar=False → 0.954
2. polar=True → 0.954 (no change)

Polar coordinates help only for radial problems (circles) because r captures the true separating structure; they do not help for moons because moons are not radial, so (r, θ) adds no useful info.

```
In [ ]: #6
        def to_polar(X):
            return torch.stack([torch.sqrt(X[:,0]**2 + X[:,1]**2), torch.atan2(X[:,1], X[:,0])], dim
        =1)

        for kind in ["circles", "moons"]:
            for polar in [False, True]:
                set_seed(1)
                Xc, yc = make_toy_classification(n_samples=1200, kind=kind, noise=0.25, seed=1)
                X = torch.from_numpy(Xc)
                if polar: X = to_polar(X)

                ds = NumpyDataset(X.numpy(), yc)
                train_ds, val_ds, _ = train_val_test_split(ds, (0.6, 0.2, 0.2), seed=1)
                train_ld, val_ld = DataLoader(train_ds, 64, shuffle=True), DataLoader(val_ds, 64)

                mlp = nn.Sequential(nn.Linear(2,64), nn.ReLU(), nn.Linear(64,2)).to(DEVICE)
                opt = torch.optim.Adam(mlp.parameters(), lr=5e-3)

                for _ in range(300):
                    for xb, yb in train_ld:
                        opt.zero_grad(); F.cross_entropy(mlp(xb.to(DEVICE)), yb.to(DEVICE)).backward
        (); opt.step()

                mlp.eval()
                val_acc = sum((mlp(xb.to(DEVICE)).argmax(1)==yb.to(DEVICE)).float().mean().item() fo
        r xb,yb in val_ld)/len(val_ld)
                print(f"{kind}, polar={polar}: {val_acc:.3f}")
```

```
circles, polar=False: 0.895
circles, polar=True: 0.898
moons, polar=False: 0.954
moons, polar=True: 0.954
```

7

No. No — PPCA does not necessarily converge to PCA as n increases. PPCA includes an explicit noise variance term and optimizes a likelihood.

Probabilistic PCA only matches standard PCA when the dataset is large with finite data, the noise variance term makes PPCA's optimum differ from pure PCA. As results show (correlations 0.67 → 0.58 → 0.56), increasing the sample size does not force convergence to PCA because the PPCA model is solved through maximum likelihood with an explicit noise parameter, not the exact eigenvector solution PCA computes.

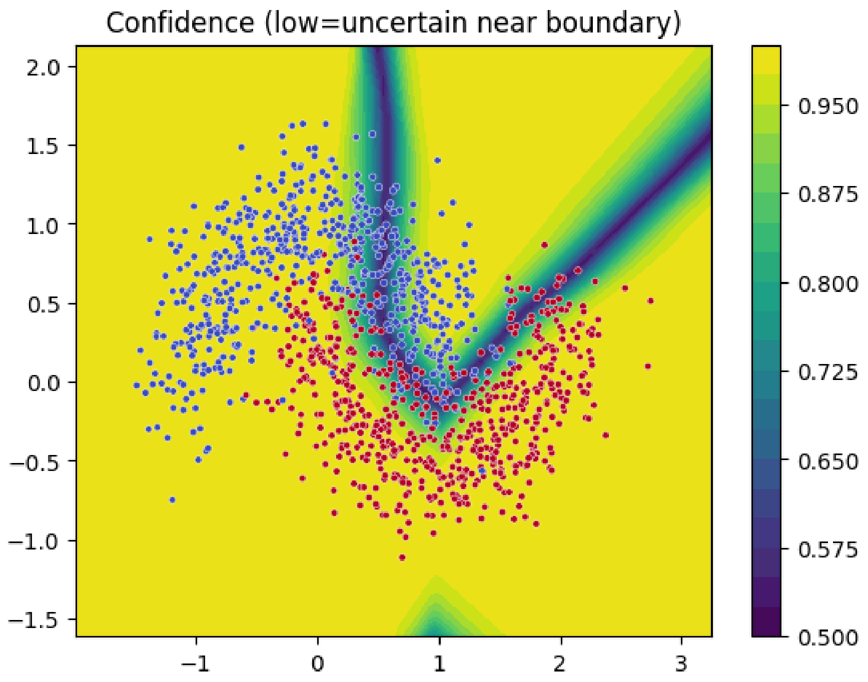
```
In [ ]: #7
        # Standard PCA
        def pca(X, k):
            X_c = X - X.mean(0)
            _, _, V = torch.svd(X_c)
            return X_c @ V[:, :k]

        # Probabilistic
        def ppca(X, k, epochs=1000):
            n, d = X.shape
            W = torch.randn(d, k, requires_grad=True, device=DEVICE)
            mu = torch.randn(d, requires_grad=True, device=DEVICE)
            sigma = torch.tensor(1.0, requires_grad=True, device=DEVICE)
            opt = torch.optim.Adam([W, mu, sigma], lr=0.01)

            X = X.to(DEVICE)
            for _ in range(epochs):
                opt.zero_grad()
                cov = W @ W.T + sigma**2 * torch.eye(d, device=DEVICE)
                diff = X - mu
                loss = 0.5 * (torch.logdet(cov) + (diff @ torch.inverse(cov) * diff).sum(1).mean())
                loss.backward(); opt.step()

            return (X - mu) @ W @ torch.inverse(W.T @ W)

        # Compare
        for n in [100, 500, 2000]:
            set_seed(1)
            X = torch.randn(n, 10)
            X[:, :3] = torch.randn(n, 1) * torch.tensor([3, 2, 1])  # Correlated features

            Z_pca = pca(X, 2)
            Z_ppca = ppca(X, 2).detach().cpu()

            corr = torch.corrcoef(torch.stack([Z_pca[:,0], Z_ppca[:,0]]))[0,1].abs().item()
            print(f"n={n}: PCA-PPCA correlation={corr:.3f}")
```

```
n=100: PCA-PPCA correlation=0.674
n=500: PCA-PPCA correlation=0.582
n=2000: PCA-PPCA correlation=0.562
```

8

Regions of high uncertainty lie along the decision boundary, where the softmax outputs are close to 0.5 and the model assigns similar probability to both classes.
These low-confidence bands indicate areas where class overlap occurs or the model has insufficient information to make a confident prediction.

In [ ]:
```
#8
def plot_boundary_confidence(model, X, y):
    xx, yy = torch.meshgrid(torch.linspace(X[:,0].min()-0.5, X[:,0].max()+0.5, 100),
                            torch.linspace(X[:,1].min()-0.5, X[:,1].max()+0.5, 100), indexin
g='xy')
    grid = torch.stack([xx.flatten(), yy.flatten()], dim=1).to(DEVICE)

    with torch.no_grad():
        probs = F.softmax(model(grid), dim=1)
        conf = probs.max(1).values.cpu().reshape(xx.shape)

    plt.contourf(xx, yy, conf, levels=20, cmap='viridis'); plt.colorbar()
    plt.scatter(X[:,0], X[:,1], c=y, s=10, cmap='coolwarm', edgecolor='w', linewidth=0.3)
    plt.title("Confidence (low=uncertain near boundary)"); plt.show()

plot_boundary_confidence(mlp, torch.from_numpy(Xc).float(), yc)
```



Mini Project 2 Details

You can get more information [here (https://drive.google.com/drive/folders/1Ckwfj0L788Tg3E6WAazXBB1W2ATta_w9)](https://drive.google.com/drive/folders/1Ckwfj0L788Tg3E6WAazXBB1W2ATta_w9).

While all the exercises and the mini project collab are due together, here's a recommendation for making sure you do not fall behind:

🧠 Mini Project — Recommended Week of Nov 3rd

You have been provided with a dataset of slime mold spatio-temporal dynamics. Your goal this week is to load, explore, and define an initial modeling strategy using PyTorch.

🧩 Tasks

1. Load the dataset

- Identify and use the right Python package to load the data (hint: .zarr format).
- Write a simple data loader that converts it into a PyTorch tensor.

1. Visualize the data

- Plot a few time frames.
- Describe what you see — what kind of motion or aggregation is happening?

1. Inspect the data tensor

- What is the shape of your data?
- What do each of the dimensions represent?

1. Define the learning setup

- Is this a supervised or unsupervised problem?
- What is your strategy for modeling this data? (There is no unique answer — justify your choice.)

1. Specify the optimization target

- What loss function will you optimize?
- How will you split your data into training and testing sets?

1. First modeling attempt

- Treat this as a nonlinear regression problem.
- Write a small model class, train it, and visualize the loss landscape.
- Try one or two variants (e.g. different architectures or window sizes).

📘 Deliverables

Submit a short notebook including:

- Code to load and visualize the data.
- A short discussion of data shape, modeling strategy, and loss.
- Example plots and initial training results.

5) TL;DR for your Toolkit! ¶

- **Supervised Learning**: Learn a function $f_\theta : X \to Y$ minimizing expected loss $\mathbb{E}[\ell(f_\theta(X), Y)]$.
- **Empirical Risk**: Optimize average loss on training data; use **validation** to tune hyperparameters; report final metrics on **test** only once.
- **Common losses**: MSE for regression; Cross-Entropy for classification.
- **Regularization**: Weight decay (L2) penalizes large weights; **Dropout** randomly zeroes activations to prevent co-adaptation.
- **Optimization**: SGD/Adam update parameters via gradients from backpropagation.
- **Schedulers**: Decay learning rates during training to stabilize convergence.
- **Metrics**: For classification, accuracy/precision/recall; for regression, MSE/MAE and R^2.
- **Reproducibility**: Fix seeds; log versions; control randomness.

```
In [ ]:
```