NNDL_Project_Notebook_Live_Submit

December 16, 2025

1 SECTION 1: Setup & Imports

[ ]:
```
from google.colab import drive
drive.mount('/content/drive')

!nvidia-smi  # just to sanity-check the GPU

!pip install wandb -q
import wandb

USE_WANDB = True
WANDB_ENTITY = "nndl-project-F25"
WANDB_PROJECT = "Multihead-Classification-Competition"

if USE_WANDB:
  wandb.login()


from datetime import datetime
import os, zipfile, random

import numpy as np
import pandas as pd
from PIL import Image

import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim

from torch.utils.data import Dataset, DataLoader, random_split
from torchvision import transforms, models

import matplotlib.pyplot as plt

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print("Using device:", device)
```

```python
# wandb run-naming schema
def make_run_name(base: str) -> str:
    """Create a unique run name with timestamp."""
    return f"{base}_{datetime.now().strftime('%Y%m%d_%H%M%S')}"

# optional: for approximate reproducibility
def set_seed(seed=42):
    random.seed(seed)
    np.random.seed(seed)
    torch.manual_seed(seed)
    torch.cuda.manual_seed_all(seed)

set_seed(42)
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call
drive.mount("/content/drive", force_remount=True).
Sun Dec 14 18:21:33 2025
+---------------------------------------------------------------------------------
----------+
| NVIDIA-SMI 550.54.15              Driver Version: 550.54.15      CUDA Version:
12.4     |
|-----------------------------------------+------------------------+------------
----------+
| GPU  Name                 Persistence-M | Bus-Id          Disp.A | Volatile
Uncorr. ECC |
| Fan  Temp   Perf          Pwr:Usage/Cap |           Memory-Usage | GPU-Util
Compute M. |
|                                         |                        |
MIG M. |
|=========================================+========================+============
==========|
|   0  NVIDIA A100-SXM4-80GB          Off |   00000000:00:05.0 Off |
0 |
| N/A   32C    P0             52W /  400W |       0MiB /  81920MiB |      0%
Default |
|                                         |                        |
Disabled |
+-----------------------------------------+------------------------+------------
----------+

+---------------------------------------------------------------------------------
----------+
| Processes:
|
|  GPU   GI   CI        PID   Type   Process name
GPU Memory |
```

```
|        ID   ID
Usage      |
|===============================================================================
==========|
|  No running processes found
|
+-------------------------------------------------------------------------------
----------+
```

wandb: Currently logged in as: akseldkw
(akseldkw07) to https://api.wandb.ai. Use `wandb login

--relogin` to force relogin

Using device: cuda

2 SECTION 2: Config & Paths

[ ]:
```
DATA_ROOT = "/content/drive/MyDrive/NNDL-Project/Project Data"

# Local scratch space on the VM / Colab
LOCAL_DATA_ROOT = "/content/local_data"
os.makedirs(LOCAL_DATA_ROOT, exist_ok=True)

train_zip_path = os.path.join(DATA_ROOT, "train_images.zip")
test_zip_path  = os.path.join(DATA_ROOT, "test_images.zip")

# Unzip to LOCAL_DATA_ROOT instead of Drive
train_out_dir = os.path.join(LOCAL_DATA_ROOT, "train_images")
test_out_dir  = os.path.join(LOCAL_DATA_ROOT, "test_images")

if not os.path.exists(train_out_dir):
    os.makedirs(train_out_dir, exist_ok=True)
    with zipfile.ZipFile(train_zip_path, 'r') as z:
        z.extractall(train_out_dir)

if not os.path.exists(test_out_dir):
    os.makedirs(test_out_dir, exist_ok=True)
    with zipfile.ZipFile(test_zip_path, 'r') as z:
        z.extractall(test_out_dir)

TRAIN_IMG_DIR = os.path.join(train_out_dir, "train_images")
TEST_IMG_DIR  = os.path.join(test_out_dir, "test_images")

TRAIN_CSV = os.path.join(DATA_ROOT, "train_data.csv")
SUPER_CSV = os.path.join(DATA_ROOT, "superclass_mapping.csv")
SUB_CSV   = os.path.join(DATA_ROOT, "subclass_mapping.csv")
```

```
BATCH_SIZE = 64
NUM_WORKERS = 2  # can set to 0 if we hit dataloader issues

VAL_SPLIT = 0.1  # 10% validation
IMG_SIZE = 64   # our image dimensions

PROJECT_NAME = "coms4776-transfer-learning" # TBD update
APPROACH = "two_models" # "two_heads" or "two_models"
DATA_AUGMENT = True

# Indices for "novel" classes (per provided data)
NOVEL_SUPER_IDX = 3     # superclass index for novel
NOVEL_SUB_IDX = 87      # subclass index for novel

# Number of times run full-batch
EPOCHS = 15

# Learning rates
LR = 1e-4  # overall learning rate
LR_HEAD = 1e-2 # head learning rate, used when freezing backbone
WEIGHT_DECAY = 1e-4 # seems standard
BACKBONE = "resnet50" # "resnet18" or "resnet50"

# Novel-super CIFAR integration (more images)
# Options: "none", "small" (~1000 samples), "large" (~5000 samples)
CIFAR_NOVEL_MODE = "large"    # "large" or "small" or "none"

# Path to store metadata about CIFAR novel images
CIFAR_NOVEL_CSV_PATH = os.path.join(LOCAL_DATA_ROOT, "cifar_novel_data.csv")

# Fine-tuning mode for ResNet backbone
# "full"   = train all layers (what you're currently doing)
# "frozen" = freeze backbone, train only the heads on top
FINE_TUNE_MODE = "full"    # or "frozen"

# Initial novelty thresholds (starting points, will tune further)
TAU_SUPER = 0.99        # NOTE: per calibration with validation data. if max superclass prob < TAU_SUPER -> predict novel superclass
TAU_SUB = 0.85          # NOTE: per calibration with validation data. if max subclass prob < TAU_SUB  -> predict novel subclass

########### MAKE SURE USE_PSEDUO_NOVEL IS FALSE BEFORE LEADERBOARD SUBMISSION ##################################################
USE_PSEUDO_NOVEL = True # to validate on held-out subclasses from training. Used to fine-tune TAU_SUB
PSEUDO_NOVEL_FRACTION = 0.15
PSEUDO_NOVEL_SEED = 123
```

[ ]:
```
# Build CIFAR-100 novel-super dataset (excluding reptiles)
from torchvision.datasets import CIFAR100

# Download CIFAR100 once (raw PIL images)
CIFAR_ROOT = os.path.join(LOCAL_DATA_ROOT, "cifar100_raw")
os.makedirs(CIFAR_ROOT, exist_ok=True)

# Only do the heavy image-copying if CSV doesn't exist
if CIFAR_NOVEL_MODE != "none" and not os.path.exists(CIFAR_NOVEL_CSV_PATH):
    print("Building CIFAR novel-super dataset (this happens once)...")

    cifar_train = CIFAR100(root=CIFAR_ROOT, train=True, download=True,␣
↪transform=None)

    # CIFAR-100 fine label names (with underscores)
    cifar_fine_names = cifar_train.classes  # e.g. "apple", "beaver",␣
↪"aquarium_fish", ...

    # Fine classes we want, based on your list, excluding reptiles
    # (these names match CIFAR-100 fine label names)
    allowed_fine_names = set([
        # aquatic mammals
        "beaver", "dolphin", "otter", "seal", "whale",
        # fish
        "aquarium_fish", "flatfish", "ray", "shark", "trout",
        # flowers
        "orchid", "poppy", "rose", "sunflower", "tulip",
        # food containers
        "bottle", "bowl", "can", "cup", "plate",
        # fruit and vegetables
        "apple", "mushroom", "orange", "pear", "sweet_pepper",
        # household electrical devices
        "clock", "keyboard", "lamp", "telephone", "television",
        # household furniture
        "bed", "chair", "couch", "table", "wardrobe",
        # insects
        "bee", "beetle", "butterfly", "caterpillar", "cockroach",
        # large carnivores
        "bear", "leopard", "lion", "tiger", "wolf",
        # large man-made outdoor things
        "bridge", "castle", "house", "road", "skyscraper",
        # large natural outdoor scenes
        "cloud", "forest", "mountain", "plain", "sea",
        # large omnivores and herbivores
        "camel", "cattle", "chimpanzee", "elephant", "kangaroo",
        # medium-sized mammals
        "fox", "porcupine", "possum", "raccoon", "skunk",
```

```
        # non-insect invertebrates
        "crab", "lobster", "snail", "spider", "worm",
        # people
        "baby", "boy", "girl", "man", "woman",
        # small mammals
        "hamster", "mouse", "rabbit", "shrew", "squirrel",
        # trees
        "maple", "oak", "palm", "pine", "willow",
        # vehicles 1
        "bicycle", "bus", "motorcycle", "pickup_truck", "train",
        # vehicles 2
        "lawn_mower", "rocket", "streetcar", "tank", "tractor",
        # NOTE: reptiles group ("crocodile", "dinosaur", "lizard", "snake",␣
↪"turtle") is *excluded* on purpose
    ])

    # Map class_name -> list of indices for that fine class
    name_to_indices = {name: [] for name in allowed_fine_names}
    for idx in range(len(cifar_train)):
        _, fine_label = cifar_train[idx]  # fine_label is int index into␣
↪cifar_fine_names
        fine_name = cifar_fine_names[fine_label]
        if fine_name in allowed_fine_names:
            name_to_indices[fine_name].append(idx)

    # Flatten candidate indices across all allowed classes
    candidate_indices = []
    for name, idx_list in name_to_indices.items():
        candidate_indices.extend(idx_list)

    print("Total candidate CIFAR images (allowed classes, excl. reptiles):",␣
↪len(candidate_indices))

    # Target total novel-super samples (max 5000, as you requested)
    TARGET_TOTAL = 5000
    random.seed(42)
    random.shuffle(candidate_indices)
    selected_indices = candidate_indices[:TARGET_TOTAL]

    print("Selected indices:", len(selected_indices))

    # Copy images into TRAIN_IMG_DIR and build CSV rows
    cifar_aug_records = []

    for idx in selected_indices:
        img, fine_label = cifar_train[idx]
        fine_name = cifar_fine_names[fine_label]
```

```
        # Unique filename to avoid collisions
        fname = f"cifar_novel_{idx}_{fine_name}.png"
        dst_path = os.path.join(TRAIN_IMG_DIR, fname)

        # img is PIL.Image when transform=None
        img.save(dst_path)

        record = {
            "image": fname,
            "superclass_index": NOVEL_SUPER_IDX,  # novel superclass
            "subclass_index": NOVEL_SUB_IDX,      # novel subclass
            "description": f"CIFAR100:{fine_name} (novel superclass)",
        }
        cifar_aug_records.append(record)

    cifar_aug_df = pd.DataFrame(cifar_aug_records)
    cifar_aug_df.to_csv(CIFAR_NOVEL_CSV_PATH, index=False)
    print("Saved CIFAR novel-super metadata to:", CIFAR_NOVEL_CSV_PATH)
    print("Images copied into TRAIN_IMG_DIR:", TRAIN_IMG_DIR)

elif CIFAR_NOVEL_MODE != "none":
    print("CIFAR novel-super CSV already exists at:", CIFAR_NOVEL_CSV_PATH)
else:
    print("CIFAR_NOVEL_MODE='none'; skipping CIFAR novel-super creation.")
```

```
CIFAR novel-super CSV already exists at:
/content/local_data/cifar_novel_data.csv
```

3 SECTION 3: Data Loading & DataLoaders

[ ]:
```
# SECTION 3: Data Loading & Dataloaders

# Base training data from class
base_train_df = pd.read_csv(TRAIN_CSV)

super_map_df = pd.read_csv(SUPER_CSV)   # columns: index, class
sub_map_df   = pd.read_csv(SUB_CSV)     # columns: index, class

num_super = len(super_map_df)
num_sub   = len(sub_map_df)

print("Num superclasses:", num_super)
print("Num subclasses:", num_sub)

# --- Integrate CIFAR novel-super examples, if enabled ---
```

```
if CIFAR_NOVEL_MODE == "none":
    train_df = base_train_df.copy()
    print("CIFAR_NOVEL_MODE='none' → using only original training data.")
else:
    if not os.path.exists(CIFAR_NOVEL_CSV_PATH):
        raise FileNotFoundError(
            f"CIFAR_NOVEL_MODE={CIFAR_NOVEL_MODE} but {CIFAR_NOVEL_CSV_PATH}␣
↪not found. "
            "Run the CIFAR novel-super build section first."
        )

    cifar_aug_df = pd.read_csv(CIFAR_NOVEL_CSV_PATH)

    if CIFAR_NOVEL_MODE == "small":
        # Use ~1000 CIFAR novel-super images
        n_small = min(1000, len(cifar_aug_df))
        cifar_aug_df = cifar_aug_df.sample(n=n_small, random_state=42).
↪reset_index(drop=True)
        print(f"CIFAR_NOVEL_MODE='small' → using {len(cifar_aug_df)} CIFAR␣
↪novel-super samples.")
    elif CIFAR_NOVEL_MODE == "large":
        # Use all available (up to 5000 created earlier)
        print(f"CIFAR_NOVEL_MODE='large' → using {len(cifar_aug_df)} CIFAR␣
↪novel-super samples.")
    else:
        raise ValueError(f"Unknown CIFAR_NOVEL_MODE: {CIFAR_NOVEL_MODE}")

    # Combine original training data with CIFAR novel-super rows
    train_df = pd.concat([base_train_df, cifar_aug_df], ignore_index=True)
    print("Combined train_df size (original + CIFAR):", len(train_df))
    print("  Novel-super count (superclass_index == NOVEL_SUPER_IDX):",
          (train_df["superclass_index"] == NOVEL_SUPER_IDX).sum())

# --- Build subclass -> superclass mapping from *combined* train_df ---
# This still satisfies "each subclass has a single superclass":
#  - Original subclasses 0..86
#  - Novel subclass 87 always maps to NOVEL_SUPER_IDX
sub_to_super = (
    train_df.groupby("subclass_index")["superclass_index"]
            .agg(lambda x: x.value_counts().index[0])
            .to_dict()
)

print("Example sub_to_super mapping (first 10):",
      dict(list(sub_to_super.items())[:10]))
```

```
Num superclasses: 4
```

```
Num subclasses: 88
CIFAR_NOVEL_MODE='large' → using 5000 CIFAR novel-super samples.
Combined train_df size (original + CIFAR): 11288
  Novel-super count (superclass_index == NOVEL_SUPER_IDX): 5000
Example sub_to_super mapping (first 10): {0: 1, 1: 2, 2: 1, 3: 2, 4: 0, 5: 0, 6:
0, 7: 1, 8: 0, 9: 1}
```

[ ]:
```python
# Dataset functions
class BirdDogReptileDataset(Dataset):
    def __init__(self, df, img_dir, transform=None):
        self.df = df.reset_index(drop=True)
        self.img_dir = img_dir
        self.transform = transform

    def __len__(self):
        return len(self.df)

    def __getitem__(self, idx):
        row = self.df.iloc[idx]
        img_name = row["image"]
        img_path = os.path.join(self.img_dir, img_name)

        image = Image.open(img_path).convert("RGB")
        if self.transform:
            image = self.transform(image)

        super_idx = int(row["superclass_index"])
        sub_idx = int(row["subclass_index"])
        return image, super_idx, sub_idx
```

[ ]:
```python
# Test dataset (for leaderboard predictions)

class BirdDogReptileTestDataset(Dataset):
    def __init__(self, img_dir, transform=None):
        self.img_dir = img_dir
        self.transform = transform
        # assumes images are named 0.jpg, 1.jpg, ..., N-1.jpg
        self.filenames = sorted(os.listdir(img_dir), key=lambda x: int(os.path.
 ↪splitext(x)[0]))

    def __len__(self):
        return len(self.filenames)

    def __getitem__(self, idx):
        img_name = self.filenames[idx]
        img_path = os.path.join(self.img_dir, img_name)
```

```
        image = Image.open(img_path).convert("RGB")
        if self.transform:
            image = self.transform(image)

        return image, img_name
```

[ ]:
```
# Transforms

if DATA_AUGMENT:
    train_transform = transforms.Compose([
        transforms.Resize((IMG_SIZE, IMG_SIZE)),
        transforms.RandomHorizontalFlip(),
        transforms.RandomRotation(10),
        transforms.ToTensor(),
        transforms.Normalize(mean=[0.485, 0.456, 0.406],
                             std=[0.229, 0.224, 0.225]),
    ])
else:
    train_transform = transforms.Compose([
        transforms.Resize((IMG_SIZE, IMG_SIZE)),
        transforms.ToTensor(),
        transforms.Normalize(mean=[0.485, 0.456, 0.406],
                             std=[0.229, 0.224, 0.225]),
    ])

val_test_transform = transforms.Compose([
    transforms.Resize((IMG_SIZE, IMG_SIZE)),
    transforms.ToTensor(),
    transforms.Normalize(mean=[0.485, 0.456, 0.406],
                         std=[0.229, 0.224, 0.225]),
])
```

[ ]:
```
# Train/val split + loaders with optional pseudo-novel validation,
# ensuring novel-super examples (super == NOVEL_SUPER_IDX) appear in both train␣
↪and val.

from math import ceil

pseudo_novel_loader = None      # default; will be set if USE_PSEUDO_NOVEL
heldout_subclasses = None       # to inspect later if needed

def split_seen_vs_novel_super(df, val_split, novel_super_idx, rng_seed=42):
    """
    Split dataframe into train/val, ensuring that both seen-super (0/1/2)
    and novel-super (== novel_super_idx) appear in both splits if present.
    """
    rng = np.random.default_rng(rng_seed)
```

```
    df_novel_super = df[df["superclass_index"] == novel_super_idx]
    df_seen_super  = df[df["superclass_index"] != novel_super_idx]

    print("  Seen-super samples:", len(df_seen_super))
    print("  Novel-super samples:", len(df_novel_super))

    # Split seen-super part
    if len(df_seen_super) > 0:
        val_seen_size = int(len(df_seen_super) * val_split)
        val_seen_indices = rng.choice(len(df_seen_super), size=val_seen_size,␣
↪replace=False)
        val_seen_df = df_seen_super.iloc[val_seen_indices]
        train_seen_df = df_seen_super.drop(val_seen_df.index)
    else:
        val_seen_df = df_seen_super.iloc[0:0]
        train_seen_df = df_seen_super.iloc[0:0]

    # Split novel-super part (if any)
    if len(df_novel_super) > 0:
        val_novel_size = max(1, int(len(df_novel_super) * val_split))
        val_novel_indices = rng.choice(len(df_novel_super),␣
↪size=val_novel_size, replace=False)
        val_novel_df = df_novel_super.iloc[val_novel_indices]
        train_novel_df = df_novel_super.drop(val_novel_df.index)
    else:
        val_novel_df = df_novel_super.iloc[0:0]
        train_novel_df = df_novel_super.iloc[0:0]

    # Combine splits and shuffle
    train_split_df = pd.concat([train_seen_df, train_novel_df],␣
↪ignore_index=True)
    val_split_df   = pd.concat([val_seen_df,   val_novel_df],   ␣
↪ignore_index=True)

    train_split_df = train_split_df.sample(frac=1.0, random_state=rng_seed).
↪reset_index(drop=True)
    val_split_df   = val_split_df.sample(frac=1.0,   random_state=rng_seed + 1).
↪reset_index(drop=True)

    print("  Final split sizes:")
    print("    train:", len(train_split_df))
    print("    val:  ", len(val_split_df))
    print("    train novel-super:",
          (train_split_df["superclass_index"] == novel_super_idx).sum())
    print("    val novel-super:  ",
```

```
        (val_split_df["superclass_index"] == novel_super_idx).sum())

    return train_split_df, val_split_df


if not USE_PSEUDO_NOVEL:
    # -------------------------
    # Simple split, but novel-super-aware
    # -------------------------
    print("[Simple split, novel-super aware]")

    train_split_df, val_split_df = split_seen_vs_novel_super(
        train_df,
        VAL_SPLIT,
        NOVEL_SUPER_IDX,
        rng_seed=42,
    )

    train_dataset = BirdDogReptileDataset(
        train_split_df,
        TRAIN_IMG_DIR,
        transform=train_transform,
    )
    val_dataset = BirdDogReptileDataset(
        val_split_df,
        TRAIN_IMG_DIR,
        transform=val_test_transform,
    )

    train_loader = DataLoader(
        train_dataset,
        batch_size=BATCH_SIZE,
        shuffle=True,
        num_workers=NUM_WORKERS,
        pin_memory=True,
    )
    val_loader = DataLoader(
        val_dataset,
        batch_size=BATCH_SIZE,
        shuffle=False,
        num_workers=NUM_WORKERS,
        pin_memory=True,
    )

    print(f"[Simple split] Train size: {len(train_dataset)}, Val size:␣
 ↪{len(val_dataset)}")
```

```
else:
    # -------------------------
    # Pseudo-novel setup: hold out some subclasses entirely for pseudo-novel␣
↪validation
    # while still keeping novel-super in both train and val.
    # -------------------------

    print("[Pseudo-novel subclass split + novel-super-aware train/val]")

    # 1) choose subset of subclasses to treat as pseudo-novel
    all_subclasses = sorted(train_df["subclass_index"].unique())
    # Do NOT hold out the novel subclass itself (87)
    all_subclasses_no_novel = [c for c in all_subclasses if c != NOVEL_SUB_IDX]

    rng = np.random.default_rng(PSEUDO_NOVEL_SEED)

    num_holdout = max(1, int(len(all_subclasses_no_novel) *␣
↪PSEUDO_NOVEL_FRACTION))
    heldout_subclasses = set(
        rng.choice(all_subclasses_no_novel, size=num_holdout, replace=False).
↪tolist()
    )
    seen_subclasses = [c for c in all_subclasses if c not in heldout_subclasses]

    print(f"[Pseudo-novel] Total subclasses (excl. novel):␣
↪{len(all_subclasses_no_novel)}")
    print(f"[Pseudo-novel] Held-out subclasses (pseudo-novel):␣
↪{sorted(heldout_subclasses)}")
    print(f"[Pseudo-novel] Seen subclasses (incl. novel-sub):␣
↪{len(seen_subclasses)}")

    # 2) split dataframe into seen vs pseudo-novel (by subclass)
    seen_mask = ~train_df["subclass_index"].isin(heldout_subclasses)
    seen_df = train_df[seen_mask].reset_index(drop=True)
    pseudo_novel_df = train_df[~seen_mask].reset_index(drop=True)

    print(f"[Pseudo-novel] Seen samples: {len(seen_df)}, Pseudo-novel samples:␣
↪{len(pseudo_novel_df)}")

    # 3) Train/val split on seen data, but ensure novel-super in both
    train_split_df, val_split_df = split_seen_vs_novel_super(
        seen_df,
        VAL_SPLIT,
        NOVEL_SUPER_IDX,
        rng_seed=PSEUDO_NOVEL_SEED,
    )
```

```python
    train_dataset = BirdDogReptileDataset(
        train_split_df,
        TRAIN_IMG_DIR,
        transform=train_transform,
    )
    val_seen_dataset = BirdDogReptileDataset(
        val_split_df,
        TRAIN_IMG_DIR,
        transform=val_test_transform,
    )

    train_loader = DataLoader(
        train_dataset,
        batch_size=BATCH_SIZE,
        shuffle=True,
        num_workers=NUM_WORKERS,
        pin_memory=True,
    )
    val_loader = DataLoader(
        val_seen_dataset,
        batch_size=BATCH_SIZE,
        shuffle=False,
        num_workers=NUM_WORKERS,
        pin_memory=True,
    )

    # 4) pseudo-novel validation loader (all held-out subclasses, val-style␣
↪transform)
    pseudo_novel_dataset = BirdDogReptileDataset(
        pseudo_novel_df,
        TRAIN_IMG_DIR,
        transform=val_test_transform,
    )
    pseudo_novel_loader = DataLoader(
        pseudo_novel_dataset,
        batch_size=BATCH_SIZE,
        shuffle=False,
        num_workers=NUM_WORKERS,
        pin_memory=True,
    )

    print(f"[Pseudo-novel] Train size: {len(train_dataset)}, "
          f"Seen-val size: {len(val_seen_dataset)}, "
          f"Pseudo-novel val size: {len(pseudo_novel_dataset)}")

# Test loader is the same regardless
```

```
test_dataset = BirdDogReptileTestDataset(TEST_IMG_DIR,␣
↪transform=val_test_transform)
test_loader = DataLoader(test_dataset, batch_size=64,
                         shuffle=False, num_workers=NUM_WORKERS)
# change batch size back to 1 if see any errors

print(f"Test size: {len(test_dataset)}")
```

```
[Pseudo-novel subclass split + novel-super-aware train/val]
[Pseudo-novel] Total subclasses (excl. novel): 87
[Pseudo-novel] Held-out subclasses (pseudo-novel): [1, 4, 14, 15, 17, 20, 27,
29, 39, 45, 51, 69, 71]
[Pseudo-novel] Seen subclasses (incl. novel-sub): 75
[Pseudo-novel] Seen samples: 10340, Pseudo-novel samples: 948
  Seen-super samples: 5340
  Novel-super samples: 5000
  Final split sizes:
    train: 9306
    val:   1034
    train novel-super: 4500
    val novel-super:   500
[Pseudo-novel] Train size: 9306, Seen-val size: 1034, Pseudo-novel val size: 948
Test size: 11180
```

4 SECTION 4: Backbone & Model Definitions

[ ]:
```
# Backbone builder

# Using ImageNet pretrained ResNet backbone, and chopping off FC head to␣
↪Transfer Learn

def build_resnet_backbone():
    # Using torchvision ResNet-18 with ImageNet weights
    if BACKBONE == "resnet18":
        base = models.resnet18(weights=models.ResNet18_Weights.IMAGENET1K_V1)
    elif BACKBONE == "resnet50":
        base = models.resnet50(weights=models.ResNet50_Weights.IMAGENET1K_V1)
    else:
        raise ValueError(f"Unknown BACKBONE: {BACKBONE}")
    # Remove the final classification layer
    in_features = base.fc.in_features
    base.fc = nn.Identity()
    return base, in_features
```

[ ]:
```
# Methods for Shared backbone + two heads + KL divergence

class SharedBackboneTwoHeads(nn.Module):
```

```
    def __init__(self, num_super, num_sub):
        super().__init__()
        self.backbone, feat_dim = build_resnet_backbone()
        self.super_head = nn.Linear(feat_dim, num_super)
        self.sub_head = nn.Linear(feat_dim, num_sub)

    def forward(self, x):
        feats = self.backbone(x)
        super_logits = self.super_head(feats)
        sub_logits = self.sub_head(feats)
        return super_logits, sub_logits
```

[ ]:
```
# KL helper that maps subclass probs to superclass probs using sub_to_super␣
↪mapping

def sub_probs_to_super_probs(sub_probs, sub_to_super, num_super):
    """
    sub_probs: (B, num_sub), softmax over subclasses
    returns: (B, num_super), summed probs per super-class
    """
    B, num_sub = sub_probs.shape
    super_probs = torch.zeros(B, num_super, device=sub_probs.device)

    for sub_idx, super_idx in sub_to_super.items():
        super_probs[:, super_idx] += sub_probs[:, sub_idx]

    # For safety: re-normalize in case of any numeric drift
    super_probs = super_probs / (super_probs.sum(dim=1, keepdim=True) + 1e-8)
    return super_probs
```

[ ]:
```
# Single-head model for 2-separate models approach
# Each model is just a backbone + one linear head

# to instantiate, one has num_classes = num_super, other has num_classes =␣
↪num_sub

class SingleHeadModel(nn.Module):
    def __init__(self, num_classes):
        super().__init__()
        self.backbone, feat_dim = build_resnet_backbone()
        self.head = nn.Linear(feat_dim, num_classes)

    def forward(self, x):
        feats = self.backbone(x)
        logits = self.head(feats)
        return logits
```

5 SECTION 5: Training & evaluation utilities

[ ]:
```
# functions for training

# we pass a flag mode to indicate which model using either:
# "two_heads_kl", "single_head_super" or "single_head"sub"


def accuracy_from_logits(logits, targets):
    preds = logits.argmax(dim=1)
    correct = (preds == targets).sum().item()
    total = targets.size(0)
    return correct, total


def train_one_epoch(model, optimizer, loader, criterion, mode,␣
↪sub_to_super=None,
                    num_super=None, alpha_kl=0.1, temperature=1.0):
    model.train()
    running_loss = 0.0
    super_correct = sub_correct = 0
    super_total = sub_total = 0

    for images, super_labels, sub_labels in loader:
        images = images.to(device)
        super_labels = super_labels.to(device)
        sub_labels = sub_labels.to(device)

        optimizer.zero_grad()

        if mode == "two_heads_kl":
            super_logits, sub_logits = model(images)
            # CE losses
            loss_super = criterion(super_logits, super_labels)
            loss_sub = criterion(sub_logits, sub_labels)

            # KL term between super head and aggregated subclass head
            with torch.no_grad():
                # target: super_probs
                super_probs = F.softmax(super_logits / temperature, dim=1)
            sub_probs = F.softmax(sub_logits / temperature, dim=1)
            agg_super_probs = sub_probs_to_super_probs(sub_probs, sub_to_super,␣
↪num_super)

            # KL(super || agg_super) = sum p * (log p - log q)
            # using KLDivLoss with log_softmax input and probs target:
            kl_loss = F.kl_div(
```

```
                input=torch.log(agg_super_probs + 1e-8),
                target=super_probs,
                reduction="batchmean"
            )

            loss = loss_super + loss_sub + alpha_kl * kl_loss

            sc, st = accuracy_from_logits(super_logits, super_labels)
            suc, sut = accuracy_from_logits(sub_logits, sub_labels)
            super_correct += sc
            super_total += st
            sub_correct += suc
            sub_total += sut

        elif mode in ("single_head_super", "single_head_sub"):
            logits = model(images)
            if mode == "single_head_super":
                loss = criterion(logits, super_labels)
                sc, st = accuracy_from_logits(logits, super_labels)
                super_correct += sc
                super_total += st
            else:
                loss = criterion(logits, sub_labels)
                suc, sut = accuracy_from_logits(logits, sub_labels)
                sub_correct += suc
                sub_total += sut
        else:
            raise ValueError(f"Unknown mode {mode}")

        loss.backward()
        optimizer.step()

        running_loss += loss.item()

    avg_loss = running_loss / len(loader)
    metrics = {"loss": avg_loss}
    if super_total > 0:
        metrics["acc_super"] = super_correct / super_total
    if sub_total > 0:
        metrics["acc_sub"] = sub_correct / sub_total

    return metrics


@torch.no_grad()
def eval_one_epoch(model, loader, criterion, mode, sub_to_super=None,
                   num_super=None, alpha_kl=0.1, temperature=1.0):
```

```
    model.eval()
    running_loss = 0.0
    super_correct = sub_correct = 0
    super_total = sub_total = 0

    for images, super_labels, sub_labels in loader:
        images = images.to(device)
        super_labels = super_labels.to(device)
        sub_labels = sub_labels.to(device)

        if mode == "two_heads_kl":
            super_logits, sub_logits = model(images)
            loss_super = criterion(super_logits, super_labels)
            loss_sub = criterion(sub_logits, sub_labels)

            with torch.no_grad():
                super_probs = F.softmax(super_logits / temperature, dim=1)
            sub_probs = F.softmax(sub_logits / temperature, dim=1)
            agg_super_probs = sub_probs_to_super_probs(sub_probs, sub_to_super, num_super)

            kl_loss = F.kl_div(
                input=torch.log(agg_super_probs + 1e-8),
                target=super_probs,
                reduction="batchmean"
            )

            loss = loss_super + loss_sub + alpha_kl * kl_loss

            sc, st = accuracy_from_logits(super_logits, super_labels)
            suc, sut = accuracy_from_logits(sub_logits, sub_labels)
            super_correct += sc
            super_total += st
            sub_correct += suc
            sub_total += sut

        elif mode in ("single_head_super", "single_head_sub"):
            logits = model(images)
            if mode == "single_head_super":
                loss = criterion(logits, super_labels)
                sc, st = accuracy_from_logits(logits, super_labels)
                super_correct += sc
                super_total += st
            else:
                loss = criterion(logits, sub_labels)
                suc, sut = accuracy_from_logits(logits, sub_labels)
                sub_correct += suc
```

```
                sub_total += sut

        running_loss += loss.item()

    avg_loss = running_loss / len(loader)
    metrics = {"val_loss": avg_loss}
    if super_total > 0:
        metrics["val_acc_super"] = super_correct / super_total
    if sub_total > 0:
        metrics["val_acc_sub"] = sub_correct / sub_total

    return metrics
```

[ ]:
```
# Analysis and Visualize: for Novel Subclass fine tuning
# Determines optimal threshold value from training data (except held out) vs.␣
 ↪held out (pseudo-novel) subclass data

@torch.no_grad()
def collect_max_probs_sub(model, loader, mode="two_heads"):
    """
    Collect max softmax probabilities from the subclass head.

    mode:
      - "two_heads": model(images) -> (super_logits, sub_logits)
      - "sub_single_head": model(images) -> sub_logits
    """
    model.eval()
    probs = []

    for batch in loader:
        images = batch[0].to(device)

        if mode == "two_heads":
            _, sub_logits = model(images)
        elif mode == "sub_single_head":
            sub_logits = model(images)
        else:
            raise ValueError(f"Unknown mode: {mode}")

        # Softmax over subclasses, then take max per sample
        p = F.softmax(sub_logits, dim=1).max(dim=1).values
        probs.extend(p.cpu().numpy().tolist())

    return np.array(probs)

@torch.no_grad()
def analyze_tau_sub(model, mode="two_heads"):
```

```
"""
Compare max subclass probabilities on:
  - seen validation (val_loader)
  - pseudo-novel validation (pseudo_novel_loader)
and suggest TAU_SUB candidates.
"""

if pseudo_novel_loader is None:
    print("pseudo_novel_loader is None. "
          "Set USE_PSEUDO_NOVEL = True before building loaders to use this␣
↪analysis.")
    return

# Collect max probs
seen_probs = collect_max_probs_sub(model, val_loader, mode=mode)
pseudo_probs = collect_max_probs_sub(model, pseudo_novel_loader, mode=mode)

# Summary stats
def summarize(name, arr):
    print(f"\n{name} subclass max-prob stats:")
    print(f"  count = {len(arr)}")
    print(f"  mean  = {arr.mean():.3f}")
    print(f"  std   = {arr.std():.3f}")
    percentiles = [1, 5, 10, 25, 50, 75, 90, 95, 99]
    pvals = {p: float(np.percentile(arr, p)) for p in percentiles}
    print("  percentiles:")
    for p in percentiles:
        print(f"    p{p:>2}: {pvals[p]:.3f}")
    return pvals

seen_p = summarize("Seen", seen_probs)
pseudo_p = summarize("Pseudo-novel", pseudo_probs)

# Simple candidate thresholds
# 1) 10th percentile of seen (reject only the lowest-confidence seen examples)
tau_candidate_1 = seen_p[10]

# 2) Midpoint between mean(seen) and mean(pseudo)
tau_candidate_2 = 0.5 * (seen_probs.mean() + pseudo_probs.mean())

print("\nSuggested TAU_SUB candidates:")
print(f"  tau_sub  10th percentile of seen: {tau_candidate_1:.3f}")
print(f"  tau_sub  mean(seen + pseudo)/2:  {tau_candidate_2:.3f}")
print("\nYou can start with one of these for TAU_SUB and adjust based on␣
↪leaderboard/behavior.")

# Histogram visualization
```

```
plt.figure(figsize=(8, 5))
plt.hist(seen_probs, bins=30, alpha=0.5, label="Seen subclasses")
plt.hist(pseudo_probs, bins=30, alpha=0.5, label="Pseudo-novel subclasses")
plt.axvline(tau_candidate_1, linestyle="--", label=f"p10 seen ~␣
↪{tau_candidate_1:.2f}")
plt.axvline(tau_candidate_2, linestyle=":", label=f"mean midpoint ~␣
↪{tau_candidate_2:.2f}")
plt.xlabel("Max softmax probability (subclass head)")
plt.ylabel("Count")
plt.title("Subclass max-prob: seen vs pseudo-novel")
plt.legend()
plt.tight_layout()
plt.show()

# Optional: log histograms and candidates to W&B
if USE_WANDB:
    try:
        import wandb
        wandb.log({
            "sub_seen_maxprob_hist": wandb.Histogram(seen_probs),
            "sub_pseudo_maxprob_hist": wandb.Histogram(pseudo_probs),
            "tau_sub_candidate_p10_seen": tau_candidate_1,
            "tau_sub_candidate_mean_midpoint": tau_candidate_2,
        })
        print("Logged histograms and tau_sub candidates to Weights & Biases.")
    except Exception as e:
        print("Could not log to W&B:", e)
```

[ ]:
```
# Analysis and Visualize: for Novel Superclass fine tuning
# Determines the optimal threshold from provided training data vs. Novel Super␣
↪data (more images)

@torch.no_grad()
def collect_max_probs_super(model, loader, mode="two_heads"):
    """
    Collect max softmax probabilities from the superclass head.

    mode:
      - "two_heads": model(images) -> (super_logits, sub_logits)
      - "super_single_head": model(images) -> super_logits
    """
    model.eval()
    probs = []

    for batch in loader:
        images = batch[0].to(device)
```

```python
        if mode == "two_heads":
            super_logits, _ = model(images)
        elif mode == "super_single_head":
            super_logits = model(images)
        else:
            raise ValueError(f"Unknown mode: {mode}")

        p = F.softmax(super_logits, dim=1).max(dim=1).values
        probs.extend(p.cpu().numpy().tolist())

    return np.array(probs)

@torch.no_grad()
def analyze_tau_super(model, mode="two_heads"):
    """
    Analyze max superclass probabilities on validation set, split into:
      - seen superclasses (super != NOVEL_SUPER_IDX)
      - novel superclasses (super == NOVEL_SUPER_IDX)

    This assumes:
      - val_loader batches look like (images, super_labels, sub_labels, ...)
      - NOVEL_SUPER_IDX is defined (e.g. 3)
    """

    model.eval()

    seen_probs = []
    novel_probs = []

    for batch in val_loader:
        images = batch[0].to(device)
        super_labels = batch[1].to(device)   # assumes (images, super, sub, ...)

        # Forward
        if mode == "two_heads":
            super_logits, _ = model(images)
        elif mode == "super_single_head":
            super_logits = model(images)
        else:
            raise ValueError(f"Unknown mode: {mode}")

        probs = F.softmax(super_logits, dim=1)          # (B, num_super)
        max_probs, _ = probs.max(dim=1)                 # (B,)

        novel_mask = (super_labels == NOVEL_SUPER_IDX)
        seen_mask = ~novel_mask
```

```
        if seen_mask.any():
            seen_probs.extend(max_probs[seen_mask].detach().cpu().numpy().
↪tolist())
        if novel_mask.any():
            novel_probs.extend(max_probs[novel_mask].detach().cpu().numpy().
↪tolist())

    seen_probs = np.array(seen_probs)
    novel_probs = np.array(novel_probs)

    def summarize(name, arr):
        print(f"\n{name} superclass max-prob stats:")
        print(f"  count = {len(arr)}")
        print(f"  mean  = {arr.mean():.3f}")
        print(f"  std   = {arr.std():.3f}")
        percentiles = [1, 5, 10, 25, 50, 75, 90, 95, 99]
        pvals = {p: float(np.percentile(arr, p)) for p in percentiles}
        print("  percentiles:")
        for p in percentiles:
            print(f"    p{p:>2}: {pvals[p]:.3f}")
        return pvals

    if len(seen_probs) == 0:
        print("No seen-super examples found in val_loader (super !=␣
↪NOVEL_SUPER_IDX).")
        return
    seen_p = summarize("Seen superclasses (0/1/2)", seen_probs)

    if len(novel_probs) == 0:
        print("\nNo novel-super examples (super == NOVEL_SUPER_IDX) in␣
↪val_loader yet.")
        novel_p = None
    else:
        novel_p = summarize("Novel superclasses (== NOVEL_SUPER_IDX)",␣
↪novel_probs)

    # ---- Candidate thresholds ----
    # Start from seen distribution:
    tau_p10_seen = seen_p[10]
    tau_p5_seen  = seen_p[5]
    tau_mean_minus_std = max(0.0, min(1.0, seen_probs.mean() - seen_probs.
↪std()))

    # If we have novel-super stats, try to place tau between seen & novel means/
↪percentiles
    if novel_p is not None:
```

```
        # Midpoint between seen mean and novel mean
        tau_mean_mid = 0.5 * (seen_probs.mean() + novel_probs.mean())
        print("\nSuggested TAU_SUPER candidates (using seen + novel):")
        print(f"  tau_super  10th percentile of seen:      {tau_p10_seen:.3f}")
        print(f"  tau_super  5th percentile of seen:       {tau_p5_seen:.3f}")
        print(f"  tau_super  mean(seen) - std(seen):       {tau_mean_minus_std:.3f}")
        print(f"  tau_super  mean(seen & novel) midpoint:  {tau_mean_mid:.3f}")
        tau_candidates = [tau_p10_seen, tau_p5_seen, tau_mean_minus_std, tau_mean_mid]
    else:
        print("\nSuggested TAU_SUPER candidates (seen only):")
        print(f"  tau_super  10th percentile of seen:      {tau_p10_seen:.3f}")
        print(f"  tau_super  5th percentile of seen:       {tau_p5_seen:.3f}")
        print(f"  tau_super  mean(seen) - std(seen):       {tau_mean_minus_std:.3f}")
        tau_candidates = [tau_p10_seen, tau_p5_seen, tau_mean_minus_std]

    # ---- Histogram plot ----
    plt.figure(figsize=(8, 5))
    plt.hist(seen_probs, bins=30, alpha=0.6, label="Seen superclasses (0/1/2)")
    if len(novel_probs) > 0:
        plt.hist(novel_probs, bins=30, alpha=0.6, label="Novel superclasses (3)")

    # Draw candidate lines (use a couple of them for visual reference)
    for tau in tau_candidates[:3]:
        plt.axvline(tau, linestyle="--", alpha=0.7)

    plt.xlabel("Max softmax probability (superclass head)")
    plt.ylabel("Count")
    plt.title("Superclass max-prob: seen vs novel-super on validation")
    plt.legend()
    plt.tight_layout()
    plt.show()

    # ---- Optional: log to W&B ----
    if USE_WANDB:
        try:
            import wandb
            log_dict = {
                "super_seen_maxprob_hist": wandb.Histogram(seen_probs),
            }
```

```
            if len(novel_probs) > 0:
                log_dict["super_novel_maxprob_hist"] = wandb.
↪Histogram(novel_probs)
            # Also log first few tau candidates
            log_dict["tau_super_candidate_1"] = float(tau_candidates[0])
            if len(tau_candidates) > 1:
                log_dict["tau_super_candidate_2"] = float(tau_candidates[1])
            if len(tau_candidates) > 2:
                log_dict["tau_super_candidate_3"] = float(tau_candidates[2])
            wandb.log(log_dict)
            print("Logged superclass histograms and tau_super candidates to␣
↪Weights & Biases.")
        except Exception as e:
            print("Could not log to W&B:", e)
```

[ ]:
```
# Additional eval helper functions

# This calculates the following:
# 1. How often we correctly keep seen classes (low false "novel" rate)
# 2. How often we correctly identify CIFAR "novel super" samples (new data)

@torch.no_grad()
def evaluate_on_val_with_novelty(model, mode="two_heads",
                                 tau_super=TAU_SUPER, tau_sub=TAU_SUB,
                                 loader=None, name="val"):
    """
    Evaluate a model on a loader with novel thresholds applied.

    For subclasses, we ONLY care about:
      - overall subclass acc
      - seen-subclass acc / false-novel rate

    We DO NOT report "novel-subclass accuracy" here because there are no
    ground-truth novel-sub labels in the original validation data.
    """
    if loader is None:
        loader = val_loader

    model.eval()

    total = 0
    super_correct = 0
    sub_correct = 0

    seen_super_correct = seen_super_total = 0
    novel_super_correct = novel_super_total = 0
```

```python
    seen_sub_correct = seen_sub_total = 0
    novel_sub_correct = novel_sub_total = 0  # still counted but not reported

    for batch in loader:
        images = batch[0].to(device)
        super_true = batch[1].to(device)
        sub_true   = batch[2].to(device)

        if mode == "two_heads":
            super_logits, sub_logits = model(images)
        elif mode == "super_single_head":
            super_logits = model(images); sub_logits = None
        elif mode == "sub_single_head":
            super_logits = None; sub_logits = model(images)
        else:
            raise ValueError(f"Unknown mode: {mode}")

        batch_size = images.size(0)
        total += batch_size

        # --- Superclass ---
        if super_logits is not None:
            super_probs = F.softmax(super_logits, dim=1)
            max_super_probs, super_idx = super_probs.max(dim=1)

            super_pred = super_idx.clone()
            novel_mask_super = max_super_probs < tau_super
            super_pred[novel_mask_super] = NOVEL_SUPER_IDX

            match_super = (super_pred == super_true)
            super_correct += match_super.sum().item()

            seen_mask_super = (super_true != NOVEL_SUPER_IDX)
            novel_mask_super_label = (super_true == NOVEL_SUPER_IDX)

            if seen_mask_super.any():
                seen_super_correct += match_super[seen_mask_super].sum().item()
                seen_super_total   += seen_mask_super.sum().item()
            if novel_mask_super_label.any():
                novel_super_correct += match_super[novel_mask_super_label].
↪sum().item()
                novel_super_total   += novel_mask_super_label.sum().item()

        # --- Subclass ---
        if sub_logits is not None:
            sub_probs = F.softmax(sub_logits, dim=1)
            max_sub_probs, sub_idx = sub_probs.max(dim=1)
```

```
            sub_pred = sub_idx.clone()
            novel_mask_sub = max_sub_probs < tau_sub
            sub_pred[novel_mask_sub] = NOVEL_SUB_IDX

            match_sub = (sub_pred == sub_true)
            sub_correct += match_sub.sum().item()

            seen_mask_sub = (sub_true != NOVEL_SUB_IDX)
            novel_mask_sub_label = (sub_true == NOVEL_SUB_IDX)

            if seen_mask_sub.any():
                seen_sub_correct += match_sub[seen_mask_sub].sum().item()
                seen_sub_total   += seen_mask_sub.sum().item()
            if novel_mask_sub_label.any():
                # counted but not reported; there shouldn't be any in original val
                novel_sub_correct += match_sub[novel_mask_sub_label].sum().item()
                novel_sub_total   += novel_mask_sub_label.sum().item()

    # ----- Compute metrics dict -----
    metrics = {}

    if total > 0:
        if super_correct > 0 or seen_super_total + novel_super_total > 0:
            metrics["overall_super_acc"] = super_correct / total
        if sub_correct > 0 or seen_sub_total + novel_sub_total > 0:
            metrics["overall_sub_acc"] = sub_correct / total

    if seen_super_total > 0:
        metrics["seen_super_acc"] = seen_super_correct / seen_super_total
        metrics["seen_super_false_novel"] = 1.0 - metrics["seen_super_acc"]
    if novel_super_total > 0:
        metrics["novel_super_acc"] = novel_super_correct / novel_super_total

    if seen_sub_total > 0:
        metrics["seen_sub_acc"] = seen_sub_correct / seen_sub_total
        metrics["seen_sub_false_novel"] = 1.0 - metrics["seen_sub_acc"]
    # NOTE: we deliberately do NOT add novel-sub metrics to `metrics`,
    # because they are not meaningful for this dataset.

    # ----- Print summary -----
    print(f"\n=== Evaluation on {name} ===")
    if "overall_super_acc" in metrics:
        print(f"Overall superclass acc: {metrics['overall_super_acc']:.4f}")
    if "overall_sub_acc" in metrics:
```

```python
        print(f"Overall subclass acc:   {metrics['overall_sub_acc']:.4f}")

    if "seen_super_acc" in metrics:
        print(f"Seen superclass acc (true super != novel):  {metrics['seen_super_acc']:.4f}")
        print(f"Seen superclass false-novel rate:           {metrics['seen_super_false_novel']:.4f}")
    if "novel_super_acc" in metrics:
        print(f"Novel superclass acc (true super == novel): {metrics['novel_super_acc']:.4f}")

    if "seen_sub_acc" in metrics:
        print(f"Seen subclass acc (true sub != novel):      {metrics['seen_sub_acc']:.4f}")
        print(f"Seen subclass false-novel rate:             {metrics['seen_sub_false_novel']:.4f}")

    # ----- Optional: log to W&B (only real metrics) -----
    if USE_WANDB:
        log_dict = {}
        for k, v in metrics.items():
            log_dict[f"{name}_{k}"] = v
        if log_dict:
            wandb.log(log_dict)

    return metrics




# This enables us to evaluate how often we correctly mark held-out subclasses as novel (proxy for leaderboard performance on subclasses)
@torch.no_grad()
def evaluate_pseudo_novel_sub_with_novelty(model, mode="two_heads",
                                           tau_sub=TAU_SUB,
                                           loader=None,
                                           name="pseudo_novel_sub"):
    """
    Evaluate how well the model flags held-out subclasses as novel.

    Assumes:
      - loader yields only *held-out* subclasses (true unseen subclasses)
      - true labels are NOT NOVEL_SUB_IDX, but we *want* the model to predict NOVEL_SUB_IDX.
    """
    if loader is None:
```

```
        loader = pseudo_novel_loader

    if loader is None:
        print("No pseudo_novel_loader available.")
        return {}

    model.eval()

    total = 0
    predicted_novel = 0
    predicted_seen = 0

    for batch in loader:
        images = batch[0].to(device)
        # we don't actually need the labels here for correctness, only for counting

        if mode == "two_heads":
            _, sub_logits = model(images)
        elif mode == "sub_single_head":
            sub_logits = model(images)
        else:
            raise ValueError(f"Unknown mode for pseudo-novel eval: {mode}")

        sub_probs = F.softmax(sub_logits, dim=1)
        max_sub_probs, sub_idx = sub_probs.max(dim=1)

        sub_pred = sub_idx.clone()
        novel_mask_sub = max_sub_probs < tau_sub
        sub_pred[novel_mask_sub] = NOVEL_SUB_IDX

        batch_size = images.size(0)
        total += batch_size

        predicted_novel += (sub_pred == NOVEL_SUB_IDX).sum().item()
        predicted_seen  += (sub_pred != NOVEL_SUB_IDX).sum().item()

    metrics = {}
    if total > 0:
        metrics["pseudo_novel_sub_novel_rate"] = predicted_novel / total
        metrics["pseudo_novel_sub_false_seen"] = predicted_seen / total

    print(f"\n=== Evaluation on {name} (held-out subclasses) ===")
    if total > 0:
        print(f"Fraction flagged as novel (good): {metrics['pseudo_novel_sub_novel_rate']:.4f}")
```

```
        print(f"Fraction mapped to seen subclasses (bad):␣
↪{metrics['pseudo_novel_sub_false_seen']:.4f}")

    if USE_WANDB and metrics:
        log_dict = {f"{name}_{k}": v for k, v in metrics.items()}
        wandb.log(log_dict)

    return metrics
```

[ ]:
```
# Dashboard for our evals so we can determine how model will likely perform on␣
↪leaderboard evaluation

@torch.no_grad()
def novelty_dashboard(model, mode="two_heads",
                      tau_super=TAU_SUPER, tau_sub=TAU_SUB,
                      include_pseudo=True):
    """
    Run thresholded evals and show a compact table of key metrics.

    Subclass side focuses on:
      - seen subclasses (false-novel rate)
      - held-out pseudo-novel subclasses (how often marked as novel)
    """
    rows = []

    # --- Main val_loader stats (seen + CIFAR-novel) ---
    val_metrics = evaluate_on_val_with_novelty(
        model,
        mode=mode,
        tau_super=tau_super,
        tau_sub=tau_sub,
        loader=val_loader,
        name="val",
    )

    # Superclass (val)
    if "seen_super_acc" in val_metrics:
        rows.append({
            "Split": "val",
            "Head": "super",
            "Metric": "Seen superclass accuracy",
            "Meaning": "Correctly keep seen superclasses as seen",
            "Value": float(val_metrics["seen_super_acc"]),
        })
        if "seen_super_false_novel" in val_metrics:
          rows.append({
                "Split": "val",
```

```
                "Head": "super",
                "Metric": "Seen superclass false-novel rate",
                "Meaning": "Seen superclasses incorrectly flipped to novel",
                "Value": float(val_metrics["seen_super_false_novel"]),
            })

    if "novel_super_acc" in val_metrics:
        rows.append({
            "Split": "val",
            "Head": "super",
            "Metric": "Novel superclass accuracy (CIFAR)",
            "Meaning": "CIFAR novel-super samples correctly predicted as novel",
            "Value": float(val_metrics["novel_super_acc"]),
        })

    # Subclass (val) - ONLY seen-subclass metrics
    if "seen_sub_acc" in val_metrics:
        rows.append({
            "Split": "val",
            "Head": "sub",
            "Metric": "Seen subclass accuracy",
            "Meaning": "Correctly keep seen subclasses as seen",
            "Value": float(val_metrics["seen_sub_acc"]),
        })
        if "seen_sub_false_novel" in val_metrics:
            rows.append({
                "Split": "val",
                "Head": "sub",
                "Metric": "Seen subclass false-novel rate",
                "Meaning": "Seen subclasses incorrectly flipped to novel",
                "Value": float(val_metrics["seen_sub_false_novel"]),
            })
    # NOTE: we deliberately do NOT add a "novel subclass accuracy" row here.

    # --- Pseudo-novel subclass stats (held-out subclasses) ---
    pseudo_metrics = {}
    if include_pseudo and pseudo_novel_loader is not None and mode in␣
↪("two_heads", "sub_single_head"):
        pseudo_metrics = evaluate_pseudo_novel_sub_with_novelty(
            model,
            mode=mode,
            tau_sub=tau_sub,
            loader=pseudo_novel_loader,
            name="pseudo_novel_sub",
        )

        if "pseudo_novel_sub_novel_rate" in pseudo_metrics:
```

```python
            rows.append({
                "Split": "pseudo_novel",
                "Head": "sub",
                "Metric": "Pseudo-novel marked as novel",
                "Meaning": "Held-out subclasses correctly flagged as novel",
                "Value": float(pseudo_metrics["pseudo_novel_sub_novel_rate"]),
            })
        if "pseudo_novel_sub_false_seen" in pseudo_metrics:
            rows.append({
                "Split": "pseudo_novel",
                "Head": "sub",
                "Metric": "Pseudo-novel mapped to seen",
                "Meaning": "Held-out subclasses wrongly mapped to some seen␣
↪subclass",
                "Value": float(pseudo_metrics["pseudo_novel_sub_false_seen"]),
            })

    # --- Config / settings summary (for *printing* only) ---
    config_rows = [
        {
            "Split": "config",
            "Head": "-",
            "Metric": "BACKBONE",
            "Meaning": "Feature extractor (e.g. resnet18 / resnet50)",
            "Value": BACKBONE,
        },
        {
            "Split": "config",
            "Head": "-",
            "Metric": "TAU_SUPER",
            "Meaning": "Novelty threshold for superclass head",
            "Value": str(tau_super),
        },
        {
            "Split": "config",
            "Head": "-",
            "Metric": "TAU_SUB",
            "Meaning": "Novelty threshold for subclass head",
            "Value": str(tau_sub),
        },
        {
            "Split": "config",
            "Head": "-",
            "Metric": "CIFAR_NOVEL_MODE",
            "Meaning": "Extra novel-super CIFAR data mode",
            "Value": str(CIFAR_NOVEL_MODE),
        },
```

```
        {
            "Split": "config",
            "Head": "-",
            "Metric": "FINE_TUNE_MODE",
            "Meaning": "Backbone training mode (full vs frozen)",
            "Value": str(FINE_TUNE_MODE),
        },
        {
            "Split": "config",
            "Head": "-",
            "Metric": "APPROACH",
            "Meaning": "Model architecture (two_heads vs two_models)",
            "Value": str(APPROACH),
        },
        {
            "Split": "config",
            "Head": "-",
            "Metric": "USE_PSEUDO_NOVEL",
            "Meaning": "Using held-out subclasses for pseudo-novel eval",
            "Value": str(bool(USE_PSEUDO_NOVEL)),
        },
        {
            "Split": "config",
            "Head": "-",
            "Metric": "DATA_AUGMENT",
            "Meaning": "Whether data augmentation is enabled for training",
            "Value": str(bool(DATA_AUGMENT)),
        },
    ]

    rows.extend(config_rows)

    if not rows:
        print("No metrics to display in dashboard.")
        return None

    dashboard_df = pd.DataFrame(rows)
    dashboard_df = dashboard_df.sort_values(
        by=["Split", "Head", "Metric"]
    ).reset_index(drop=True)

    print("\n==== Novelty Dashboard ====")
    print(dashboard_df)

    # --- Log to W&B: metrics only, numeric Value column ---
    if USE_WANDB:
        try:
```

```
            wandb_table_df = dashboard_df.copy()

            def _to_str(v):
                if isinstance(v, float):
                    return f"{v:.6f}"
                return str(v)

            wandb_table_df["Split"] = wandb_table_df["Split"].astype(str)
            wandb_table_df["Head"] = wandb_table_df["Head"].astype(str)
            wandb_table_df["Metric"] = wandb_table_df["Metric"].astype(str)
            wandb_table_df["Meaning"] = wandb_table_df["Meaning"].astype(str)
            wandb_table_df["Value"] = wandb_table_df["Value"].apply(_to_str)

            wandb.log({"novelty_dashboard": wandb.
 ↪Table(dataframe=wandb_table_df)})
        except Exception as e:
            print("Could not log dashboard table to W&B:", e)

    return dashboard_df
```

[ ]:
```
# Helper to choose backbone (freeze or full) and choose optimizer parameter

def setup_backbone_training(model, fine_tune_mode="full", lr_full=1e-4,␣
 ↪lr_head=1e-3):
    """
    Given a model with attributes:
        - model.backbone  (all feature extractor layers)
        - head layers (e.g. super/sub heads) as other modules,
    freeze or unfreeze the backbone and return an optimizer.

    Returns:
        optimizer, effective_lr
    """
    if fine_tune_mode == "full":
        # Everything trainable
        for p in model.parameters():
            p.requires_grad = True
        trainable_params = model.parameters()
        lr = lr_full
    elif fine_tune_mode == "frozen":
        # Freeze backbone, train only heads
        for p in model.backbone.parameters():
            p.requires_grad = False
        # Only parameters that still require grad will be optimized
        trainable_params = [p for p in model.parameters() if p.requires_grad]
        lr = lr_head
```

```
        print(f"Freezing backbone; training {len(trainable_params)} parameter␣
↪tensors in heads only.")
    else:
        raise ValueError(f"Unknown FINE_TUNE_MODE: {fine_tune_mode}")

    optimizer = optim.Adam(trainable_params, lr=lr, weight_decay=WEIGHT_DECAY)
    return optimizer
```

6 SECTION 6: Approach A: Shared backbone, two heads + KL

[ ]:
```
# Original idea

LR = 1e-4 # maybe two different learning rates
ALPHA_KL = 0.1
TEMPERATURE = 1.0

if APPROACH == "two_heads":
    model_two_heads = SharedBackboneTwoHeads(
        num_super=num_super,
        num_sub=num_sub
    ).to(device)

    criterion = nn.CrossEntropyLoss()
    optimizer = setup_backbone_training(
        model_two_heads,
        fine_tune_mode=FINE_TUNE_MODE,
        lr_full=LR,
        lr_head=LR_HEAD,
    )

    run_two_heads = None
    if USE_WANDB:
        run_two_heads = wandb.init(
            entity=WANDB_ENTITY,
            project=WANDB_PROJECT,
            name=make_run_name("two_heads_kl_resnet"),
            group="two_heads",  # to group/filter all two_heads runs
            config={
                "approach": "two_heads_kl",
                "backbone": BACKBONE,
                "epochs": EPOCHS,
                "lr_full": LR,
                "lr_head": LR_HEAD,
                "fine_tune_mode": FINE_TUNE_MODE,
                "alpha_kl": ALPHA_KL,
                "temperature": TEMPERATURE,
```

```
            "img_size": IMG_SIZE,
        },
    )

best_val_score = 0.0

print("Training shared-backbone two-heads model (KL-coupled):")
for epoch in range(1, EPOCHS + 1):
    train_metrics = train_one_epoch(
        model_two_heads,
        optimizer,
        train_loader,
        criterion,
        mode="two_heads_kl",
        sub_to_super=sub_to_super,
        num_super=num_super,
        alpha_kl=ALPHA_KL,
        temperature=TEMPERATURE,
    )

    val_metrics = eval_one_epoch(
        model_two_heads,
        val_loader,
        criterion,
        mode="two_heads_kl",
        sub_to_super=sub_to_super,
        num_super=num_super,
        alpha_kl=ALPHA_KL,
        temperature=TEMPERATURE,
    )

    val_acc_super = val_metrics.get("val_acc_super", 0.0)
    val_acc_sub = val_metrics.get("val_acc_sub", 0.0)
    val_loss = val_metrics["val_loss"]

    print(
        f"[Two-heads] Epoch {epoch}: "
        f"train_loss={train_metrics['loss']:.4f}, "
        f"val_loss={val_loss:.4f}, "
        f"val_acc_super={val_acc_super:.4f}, "
        f"val_acc_sub={val_acc_sub:.4f}"
    )

    if USE_WANDB:
        # prefix metrics so they don't collide with two-model ones
        log_dict = {
            "epoch": epoch,
```

```
                "two_heads_train_loss": train_metrics["loss"],
                "two_heads_val_loss": val_loss,
                "two_heads_val_acc_super": val_acc_super,
                "two_heads_val_acc_sub": val_acc_sub,
            }
            wandb.log(log_dict, step=epoch)

        # simple combined score: average of super/sub val accuracy
        val_score = 0.5 * val_acc_super + 0.5 * val_acc_sub
        if val_score > best_val_score:
            best_val_score = val_score
            torch.save(
                model_two_heads.state_dict(),
                os.path.join(DATA_ROOT, "best_two_heads_kl.pth"),
            )
            print("  Saved new best two-heads model")


    best_ckpt_path = os.path.join(DATA_ROOT, "best_two_heads_kl.pth")
    model_two_heads.load_state_dict(torch.load(best_ckpt_path,␣
 ↪map_location=device))


    analyze_tau_sub(model_two_heads, mode="two_heads")
    analyze_tau_super(model_two_heads, mode="two_heads")
    evaluate_on_val_with_novelty(model_two_heads, mode="two_heads",
                                 tau_super=TAU_SUPER, tau_sub=TAU_SUB,
                                 loader=val_loader, name="val_two_heads")
    evaluate_pseudo_novel_sub_with_novelty(
        model_two_heads, mode="two_heads", tau_sub=TAU_SUB
    )
    novelty_dashboard(model_two_heads, mode="two_heads",
                      tau_super=TAU_SUPER, tau_sub=TAU_SUB)

    if run_two_heads is not None:
        run_two_heads.finish()

else:
    print("APPROACH is not 'two_heads'; skipping two-heads training in this␣
 ↪cell.")
```

```
APPROACH is not 'two_heads'; skipping two-heads training in this cell.
```

7 Aksel Modifications

7.1 Newer Resnet

[ ]:
```python
def build_resnet_backbone(backbone: str=BACKBONE):
    # Using torchvision ResNet-18 with ImageNet weights
    if backbone == "resnet18":
        base = models.resnet18(weights=models.ResNet18_Weights.IMAGENET1K_V1)
    elif backbone == "resnet50":
        base = models.resnet50(weights=models.ResNet50_Weights.IMAGENET1K_V2)
    else:
        raise ValueError(f"Unknown BACKBONE: {backbone}")
    # Remove the final classification layer
    in_features = base.fc.in_features
    base.fc = nn.Identity()  # type: ignore[assignment]
    return base, in_features
```

7.2 New training routine

[ ]:
```python
def train_one_epoch(
    model: nn.Module,
    optimizer: torch.optim.Optimizer,
    loader: torch.utils.data.DataLoader,
    criterion: nn.Module,
    mode: str,
    sub_to_super: dict|None = None,
    num_super: int | None = None,
    trained_superclass_model: nn.Module | None = None,
    alpha_kl=0.1,
    temperature=1.0,
):
    """
    Optionally, add super class to calculate KL divergence penalty
    """
    model.train()
    running_loss = 0.0
    super_correct = sub_correct = 0
    super_total = sub_total = 0
    loss: torch.Tensor

    for images, super_labels, sub_labels in loader:
        images: torch.Tensor
        super_labels: torch.Tensor
        sub_labels: torch.Tensor
        images = images.to(device)
        super_labels = super_labels.to(device)
        sub_labels = sub_labels.to(device)
```

```
        optimizer.zero_grad()

        if mode == "two_heads_kl":
            super_logits, sub_logits = model(images)
            # CE losses
            loss_super = criterion(super_logits, super_labels)
            loss_sub = criterion(sub_logits, sub_labels)

            # KL term between super head and aggregated subclass head
            with torch.no_grad():
                # target: super_probs
                super_probs = F.softmax(super_logits / temperature, dim=1)
            sub_probs = F.softmax(sub_logits / temperature, dim=1)
            agg_super_probs = sub_probs_to_super_probs(sub_probs, sub_to_super,␣
↪num_super)

            # KL(super || agg_super) = sum p * (log p - log q)
            # using KLDivLoss with log_softmax input and probs target:
            kl_loss = F.kl_div(
                F.log_softmax(super_logits / temperature, dim=1),
                (agg_super_probs + 1e-8).log(),
                reduction="batchmean",
                log_target=True,
            )

            loss = loss_super + loss_sub + alpha_kl * kl_loss

            sc, st = accuracy_from_logits(super_logits, super_labels)
            suc, sut = accuracy_from_logits(sub_logits, sub_labels)
            super_correct += sc
            super_total += st
            sub_correct += suc
            sub_total += sut

        elif mode in ("single_head_super", "single_head_sub"):
            logits: torch.Tensor = model(images)
            if mode == "single_head_super":
                loss = criterion(logits, super_labels)
                sc, st = accuracy_from_logits(logits, super_labels)
                super_correct += sc
                super_total += st
            else:
                # Base subclass CE loss
                loss_sub = criterion(logits, sub_labels)

                # Optional: superclass-consistency penalty using a pretrained␣
↪superclass "teacher"
```

```
            # Idea: teacher gives p(super|x). We aggregate the subclass␣
↪head's probabilities into
            # q(super|x) by summing subclass probs within each super.␣
↪Penalize mismatch.
            loss_consistency = torch.zeros((), device=device)

            if trained_superclass_model is not None:
                assert sub_to_super is not None, "sub_to_super mapping␣
↪required for superclass-consistency"

                with torch.no_grad():
                    super_teacher_logits = trained_superclass_model(images)
                    super_teacher_probs = F.softmax(super_teacher_logits,␣
↪dim=1)

                # Aggregate subclass probs to super probs
                sub_probs = F.softmax(logits, dim=1)
                agg_super_probs = sub_probs_to_super_probs(sub_probs,␣
↪sub_to_super, num_super)

                # Consistency loss option A (soft): KL( teacher ||␣
↪agg_super )
                # Avoid 0 * log 0 by clamping.
                eps = 1e-8
                loss_consistency = F.kl_div(
                    (agg_super_probs.clamp_min(eps)).log(),
                    super_teacher_probs,
                    reduction="batchmean",
                )

                # Consistency loss option B (hard): encourage probability␣
↪mass to fall inside the teacher's top super
                # Uncomment to add this as well.
                # in_super_prob = agg_super_probs.gather(1,␣
↪super_pred_indices.unsqueeze(1)).squeeze(1)
                # loss_consistency = loss_consistency + (-torch.
↪log(in_super_prob.clamp_min(eps))).mean()

            # Weight the consistency term (tune as needed)
            loss = loss_sub + ALPHA_SUPER_CONSISTENCY * loss_consistency

            suc, sut = accuracy_from_logits(logits, sub_labels)
            sub_correct += suc
            sub_total += sut
    else:
        raise ValueError(f"Unknown mode {mode}")
```

```
        loss.backward()
        optimizer.step()

        running_loss += loss.item()

    avg_loss = running_loss / len(loader)
    metrics = {"loss": avg_loss}
    if super_total > 0:
        metrics["acc_super"] = super_correct / super_total
    if sub_total > 0:
        metrics["acc_sub"] = sub_correct / sub_total

    return metrics
```

7.3 New Single Head

```
[ ]: # Single-head model for 2-separate models approach
# Each model is just a backbone + one linear head

# to instantiate, one has num_classes = num_super, other has num_classes =␣
↪num_sub

class CosineClassifier(nn.Module):
    """
    Cosine-similarity classifier (normalized linear head).
    logits = scale * cos(theta), where cos(theta)=<normalize(x), normalize(W)>.
    """

    def __init__(self, in_features: int, out_features: int, scale: float = 30.
↪0, learn_scale: bool = True):
        super().__init__()
        self.weight = nn.Parameter(torch.empty(out_features, in_features))
        nn.init.xavier_uniform_(self.weight)

        if learn_scale:
            self.scale = nn.Parameter(torch.tensor(float(scale)))
        else:
            self.register_buffer("scale", torch.tensor(float(scale)))

    def forward(self, x: torch.Tensor) -> torch.Tensor:
        x = F.normalize(x, p=2, dim=1)  # [B, D]
        w = F.normalize(self.weight, p=2, dim=1)  # [C, D]
        logits = x @ w.t()  # [B, C]
        return logits * self.scale
```

```python
class SingleHeadModel(nn.Module):
    def __init__(
        self,
        num_classes: int,
        head: str,  # "linear" or "cosine"
        cosine_scale: float = 30.0,
        learn_scale: bool = True,
    ):
        super().__init__()
        self.backbone, feat_dim = build_resnet_backbone()

        if head == "cosine":
            self.head = nn.Sequential(
                CosineClassifier(
                    in_features=feat_dim,
                    out_features=(out := num_classes),
                    scale=cosine_scale,
                    learn_scale=learn_scale,
                ),
                nn.ReLU(),
                nn.Linear(out, num_classes),
            )
        elif head == "linear":
            self.head = nn.Linear(feat_dim, num_classes)
    def forward(self, x: torch.Tensor) -> torch.Tensor:
        feats = self.backbone(x)
        logits = self.head(feats)
        return logits
```

8 Print Vars

[ ]:
```python
SUPER_HEAD_TYPE = "linear"   # "linear" or "cosine"
SUB_HEAD_TYPE = "cosine"   # "linear" or "cosine"
ALPHA_SUPER_CONSISTENCY = 0.2 # unused
USE_PSUDEO_NOVEL = False
```

[ ]:
```python
print(BACKBONE, FINE_TUNE_MODE, SUPER_HEAD_TYPE, SUB_HEAD_TYPE,
  USE_PSEUDO_NOVEL)
```

```
resnet50 full linear cosine True
```

9 SECTION 7: Approach B - Two separate models

9.1 Train Super

[ ]:
```
# Second idea to compare

LR = 1e-4

if APPROACH == "two_models":
    # Superclass model
    model_super = SingleHeadModel(num_classes=num_super, head=SUPER_HEAD_TYPE).
 ↪to(device)
    criterion_super = nn.CrossEntropyLoss()
    optimizer_super = setup_backbone_training(
        model_super,
        fine_tune_mode=FINE_TUNE_MODE,
        lr_full=LR,
        lr_head=LR_HEAD,
    )

    run_super = None
    if USE_WANDB:
        run_super = wandb.init(
            entity=WANDB_ENTITY,
            project=WANDB_PROJECT,
            name=make_run_name("two_models_super_resnet"),
            group="two_models",   # to filter all two_models runs together
            config={
                "approach": "two_models",
                "head": "super",
                "backbone": BACKBONE,
                "epochs": EPOCHS,
                "lr_full": LR,
                "lr_head": LR_HEAD,
                "fine_tune_mode": FINE_TUNE_MODE,
                "img_size": IMG_SIZE,
                'super_head_type': SUPER_HEAD_TYPE,
            },
        )

    best_val_super = 0.0

    print("Training superclass model:")
    for epoch in range(1, EPOCHS + 1):
        train_metrics = train_one_epoch(
            model_super,
            optimizer_super,
```

```
            train_loader,
            criterion_super,
            mode="single_head_super",
        )
        val_metrics = eval_one_epoch(
            model_super,
            val_loader,
            criterion_super,
            mode="single_head_super",
        )

        val_acc = val_metrics.get("val_acc_super", 0.0)
        print(
            f"[Super] Epoch {epoch}: "
            f"train_loss={train_metrics['loss']:.4f}, "
            f"val_loss={val_metrics['val_loss']:.4f}, "
            f"val_acc_super={val_acc:.4f}"
        )

        if USE_WANDB:
            wandb.log(
                {
                    "epoch": epoch,
                    "super_train_loss": train_metrics["loss"],
                    "super_val_loss": val_metrics["val_loss"],
                    "super_val_acc": val_acc,
                },
                step=epoch,
            )

        if val_acc > best_val_super:
            best_val_super = val_acc
            torch.save(
                model_super.state_dict(),
                os.path.join(DATA_ROOT, "best_super_model.pth"),
            )
            print("  Saved new best superclass model")
        if val_acc ==1.0:
          print('ACHIEVED PERFECT SCORE.')

    if run_super is not None:
        run_super.finish()
```

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Training superclass model:
[Super] Epoch 1: train_loss=0.2098, val_loss=0.0126, val_acc_super=0.9932
  Saved new best superclass model
[Super] Epoch 2: train_loss=0.0141, val_loss=0.0059, val_acc_super=0.9981
  Saved new best superclass model
[Super] Epoch 3: train_loss=0.0077, val_loss=0.0042, val_acc_super=0.9990
  Saved new best superclass model
[Super] Epoch 4: train_loss=0.0044, val_loss=0.0016, val_acc_super=1.0000
  Saved new best superclass model
ACHIEVED PERFECT SCORE.
[Super] Epoch 5: train_loss=0.0033, val_loss=0.0036, val_acc_super=0.9990
[Super] Epoch 6: train_loss=0.0037, val_loss=0.0045, val_acc_super=0.9990
[Super] Epoch 7: train_loss=0.0021, val_loss=0.0077, val_acc_super=0.9981
[Super] Epoch 8: train_loss=0.0016, val_loss=0.0018, val_acc_super=0.9990
[Super] Epoch 9: train_loss=0.0018, val_loss=0.0082, val_acc_super=0.9971
[Super] Epoch 10: train_loss=0.0007, val_loss=0.0012, val_acc_super=1.0000
ACHIEVED PERFECT SCORE.
[Super] Epoch 11: train_loss=0.0029, val_loss=0.0012, val_acc_super=1.0000
ACHIEVED PERFECT SCORE.
[Super] Epoch 12: train_loss=0.0026, val_loss=0.0008, val_acc_super=1.0000
ACHIEVED PERFECT SCORE.
[Super] Epoch 13: train_loss=0.0006, val_loss=0.0017, val_acc_super=0.9990
[Super] Epoch 14: train_loss=0.0059, val_loss=0.0008, val_acc_super=1.0000
ACHIEVED PERFECT SCORE.
[Super] Epoch 15: train_loss=0.0033, val_loss=0.0004, val_acc_super=1.0000
ACHIEVED PERFECT SCORE.

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```

9.2 Sub Class Training

[ ]:
```
if APPROACH == "two_models":
    # Subclass model
    model_sub = SingleHeadModel(num_classes=num_sub, head=SUB_HEAD_TYPE).
↪to(device)
    criterion_sub = nn.CrossEntropyLoss()
    optimizer_sub = setup_backbone_training(
        model_sub,
        fine_tune_mode=FINE_TUNE_MODE,
```

```python
        lr_full=LR,
        lr_head=LR_HEAD,
    )

    run_sub = None
    if USE_WANDB:
        run_sub = wandb.init(
            entity=WANDB_ENTITY,
            project=WANDB_PROJECT,
            name=make_run_name("two_models_sub_resnet"),
            group="two_models",
            config={
                "approach": "two_models",
                "head": "sub",
                "backbone": BACKBONE,
                "epochs": EPOCHS,
                "lr_full": LR,
                "lr_head": LR_HEAD,
                "fine_tune_mode": FINE_TUNE_MODE,
                "img_size": IMG_SIZE,
                'sub_head_type': SUB_HEAD_TYPE,
            },
        )

    best_val_sub = 0.0

    print("\nTraining subclass model:")
    for epoch in range(1, EPOCHS + 1):
        train_metrics = train_one_epoch(
            model_sub,
            optimizer_sub,
            train_loader,
            criterion_sub,
            mode="single_head_sub",
        )
        val_metrics = eval_one_epoch(
            model_sub,
            val_loader,
            criterion_sub,
            mode="single_head_sub",
        )

        val_acc = val_metrics.get("val_acc_sub", 0.0)
        print(
            f"[Sub] Epoch {epoch}: "
            f"train_loss={train_metrics['loss']:.4f}, "
            f"val_loss={val_metrics['val_loss']:.4f}, "
```

```python
            f"val_acc_sub={val_acc:.4f}"
        )

        if USE_WANDB:
            wandb.log(
                {
                    "epoch": epoch,
                    "sub_train_loss": train_metrics["loss"],
                    "sub_val_loss": val_metrics["val_loss"],
                    "sub_val_acc": val_acc,
                },
                step=epoch,
            )

        if val_acc > best_val_sub:
            best_val_sub = val_acc
            torch.save(
                model_sub.state_dict(),
                os.path.join(DATA_ROOT, "best_sub_model.pth"),
            )
            print("  Saved new best subclass model")

    if run_sub is not None:
        run_sub.finish()
```

```
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```

```
Training subclass model:
[Sub] Epoch 1: train_loss=2.4963, val_loss=1.4422, val_acc_sub=0.7602
  Saved new best subclass model
[Sub] Epoch 2: train_loss=0.8537, val_loss=0.3808, val_acc_sub=0.9352
  Saved new best subclass model
[Sub] Epoch 3: train_loss=0.2495, val_loss=0.1471, val_acc_sub=0.9642
  Saved new best subclass model
[Sub] Epoch 4: train_loss=0.1251, val_loss=0.1204, val_acc_sub=0.9623
[Sub] Epoch 5: train_loss=0.0797, val_loss=0.1175, val_acc_sub=0.9613
[Sub] Epoch 6: train_loss=0.0569, val_loss=0.1131, val_acc_sub=0.9652
  Saved new best subclass model
[Sub] Epoch 7: train_loss=0.0529, val_loss=0.1042, val_acc_sub=0.9681
  Saved new best subclass model
```

```
[Sub] Epoch 8: train_loss=0.0372, val_loss=0.0824, val_acc_sub=0.9749
  Saved new best subclass model
[Sub] Epoch 9: train_loss=0.0328, val_loss=0.0974, val_acc_sub=0.9671
[Sub] Epoch 10: train_loss=0.0302, val_loss=0.1236, val_acc_sub=0.9652
[Sub] Epoch 11: train_loss=0.0179, val_loss=0.0716, val_acc_sub=0.9787
  Saved new best subclass model
[Sub] Epoch 12: train_loss=0.0262, val_loss=0.1177, val_acc_sub=0.9671
[Sub] Epoch 13: train_loss=0.0258, val_loss=0.0949, val_acc_sub=0.9691
[Sub] Epoch 14: train_loss=0.0225, val_loss=0.0767, val_acc_sub=0.9807
  Saved new best subclass model
[Sub] Epoch 15: train_loss=0.0185, val_loss=0.0988, val_acc_sub=0.9739
```

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```

9.3 Eval

[ ]:
```
TAU_SUB = 0.85
```

[ ]:
```
if APPROACH == "two_models":
    best_super_path = os.path.join(DATA_ROOT, "best_super_model.pth")
    best_sub_path   = os.path.join(DATA_ROOT, "best_sub_model.pth")
    model_super.load_state_dict(torch.load(best_super_path,␣
 ↪map_location=device))
    model_sub.load_state_dict(torch.load(best_sub_path,   map_location=device))

    run_eval = None
    if USE_WANDB:
        run_eval = wandb.init(
            entity=WANDB_ENTITY,
            project=WANDB_PROJECT,
            name=make_run_name("two_models_eval_resnet"),
            group="two_models",
            config={
                "approach": "two_models",
                "head": "sub",
                "backbone": BACKBONE,
                "epochs": EPOCHS,
                "lr_full": LR,
                "lr_head": LR_HEAD,
                "fine_tune_mode": FINE_TUNE_MODE,
                "img_size": IMG_SIZE,
                'sub_head_type': SUB_HEAD_TYPE,
                'super_head_type': SUPER_HEAD_TYPE,
```

```
                'tau_sub': TAU_SUB,
                'tau_super': TAU_SUPER,
            },
        )

    analyze_tau_sub(model_sub, mode="sub_single_head")
    analyze_tau_super(model_super, mode="super_single_head")
    evaluate_on_val_with_novelty(model_super, mode="super_single_head",
                                 tau_super=TAU_SUPER, tau_sub=TAU_SUB,
                                 loader=val_loader, name="val_super_only")
    evaluate_on_val_with_novelty(model_sub, mode="sub_single_head",
                                 tau_super=TAU_SUPER, tau_sub=TAU_SUB,
                                 loader=val_loader, name="val_sub_only")
    evaluate_pseudo_novel_sub_with_novelty(
        model_sub, mode="sub_single_head", tau_sub=TAU_SUB
    )
    novelty_dashboard(model_super, mode="super_single_head",
                      tau_super=TAU_SUPER, tau_sub=TAU_SUB,
                      include_pseudo=False)  # no pseudo-novel meaning for super␣
 ↪head
    novelty_dashboard(model_sub, mode="sub_single_head",
                      tau_super=TAU_SUPER, tau_sub=TAU_SUB,
                      include_pseudo=True)

    if run_eval is not None:
        run_eval.finish()

else:
    print("APPROACH is not 'two_models'; skipping two-model training in this␣
 ↪cell.")
```

```
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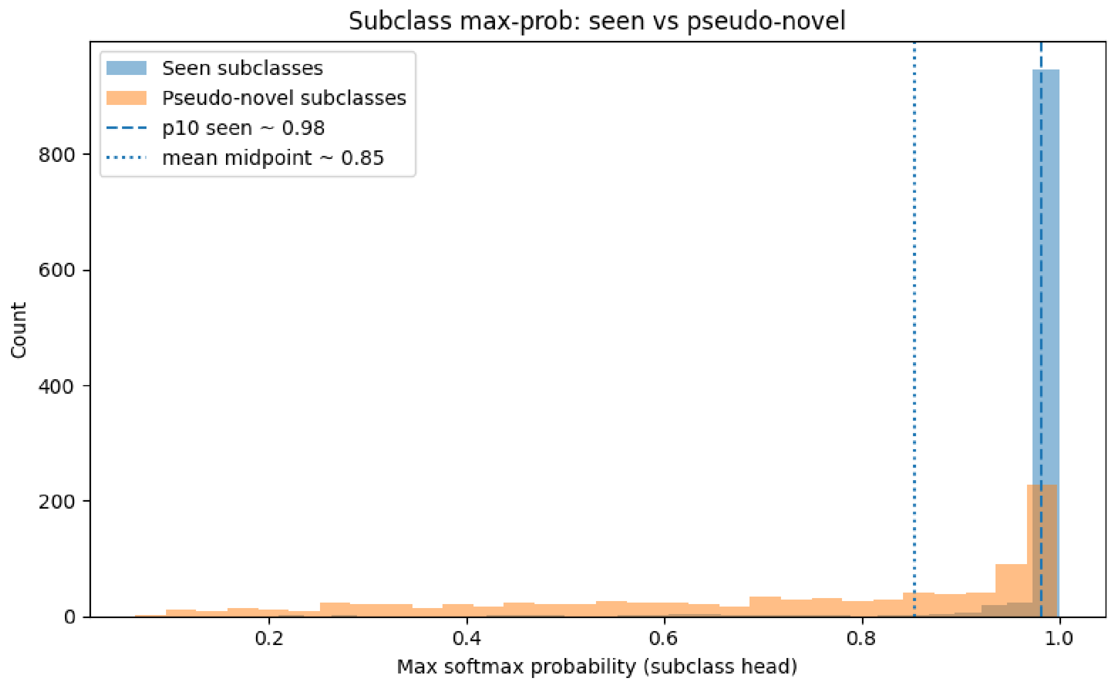
Seen subclass max-prob stats:
  count = 1034
  mean  = 0.983
  std   = 0.069
  percentiles:
    p 1: 0.612
    p 5: 0.936
```

```
    p10: 0.982
    p25: 0.996
    p50: 0.999
    p75: 1.000
    p90: 1.000
    p95: 1.000
    p99: 1.000

Pseudo-novel subclass max-prob stats:
  count = 948
  mean  = 0.724
  std   = 0.264
  percentiles:
    p 1: 0.116
    p 5: 0.226
    p10: 0.307
    p25: 0.522
    p50: 0.810
    p75: 0.964
    p90: 0.993
    p95: 0.996
    p99: 0.997

Suggested TAU_SUB candidates:
  tau_sub   10th percentile of seen: 0.982
  tau_sub   mean(seen + pseudo)/2:  0.854

You can start with one of these for TAU_SUB and adjust based on
leaderboard/behavior.
```



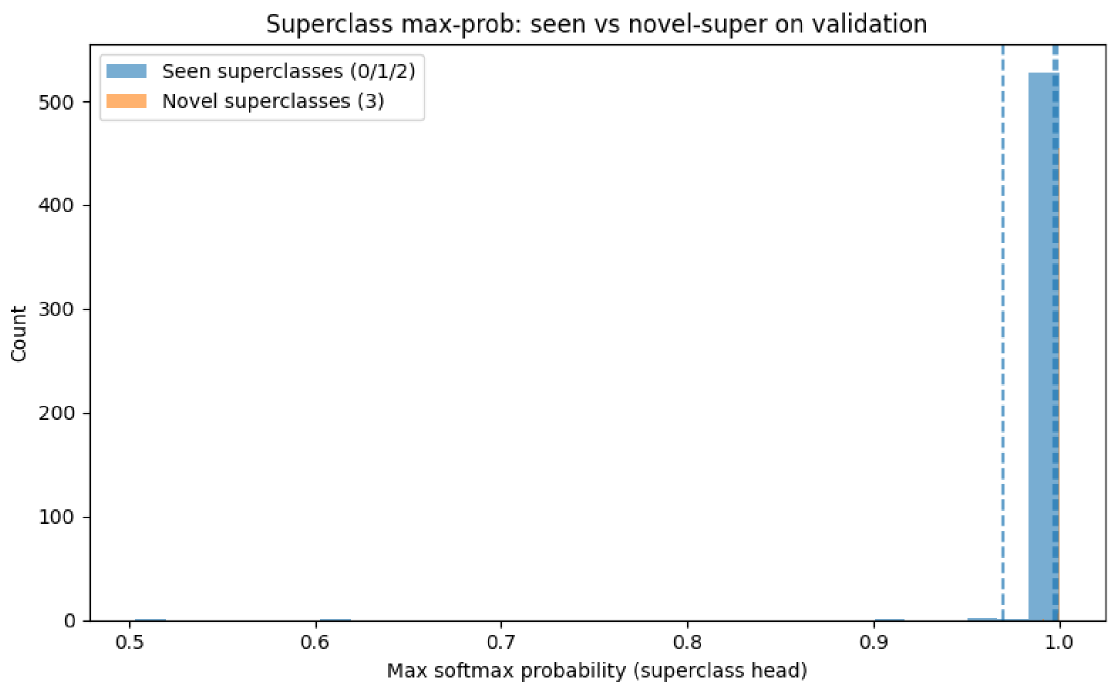

```
Logged histograms and tau_sub candidates to Weights & Biases.

Seen superclasses (0/1/2) superclass max-prob stats:
  count = 534
  mean  = 0.998
  std   = 0.028
  percentiles:
    p 1: 0.982
    p 5: 0.997
    p10: 0.999
    p25: 1.000
    p50: 1.000
    p75: 1.000
    p90: 1.000
    p95: 1.000
    p99: 1.000

Novel superclasses (== NOVEL_SUPER_IDX) superclass max-prob stats:
  count = 500
  mean  = 1.000
  std   = 0.000
  percentiles:
    p 1: 0.999
    p 5: 1.000
    p10: 1.000
```

```
    p25: 1.000
    p50: 1.000
    p75: 1.000
    p90: 1.000
    p95: 1.000
    p99: 1.000

Suggested TAU_SUPER candidates (using seen + novel):
  tau_super  10th percentile of seen:       0.999
  tau_super  5th percentile of seen:        0.997
  tau_super  mean(seen) - std(seen):        0.970
  tau_super  mean(seen & novel) midpoint:   0.999
```




```
Logged superclass histograms and tau_super candidates to Weights & Biases.

=== Evaluation on val_super_only ===
Overall superclass acc: 0.9913
Seen superclass acc (true super != novel):   0.9831
Seen superclass false-novel rate:            0.0169
Novel superclass acc (true super == novel):  1.0000

=== Evaluation on val_sub_only ===
Overall subclass acc:   0.9584
Seen subclass acc (true sub != novel):       0.9195
Seen subclass false-novel rate:              0.0805
```

```
=== Evaluation on pseudo_novel_sub (held-out subclasses) ===
Fraction flagged as novel (good): 0.5464
Fraction mapped to seen subclasses (bad): 0.4536

=== Evaluation on val ===
Overall superclass acc: 0.9913
Seen superclass acc (true super != novel):   0.9831
Seen superclass false-novel rate:            0.0169
Novel superclass acc (true super == novel):  1.0000

==== Novelty Dashboard ====
     Split   Head                             Metric  \
0   config      -                           APPROACH
1   config      -                           BACKBONE
2   config      -                   CIFAR_NOVEL_MODE
3   config      -                       DATA_AUGMENT
4   config      -                     FINE_TUNE_MODE
5   config      -                            TAU_SUB
6   config      -                          TAU_SUPER
7   config      -                   USE_PSEUDO_NOVEL
8      val  super  Novel superclass accuracy (CIFAR)
9      val  super           Seen superclass accuracy
10     val  super   Seen superclass false-novel rate

                                                Meaning       Value
0        Model architecture (two_heads vs two_models)  two_models
1        Feature extractor (e.g. resnet18 / resnet50)    resnet50
2                   Extra novel-super CIFAR data mode       large
3   Whether data augmentation is enabled for training        True
4             Backbone training mode (full vs frozen)        full
5                 Novelty threshold for subclass head        0.85
6               Novelty threshold for superclass head        0.99
7     Using held-out subclasses for pseudo-novel eval        True
8   CIFAR novel-super samples correctly predicted …        1.0
9            Correctly keep seen superclasses as seen    0.983146
10     Seen superclasses incorrectly flipped to novel    0.016854

=== Evaluation on val ===
Overall subclass acc:   0.9584
Seen subclass acc (true sub != novel):       0.9195
Seen subclass false-novel rate:              0.0805

=== Evaluation on pseudo_novel_sub (held-out subclasses) ===
Fraction flagged as novel (good): 0.5464
Fraction mapped to seen subclasses (bad): 0.4536

==== Novelty Dashboard ====
```

```
           Split Head                       Metric  \
0         config    -                     APPROACH
1         config    -                     BACKBONE
2         config    -             CIFAR_NOVEL_MODE
3         config    -                 DATA_AUGMENT
4         config    -               FINE_TUNE_MODE
5         config    -                      TAU_SUB
6         config    -                    TAU_SUPER
7         config    -             USE_PSEUDO_NOVEL
8   pseudo_novel  sub     Pseudo-novel mapped to seen
9   pseudo_novel  sub    Pseudo-novel marked as novel
10           val  sub          Seen subclass accuracy
11           val  sub   Seen subclass false-novel rate

                                              Meaning       Value
0        Model architecture (two_heads vs two_models)  two_models
1        Feature extractor (e.g. resnet18 / resnet50)    resnet50
2                   Extra novel-super CIFAR data mode       large
3   Whether data augmentation is enabled for training        True
4              Backbone training mode (full vs frozen)        full
5                  Novelty threshold for subclass head        0.85
6                Novelty threshold for superclass head        0.99
7     Using held-out subclasses for pseudo-novel eval        True
8   Held-out subclasses wrongly mapped to some see…    0.453586
9      Held-out subclasses correctly flagged as novel    0.546414
10            Correctly keep seen subclasses as seen    0.919476
11        Seen subclasses incorrectly flipped to novel    0.080524
```

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```

10 SECTION 8: Test-time Inference & CSV Export for leaderboard (two-head model)

[ ]:
```python
# Inference in order to predict "novel" superclass / subclasses


@torch.no_grad()
def predict_test_two_heads(model, test_loader, tau_super=TAU_SUPER,␣
↪tau_sub=TAU_SUB):
    """
    Inference for the two-heads model with novelty thresholds.
```

```python
    model:       SharedBackboneTwoHeads(...)
    test_loader: DataLoader yielding (images, img_names)
    tau_super:   threshold for superclass novelty
    tau_sub:     threshold for subclass novelty
    """
    model.eval()
    images_list = []
    super_preds = []
    sub_preds = []

    for images, img_names in test_loader:
        images = images.to(device, non_blocking=True)

        # Forward pass once
        super_logits, sub_logits = model(images)    # (B, num_super), (B,␣
↪num_sub)

        # --- Superclass predictions with novelty ---
        super_probs = F.softmax(super_logits, dim=1)            # (B, num_super)
        max_super_probs, super_idx = super_probs.max(dim=1)     # (B,)
        super_novel_mask = max_super_probs < tau_super
        super_idx = super_idx.clone()
        super_idx[super_novel_mask] = NOVEL_SUPER_IDX

        # --- Subclass predictions with novelty ---
        sub_probs = F.softmax(sub_logits, dim=1)                # (B, num_sub)
        max_sub_probs, sub_idx = sub_probs.max(dim=1)           # (B,)
        sub_novel_mask = max_sub_probs < tau_sub
        sub_idx = sub_idx.clone()
        sub_idx[sub_novel_mask] = NOVEL_SUB_IDX

        # Move to CPU as plain Python ints
        super_idx = super_idx.cpu().tolist()
        sub_idx   = sub_idx.cpu().tolist()

        # img_names is a list of filenames (len = B)
        images_list.extend(img_names)
        super_preds.extend(super_idx)
        sub_preds.extend(sub_idx)

    df = pd.DataFrame({
        "image": images_list,
        "superclass_index": super_preds,
        "subclass_index": sub_preds
    })
    return df
```

```
# SECTION: Test-time inference & CSV export for two-heads model

if APPROACH == "two_heads":
    # Recreate the model and load best checkpoint
    model_two_heads = SharedBackboneTwoHeads(num_super=num_super,␣
 ↪num_sub=num_sub).to(device)
    best_ckpt_path = os.path.join(DATA_ROOT, "best_two_heads_kl.pth")
    model_two_heads.load_state_dict(torch.load(best_ckpt_path,␣
 ↪map_location=device))

    test_predictions = predict_test_two_heads(
        model_two_heads,
        test_loader,
        tau_super=TAU_SUPER,
        tau_sub=TAU_SUB,
    )
    out_csv_path = os.path.join(DATA_ROOT, "two_heads_predictions.csv")
    test_predictions.to_csv(out_csv_path, index=False)
    print("Saved two-heads predictions (with novelty) to:", out_csv_path)
else:
    print("APPROACH is not 'two_heads'; skipping two-heads inference in this␣
 ↪cell.")
```

```
APPROACH is not 'two_heads'; skipping two-heads inference in this cell.
```

11 SECTION 9: Test-time Inference & CSV Export for leaderboard (two separate models)

[ ]:
```
TAU_SUB
```

[ ]:
```
0.85
```

[ ]:
```
@torch.no_grad()
def predict_test_two_models(model_super, model_sub, test_loader,
                            tau_super=TAU_SUPER, tau_sub=TAU_SUB):
    """
    Inference for the two-model setup (separate super + sub models) with␣
 ↪novelty thresholds.

    model_super: SingleHeadModel for superclass (num_classes = num_super)
    model_sub:   SingleHeadModel for subclass  (num_classes = num_sub)
    test_loader: DataLoader yielding (images, img_names)
    tau_super:   threshold for superclass novelty
    tau_sub:     threshold for subclass novelty
    """

```

```python
    model_super.eval()
    model_sub.eval()

    images_list = []
    super_preds = []
    sub_preds = []

    for images, img_names in test_loader:
        images = images.to(device, non_blocking=True)

        # Forward passes
        super_logits = model_super(images)   # (B, num_super)
        sub_logits   = model_sub(images)     # (B, num_sub)

        # --- Superclass predictions with novelty ---
        super_probs = F.softmax(super_logits, dim=1)            # (B, num_super)
        max_super_probs, super_idx = super_probs.max(dim=1)     # (B,)
        super_novel_mask = max_super_probs < tau_super
        super_idx = super_idx.clone()
        super_idx[super_novel_mask] = NOVEL_SUPER_IDX

        # --- Subclass predictions with novelty ---
        sub_probs = F.softmax(sub_logits, dim=1)                # (B, num_sub)
        max_sub_probs, sub_idx = sub_probs.max(dim=1)           # (B,)
        sub_novel_mask = max_sub_probs < tau_sub
        sub_idx = sub_idx.clone()
        sub_idx[sub_novel_mask] = NOVEL_SUB_IDX

        # Move indices to CPU as plain Python ints
        super_idx = super_idx.cpu().tolist()
        sub_idx   = sub_idx.cpu().tolist()

        # img_names is a list of filenames (len = B)
        images_list.extend(img_names)
        super_preds.extend(super_idx)
        sub_preds.extend(sub_idx)

    df = pd.DataFrame({
        "image": images_list,
        "superclass_index": super_preds,
        "subclass_index": sub_preds,
    })
    return df


if APPROACH == "two_models":
```

```
    model_super = SingleHeadModel(num_classes=num_super, head=SUPER_HEAD_TYPE).
↪to(device)
    model_sub   = SingleHeadModel(num_classes=num_sub, head=SUB_HEAD_TYPE).
↪to(device)

    model_super.load_state_dict(torch.load(os.path.join(DATA_ROOT,␣
↪"best_super_model.pth"),
                                           map_location=device))
    model_sub.load_state_dict(torch.load(os.path.join(DATA_ROOT,␣
↪"best_sub_model.pth"),
                                         map_location=device))

    test_predictions_two_models = predict_test_two_models(
        model_super, model_sub, test_loader,
        tau_super=TAU_SUPER, tau_sub=TAU_SUB,
    )

    out_csv_path = os.path.join(DATA_ROOT, "two_models_predictions.csv")
    test_predictions_two_models.to_csv(out_csv_path, index=False)
    print("Saved two-model predictions (with novelty) to:", out_csv_path)

else:
  print("APPROACH is not 'two_models'; skipping two-models inference in this␣
↪cell.")
```

```
Saved two-model predictions (with novelty) to: /content/drive/MyDrive/NNDL-
Project/Project Data/two_models_predictions.csv
```

11.1 Submission Info

Team Name: Caged Manifolds

Model Name: ResNet50v2 with Data Augmentation - Cosine Similarity heads

Description: 2 model architecture (separate super and subclass predictor), various regularization and data augmentation added, cosine classifier subhead