
Transfer Learning: Exploring Two-Headed CNN w/Interaction Loss vs. Two separate CNN Models for Superclass/Subclass Classification

Christian Montgomery and Aksel Kretsinger-Walters

Columbia University

cm4521@columbia.edu, adk2164@columbia.edu

1 Introduction

We explored optimal techniques of transfer learning for the multi-label image classification task, predicting superclass (bird/dog/reptile/novel class) and subclasses (87 seen + novel subclass) for a selection of 64×64 images. The main challenge to overcome was distribution shift between the training and test datasets, and novel classes appearing at test time (identifying both new superclasses and new subclasses as “novel”).

To maximize our performance on this classification, we explored two different model architectures: a multi-headed CNN with KL Interaction term, and separately two distinct CNN’s for each classification task. We trained detecting for “novel” superclasses via including some out-of-distribution data from CIFAR 100, and held-out some subclass images from training to assess pseudo-novel detection. For both classifications, we tuned a threshold on the max softmax score for each image, implying whether it represented a novel class or not. Two other areas we explored were varying the amount of out of distribution “novel” superclass images provided during training and experimenting with both full and frozen fine-tuning to assess generalization on unseen classes during testing.

Overall, testing showed that two-separate models performed better at identifying seen superclasses, worse at unseen superclasses, and about equivalent on subclasses overall. Interestingly, reducing the number of CIFAR 100 novel superclass images included (from 5,000 to 1,000) did not alter superclass prediction much, contrary to expectations. But it did meaningfully worsen performance on seen subclasses while meaningfully improving performance on unseen subclasses (perhaps expected from a model more “naive” to distribution of natural images). Lastly, altering the fine tuning from full to frozen changed.....

2 Background & Related Work

Our work sits at the intersection of transfer learning for vision, multi-task classification and novelty detection. A common approach in computer vision is to use a CNN pretrained on a large dataset like ImageNet and then adapt it for a downstream task. Our approach considered both ends of the fine-tuning spectrum, 1. full fine-tuning of all ResNet layers which has been shown to exhibit high performance at the potential cost of overfitting, and 2. freezing the backbone to extract features from the base model while training only the linear head on top which is known to lead to greater stability.

Prior work on multi-task and multi-label classification often uses one of two architectures, either a shared feature backbone with multiple heads, or multiple models. We decided to implement both patterns, as the shared-backbone with multiple heads is able to share features between the heads, while the two-separate model design allows each classifier to specialize. builds upon previous transfer learning experimentation and has discovered that the combination of X, Y, and Z provides the best performance for this specific task.

A key challenge is that our test data includes classes that aren’t available in training. This relates to the concept of open-set recognition and out-of-distribution (OOD) detection, where the goal is to flag samples that don’t belong to any known training class. A common approach is to apply a threshold on the maximum softmax probability, and if the model’s confidence is below this threshold, the sample is treated as “novel”, which is what we use. In order to train our model to recognize images from the subspace of “novel” superclasses, we incorporate OOD training by including images from CIFAR-100, to approximate the distribution of unknown classes. For novel subclasses, without a curated set of new dog/bird/reptile subclasses, we used a common “pseudo-novel” strategy of holding out a subset of subclasses from the training set, which allowed us to calibrate subclass thresholds.

Lastly, in the case of a single model with a shared backbone and two separate heads, it is common to use an interaction loss (KL divergence) to encourage consistency between superclass and subclass predictions (since each subclass is mapped to a unique

superclass). This type of consistency regularization relates to ideas from knowledge distillation and hierarchical classification, where one head is encouraged to agree with a derived distribution from another.

3 Methods

Overall, we built our image classification model upon a CNN-based architecture, using PyTorch within a Colab GPU and Weights & Biases for tracking training and validation error. We chose a convolutional neural network based architecture as they have repeatedly been shown to perform well on image classification tasks. We leveraged a pretrained ResNet-50 backbone trained on ImageNet to transfer learn from, and added a linear layer on top to map from final feature vectors of the pretrained model to our classification labels (both superclass and subclass). There were about $\sim 6,600$ training images, 64×64 RGB, which had superclass labels of {bird, dog, reptile} for training, 87 subclass labels within each superclass, and a “novel” label used for both unseen superclasses and unseen subclasses at test.

In processing our input data, we resized if necessary to 64×64 and then normalized with standard ImageNet normalization using the average and standard deviation of pixel values used for the RGB channels of ImageNet dataset. We randomly applied horizontal flips and random rotations by 10 degrees to our training data in order to ensure our model learned image content while remaining invariant to subject orientation.

3.1 CIFAR-100 based novel superclasses

To ensure our model was trained to generalize to images with a superclass it has never seen before (and thus should label novel), we supplemented with a subset of CIFAR-100 images which represented a novel superclass (and by extension subclass). For example, these were images that did not represent a bird, dog, or reptile, and thus we labeled them as novel. We started with 5,000 additional images (roughly double training set size) and experimented with scaling that down to only 1,000 additional images ($\sim 15\%$ of training set size). We had our validation set as 10% of total training data.

3.2 Pseudo-novel subclasses

For our model to generalize to novel subclasses, unfortunately we were limited by time and resources and could not curate a precise dataset of dogs, reptiles and birds that were exclusively not of the subclass categories provided in order to train on those novel subclasses. Instead, we used the concept of “pseudo-novel” subclasses. This entailed randomly holding out a fraction (15%) of subclasses from training entirely, then training on “seen” subclasses only, and using held-out subclasses during validation to determine an optimal confidence threshold by which to classify an image as a novel subclass. For inference, we did not hold out any subclasses so the model would have full knowledge of all subclasses in testing.

3.3 Thresholding rule

For a mechanism to infer whether a test image was of a superclass and subclass previously seen, we introduced a thresholding rule for both classification. This means that for a given percentage, (i.e. 80%), if the max softmax score for a given classification task is above 80%, the class with that softmax score is chosen as the predicted class, but if score is below, then “novel” class is chosen instead. We used separate τ_{super} and τ_{sub} for thresholding the superclass and subclass predictions respectively, which were tuned by analyzing validation performance. The below equation represents how that calculation was used at inference for both classification tasks.

$$\hat{y} = \begin{cases} \arg \max_c p(c | x), & \text{if } \max_c p(c | x) \geq \tau \\ \text{novel}, & \text{otherwise.} \end{cases}$$

Before running our model for inference, we tuned these thresholds by toggling on “pseudo-novel” so that a subset of subclasses were held out from training. We charted the results below, and decided on $\tau_{\text{super}} = 0.99$ and $\tau_{\text{sub}} = 0.85$ accordingly. The tradeoff was needing to balance between a lower threshold meant missing some “Novel” classifications, while a higher threshold would mean incorrectly classify some seen classes as “Novel”. The τ_{super} of 0.99 though high, makes sense, as we augmented training data with “Novel” CIFAR-100 images so our model actually learns about the “Novel” superclass subspace.

3.4 Approach A: Single model, 2 separate heads + KL divergence term

Our first approach in Model Architecture was utilizing a shared ResNet-50 backbone for feature learning and having two classification heads (superclass and subclass). The superclass head produced superclass logits (4 classes including novel) and the subclass head produced subclass logits. Each head is trained using its own cross-entropy loss error term, and we added an additional term to mitigate potential divergence between superclass and subclass predictions (as in, the superclass being a bird and the subclass being a golden retriever). Accordingly, we added an interaction loss term, which is the KL divergence

between: 1. Implied probability of a superclass (sum of corresponding subclass probabilities) and 2. The superclass model head's calculated probability of that subclass. Thus, the total loss reflects this term as well.

Diagram below shows our total loss computation by component.

3.5 Model Architecture

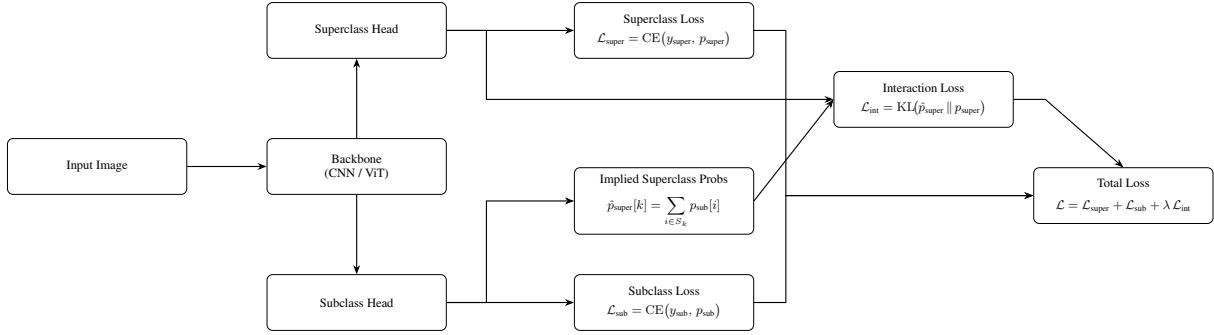


Figure 1: Model architecture and loss computation.

3.6 Interaction Loss / KL Divergence Calculations

For each superclass k , with subclass set S_k :

$$\hat{p}_{\text{super}}[k] = \sum_{i \in S_k} p_{\text{sub}}[i].$$

Then define interaction loss, e.g.:

$$\mathcal{L}_{\text{int}} = \text{KL}(\hat{p}_{\text{super}} \parallel p_{\text{super}}).$$

The Kullback–Leibler (KL) divergence between two distributions P and Q is:

$$\text{KL}(P \parallel Q) = \sum_k P(k) \log \frac{P(k)}{Q(k)}.$$

Equation below demonstrates math behind the KL divergence, which we used in Approach A.

3.7 Approach B: Two independent models, separate for superclass and subclass

Our second approach was adapting our architecture to have two separate ResNet-50 models, one for superclass and one for subclass. Each model has its own cross-entropy loss during training, and they are independently trained. At inference, their predictions are combined. The benefits of this approach are that each model can specialize for its particular classification task with little inference, the downside is more parameters and no consistency regularization.

3.8 Approach C: Two independent models, separate for superclass and subclass (cosine similarity head)

Our third approach was to modify the subclass model to implement a cosine similarity head instead of a linear feed-forward head.

3.9 Evaluation

The metrics used to evaluate model performance on unlabeled test data were: 1. cross-entropy, 2. overall accuracy, 3. seen accuracy and 4. unseen accuracy, all for both superclass and subclass. We were limited to a max of five leaderboard submissions.

4 Experimental Setup

Our hyperparameters were chosen as the following (for all models, unless denoted above): Batch size of 64, 15 training epochs, learning rate of 10^{-4} , weight decay of 10^{-4} for generalization, and Adam as optimizer. The hyperparameters used for the KL

divergence term in Approach A was an alpha value of 0.1 and a Temperature value of 1.0. Lastly, We selected a τ_{super} of 0.99 and τ_{sub} of 0.85 to threshold novel class predictions.

Below is a configuration table of our submissions, to illustrate differences in approaches.

Table 1: Configuration table of submissions.

Approach	Architecture	CIFAR novel super size	Backbone	Learning Rate	Head Type
A	Two-heads	5000	fine-tuned	.0001	Linear
B	Two models	5000	fine-tuned	.0001	Linear
C	Two models	5000	fine-tuned	.0001	Super-Linear, Sub-Linear

5 Results

Below table shows overall performance vs. baseline - the leaderboard test accuracy metrics:

Table 2: Leaderboard test accuracy metrics.

Approach	Overall Super	Seen Super	Unseen Super	Overall Sub	Seen Sub	Unseen Sub
A	83%	90%	63%	71%	84%	67%
B	85%	96%	57%	70%	83%	66%
C	90%	94%	79%	70%	75%	68%

5.1 Analysis

Overall, right from our initial Approach A and leaderboard submission we saw improved test accuracy vs. baseline in all categories except “Seen Super” where we had 90% accuracy for Approach A vs. 99% baseline. This made sense to us, as there is an inherent tradeoff in maximizing seen vs. unseen accuracies when using a threshold to predict “Novel” classes. The tradeoff is that if you set a lower threshold, say 90% threshold instead of 99% threshold as we did, we may have improved “Seen” accuracy at the expense of “Novel” accuracy since we would have reduced the rate of misclassifications labeled as “Novel” that were actually “Seen”. Since the goal was to improve the unseen accuracies vs. baseline, which we did meaningfully for both Super and Sub, we are satisfied with these results. Thus, we kept these thresholds (τ_{sub} and τ_{super}) consistent for all of our approaches accordingly. We will now review the differences each approach was meant to isolate, one by one.

5.2 Two-Heads vs. Two-Models performance

Below demonstrates the key performance differences between these two approaches, with all else held constant. Notably, only the superclass performance diverged meaningfully, as subclass performance was very similar. The superclass performance on “Seen” superclasses improved for two-models, which is intuitive as there was no interaction between the two classifier heads (as the two-headed model faced). However, the generalization worsened as the superclass performance on “Unseen” superclasses decreased for two-models, which makes sense as the superclass model became relatively more overfit without the implicit regularization of the shared backbone & KL-term.

Performance Delta Between Two-Heads and Two-Models

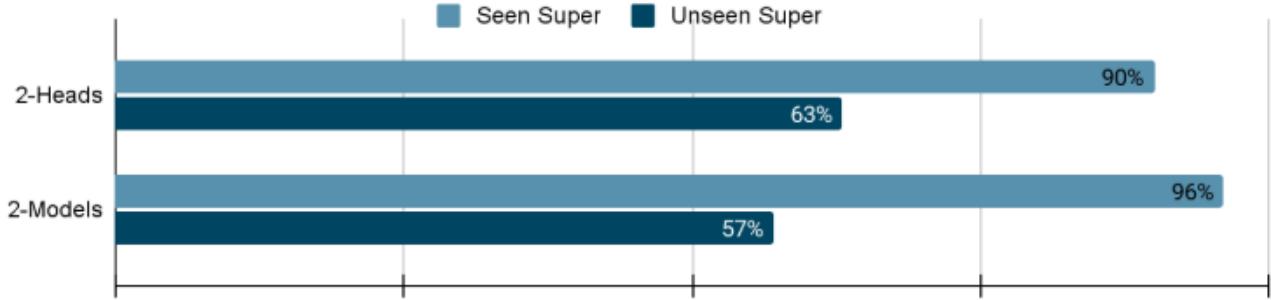


Figure 2: Performance delta between Two-Heads and Two-Models.

5.3 5,000 vs. 1,000 CIFAR-100 “Novel” Superclass Images Added performance

Interestingly, reducing the number of “Novel” class superclass images added to the training data only affected the superclass accuracy performance very little. We suppose this is from 1,000 CIFAR-100 being of sufficient size (relative to $\sim 6,600$ original training images) for the model to learn the patterns of the subspace of images that do not represent a bird, dog, or reptile, such that additional random examples from this complement space do not notably improve the accuracy.

However, for subclass accuracy, we observe meaningful differences. Notably, when we reduce the amount of images added (labeled as Novel superclass), we worsen performance on seen subclasses, but meaningfully improve performance on unseen subclasses. Given that this was tested on the two-model architecture, where the only training data with “Novel” subclasses would be images that are not birds, dogs and reptiles, the most plausible explanation is that we were “teaching” the model that novel subclasses come from a distribution beyond the superclasses of the training data. Therefore, when we relax this constraint (less images added), we reduce the “overfitting” to that constrained case of subclasses out of training distribution, and thus we improve on generalization of subclass accuracy for unseen subclasses in test data. We expect the model with less images added is more “naive” to the distribution of natural images.

Performance Delta Between 5,000 and 1,000 Superclass Images Added

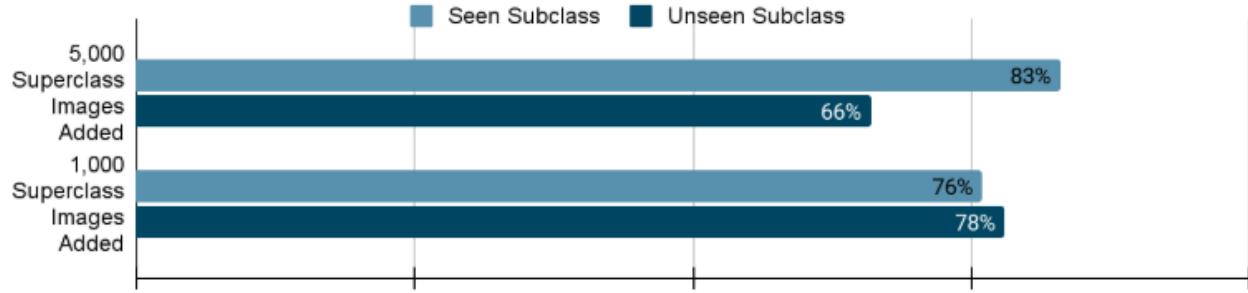


Figure 3: Performance delta between 5,000 and 1,000 superclass images added.

5.4 Amount of Fine-Tuning for Transfer Learning (Full fine-tuning vs. Fixed backbone)

Here we changed from full fine-tuning (with a learning rate of 0.0001) to fixing the ResNet50 backbone and only fine-tuning a single linear layer on top (with a learning rate of 0.01). This led to our worst performance, with the performance on subclasses meaningfully worse across the board vs. any of our other approaches (for overall, seen, and super). This makes sense as we likely had too high a learning rate to learn nuances between dogs/reptiles/birds well. The results for superclass accuracy were more interesting, as the seen superclass performance was worse, but the unseen superclass performance the best out of all of our approaches. We think this is because only the single linear layer was tuned on the superclass model, so it was able to specialize in identifying a “Novel” superclass vs. having that signal distorted when propagated across the full backbone (as in our other approaches).

Performance Delta Between Full Fine-Tuning and Fixed Backbone

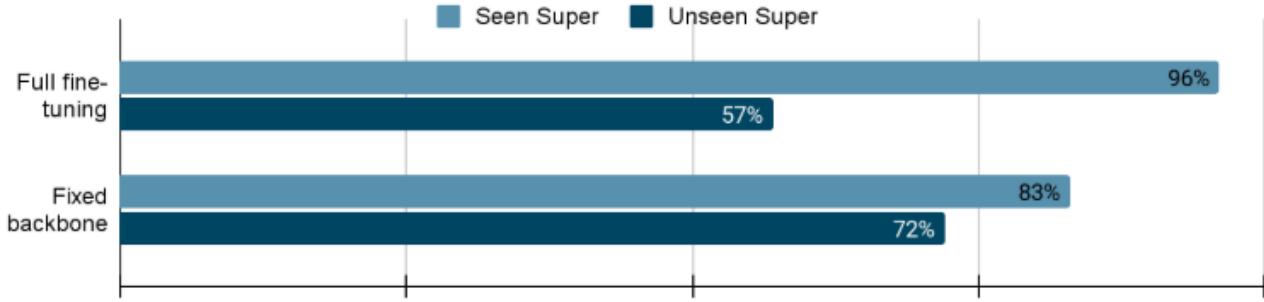


Figure 4: Performance delta between full fine-tuning and fixed backbone.

6 Discussion and Limitations

Our best model demonstrates (Approach B) demonstrates good performance on seen super and subclasses, and $\sim 60\%$ performance of catching novel super and subclasses in test data. We note that at the time of writing, this model’s performance seems to exceed that of most other ResNet-based architectures on the leaderboard, though surpassed by vision transformer-based architectures.

Limitations exist in our use of CIFAR and “pseudo-novel” subclass holdout as proxies for calibrating our thresholds for inference of “Novel” superclass and subclass respectively. CIFAR-100 served as an approximation for showing the model “out of distribution” superclass data, but did not necessarily include ambiguous data on the margin. Neither did our “pseudo-novel” technique necessarily teach our model to learn the full subspace of dog breeds (or reptiles/birds). Since there is a natural confidence overlap between seen and novel, we always faced the tradeoff in determining at what discrete point the boundary should lie.

We initially expected a single model with two heads and KL divergence term would be higher performing, due to its seemingly greater sophistication and unifying approach. We were surprised to learn, however, that two models trained separately perform better on our test data. Additionally, our initial instinct was that freezing the transfer learning backbone and only fine-tuning a layer on top would be superior, but apart from the unseen superclass evaluation metric, it was not. Lastly, it was also very surprising that reducing the amount of CIFAR superclass data affected the subclass performance much more noticeably than the superclass performance, though now we better appreciate the inherent complexity and sensitivity to change of neural networks.

7 Conclusion & Future Work

We experimented with various strategies to maximize performance on this transfer-learning image classification task. The approaches pursued were changing architecture (single model with two heads + KL divergence term vs. two models), changing number of extra images added to training data (5,000 vs. 1,000), and changing the amount of fine-tuning (full fine-tuning vs. fixed backbone). Our best model was using two separate models, with 5,000 novel superclass images added, and performing full fine-tuning.

Given further time and resources, we would have spent more time curating out of distribution datasets to add to the training data (in particular, images from novel subclasses from the given superclasses, as in new dog breeds, reptiles, and birds). We would have explored implementing more advanced and modern architecture such as Vision-Transformers.

References

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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)
```

```

# 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 |
+-----+-----+-----+
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| 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_PSEUDO_NOVEL IS FALSE BEFORE LEADERBOARD SUBMISSION #####
# Used to fine-tune TAU_SUB
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} was 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}

```

```

[ ]: # 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

```

```

[ ]: # 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, u
→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), u
→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], u
→ignore_index=True)
val_split_df = pd.concat([val_seen_df, val_novel_df], u
→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,
    )

```

```

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")
    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 ~\u2192{tau_candidate_1:.2f}")
plt.axvline(tau_candidate_2, linestyle=":", label=f"mean midpoint ~\u2192{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)

```

```

    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):      □")
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):      □")
    print(f" tau_mean_minus_std: {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

```

```

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:

```

```

        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:

```

```

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",
        "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\u20d7
        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

```
[ ]: 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

```
[ ]: 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  $p(\text{super}/x)$ . We aggregate the subclass ↵
↳ head's probabilities into
    #  $q(\text{super}/x)$  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):  $KL(\text{teacher} // \text{agg\_super})$ 
            # 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

```

```

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

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

```
[ ]: 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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```

```

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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=SUPER_HEAD_TYPE).
    ↪to(device)
    criterion_sub = nn.CrossEntropyLoss()
    optimizer_sub = setup_backbone_training(
        model_sub,
        fine_tune_mode=FINE_TUNE_MODE,

```

```

        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}, "

```

```

        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
```

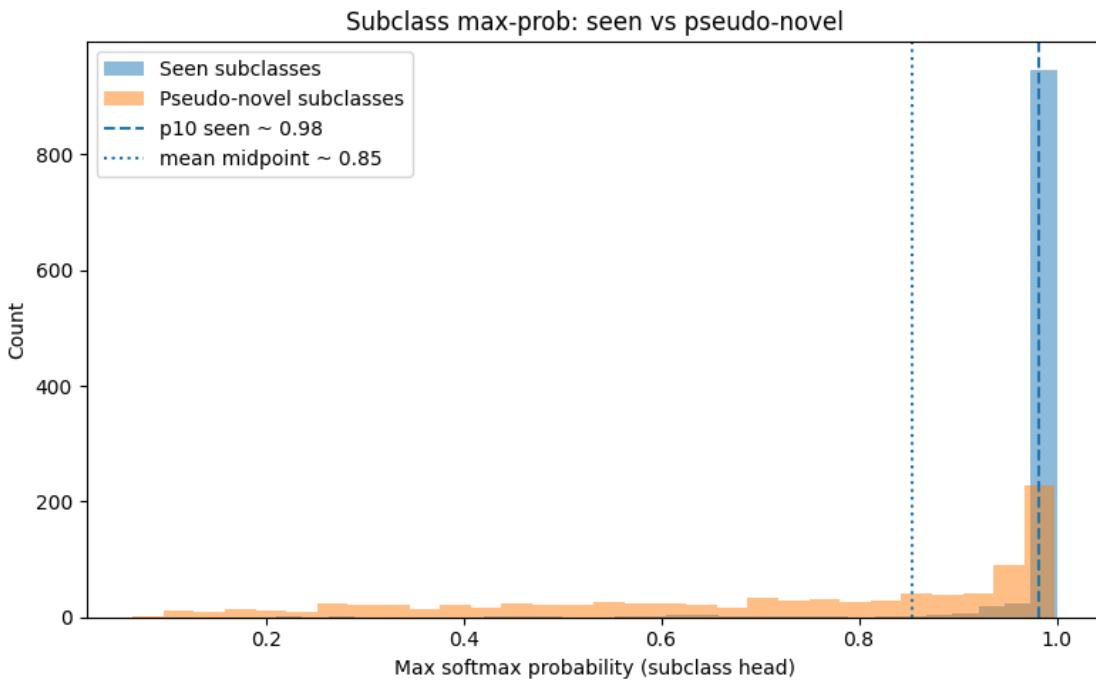
Pseudo-novel subclass max-prob stats:

```
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
```

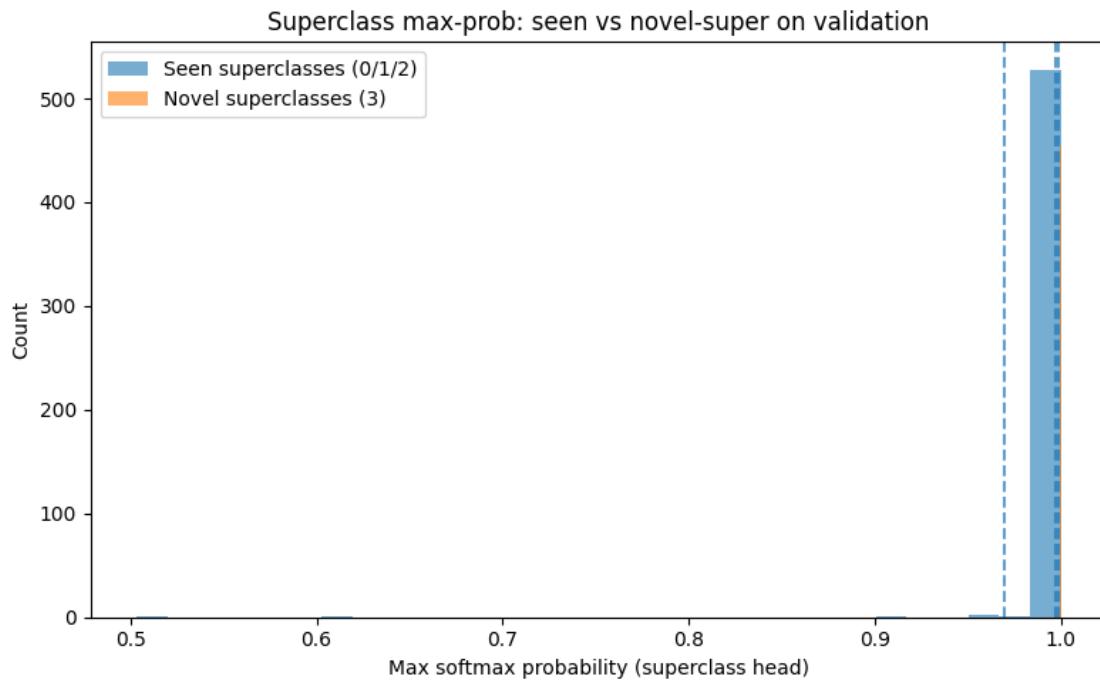
```

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 leader-board (two-head model)

```
[ ]: # 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.

```

```

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 leader-board (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
    """

```

```

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