

Lumen Data Science Team: MedMax

Technical documentation

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Introduction

This technical documentation provides an overview of our melanoma classification pipeline, developed as part of the Lumen Data Science competition during the 2024/2025 academic year. It is intended to serve both as a user guide and a developer reference for understanding, executing, and reproducing our solution.

The report is structured to walk the reader through every aspect of the system—from environment setup and modular code architecture, to training, evaluation, and deployment workflows. We explain how to use the CLI interface, modify configurations, and run trainings. Special attention is given to environment reproducibility using Docker and Conda, and to the modular design of the training components (data loading, model configuration, loss functions, and evaluation metrics).

Finally, we include a detailed reproducibility checklist—giving the exact configuration, system setup, and commands required to reproduce our best-reported results.

Project Structure and Organization

In this section, we describe the technology stack used for the project, how the codebase was organized to ensure modularity, how multi-GPU training was enabled, and how our custom DataLoader handles image loading and preprocessing. We also provide usage details for key components of the code and explain how its functionality can be easily extended.

2.1 Technology Stack

We used Python 3.10 for this project, conda for environment setup as a package manager, and PyTorch¹ as the main deep learning library. We used submittit² for submitting jobs to Slurm, Docker³ for code containerization, and tmux⁴ for running code in detached terminals and avoiding SSH interruptions. GitHub was used for version control and collaboration, while Kaggle⁵ was used for initial model exploration.

Other important libraries used include kneed⁶ for detecting the knee point of a function (useful for ITA prediction), fairlearn⁷ for fairness metric calculation, torchsampler⁸ for efficient oversampling, timm⁹ for model creation, seaborn¹⁰ and matplotlib¹¹ for visualization, and tensorboardX¹² for experiment logging. Export to ONNX¹³ and TorchScript¹⁴ is supported and described in a later section.

We also used HuggingFace¹⁵ to deploy our model and our code, making our model available for inference using Hugging Face transformers library.

```
1https://pytorch.org
2https://github.com/facebookincubator/submitit
3https://www.docker.com
4https://github.com/tmux/tmux
5https://www.kaggle.com
6https://github.com/arvkevi/kneed
7https://fairlearn.org
8https://github.com/ufoym/imbalanced-dataset-sampler
9https://github.com/huggingface/pytorch-image-models
10https://seaborn.pydata.org
11https://matplotlib.org
12https://matplotlib.org
12https://github.com/lanpa/tensorboardX
13https://onnx.ai
14https://pytorch.org/docs/stable/jit.html
15https://huggingface.co/
```

2.2 ISIC 2020 Dataset

We use the official ISIC 2020 classification dataset¹⁶, which includes dermoscopic images labeled as benign or malignant. The dataset must be downloaded and structured in the following format:

```
/path/to/isic2020_challenge/
  train/
    class1/
      img1.jpeg
    class2/
      img2.jpeg
  val/
    class1/
      img3.jpeg
    class2/
      img4.jpeg
  masks/ #optional, dataloader works without them.
    train/
      class1/
        mask1.png
      class2/
        mask2.png
    val/
      class1/
        mask3.png
      class2/
        mask4.png
```

In addition to the raw images, we provide a CSV file with following required fields: image_name, group, target, group_str, and split. This file enables metadata-based grouping (e.g., by skin tone) and train/validation splitting.

Utilities. To prepare the dataset, we provide the following scripts:

- preparer/move.py for moving images to the correct class folders.
- preparer/prepare_split.ipynb an notebook for assigning splits and verifying data organization.
- src/scripts/generate_skin_masks.py script for generating segmentation masks based on skin detection, given a source path.

For reproducibility, the metadata CSV file used during training is also included in our GitHub repository.

2.3 Code Structure

The project is organized in a modular and scalable structure. Below is a simplified directory tree (up to depth 3) that outlines the key components.

¹⁶https://challenge.isic-archive.com/data/

```
configs/
                                                # Model-specific
     training configs
                   convnext_base.py
                   convnext_large.py
3
                                                # Dockerfiles for
             docker/
     containerization
                   Dockerfile
                   Dockerfile_cpu
                                                # Conda environment
             environment.yml
     definition
            isic2020_challenge/
                                               # Dataset: splits, masks,
      and labels
                   ISIC_2020_full.csv
                   masks/
10
                         train/
11
                         valid/
12
                   train/
                         benign/
14
                         malignant/
15
                   valid/
                       benign/
17
                       malignant/
18
            melanoma_classifier_output/
                                               # Training logs, configs,
19
      and checkpoints
            melanoma_train.py
                                               # Main training script
20
            melanoma_eval.py
                                               # Evaluation script
21
            notebooks/
                                               # Exploratory notebooks
22
                   skin_tone_analysis.ipynb
23
24
                   skin_tone_estimation.ipynb
            preparer/
                                               # Data preprocessing
25
     scripts
26
                   move.py
                   prepare_split.ipynb
27
            src/
                                               # Core project modules
28
                   datasets/
29
                         data_processing.py
30
                         datasets.py # custom datasets
31
                         sampler.py
                                        # custom samplers
32
33
                   engine/
                         engine.py
                                        # train and test logic
                         scheduler.py
35
                   evaluation/
36
                                       # metric definition
37
                         metrics.py
                   models/
38
                         backbones/
                                       # models used for feature
39
     extraction, e.g. ConvNeXt, DinoV2
                                        # layers needed for models
                         layers/
40
     initialization
                                        # loss function definitions
                         losses/
41
                         melanoma_classifier.py # our classification
42
     model wrapper
                         optim_factory.py
                                               # optimizer factory
43
                         utils/
44
                   scripts/
45
                         estimate_ita.py
                                                       # script for ITAS
```

```
estimation from images
                          generate_skin_masks.py
                                                        # mask generator
47
     script
                   utils/
48
                                              # argument parsing
                          argparser.py
49
     utilities
                          distributed.py
                                             # distributed training
50
     utilities
51
                          logging_utils.py
                                             # logging utilities
                          utils.py
                                              # model saving logic
52
     utilities, etc.
                   visualization/
53
                       visualize_images.py
                                                # Testing entrypoint
55
             test.sh
             train.sh
                                                # Training entrypoint
56
                                                # Model weights directory
             weights/
57
```

Listing 2.1: Project Directory Structure

2.4 Modular Design

The main idea behind the code is modularity. We wanted to iterate quickly and try different experiment setups, which required from us to build a code that is easy to maintain and even easier to extend.

In the following sections, we will go through main components of our system, focusing on how our custom DataLoader operates, how we made it possible to add a completely new architecture with few lines of code, how we managed to handle multiple options for samplers, optimizers, losses, loss weights, metric calculations, etc.

2.4.1 Dataloader design

LocalISICDataset, as we named it, is a highly modular PyTorch Dataset implementation designed specifically for the ISIC 2020 skin lesion dataset. It supports advanced preprocessing, skin tone—aware augmentation, and segmentation-based manipulation of images, as we wanted to explore whether and how colorspace (RGB vs LAB), augmentations (skin color transformations), segmenting out skin, and oversampling helps our model to perfrom better.

Key Features:

- Input configuration: Supports directory-based dataset structure with separate folders for train/test, benign/malignant images and corresponding segmentation masks. Masks may only be used/present if we want masking out skin and learning only on the masked images.
- Skin tone integration: When a skin_color_csv is provided, the loader incorporates:
 - ITA (Individual Typology Angle)
 - Fitzpatrick skin scale
 - Group labels for skin-type-aware augmentation

- Oversampling with augmentations: For malignant samples, user-defined augmentations (e.g., rotations, brightness shifts) can be selectively applied. The loader supports sampling with an oversampling ratio derived from the number of augmentations. This was used to artificially increase the number of positives.
- Color space transformation:
 - Standard RGB pipeline
 - Optional conversion to CIELAB color space
 - Group-specific pixel-level transformations to simulate skin tone shifts ("skin-former" mode) idea is to mask out the skin from the image and with certain probability to darken it, as most of the skin color types are of lighter colors.
- Mask-based processing: If segment_out_skin=True, the loader uses segmentation masks to isolate lesions and mask out all the other pixels.

Return Values: Each call to __getitem__ returns a triplet:

```
(image: Tensor, label: int, group: int)
```

where group encodes the patient's skin tone classification, and is used for group-aware training and fairness analysis.

2.4.2 Classifier design

The classification model is implemented in src/models/melanoma_classifier.py. It is structured as a modular wrapper around backbone feature extractors, enabling flexibility in switching between different model architectures. Each backbone is followed by a classification head — a linear layer — making the overall model suitable for 2-class melanoma classification.

Skin Tone Group-Aware Extension. To support fairness-aware training, the classifier can optionally be extended to produce $num_classes \times num_groups$ outputs. This is used when performing group-aware loss computation (e.g., skin tone—sensitive learning), and allows the same model to adapt to fairness constrained tasks.

Backbone Support. The classifier supports the following pretrained architectures:

- ConvNeXt using create_convnext_model¹⁷
- ConvNeXtV2 using create_convnext_v2_model 18
- EfficientNetV2 using crete_efficientnet_v2_model¹⁹
- DINOv2 through create_dinov2_model²⁰

Each model returns either a classification token (e.g., in ViT/DINOv2) or pooled feature vector (e.g., in CNNs), which is then passed to a fully connected nn.Linear head layer. The head is dynamically adjusted to match the number of target classes.

¹⁷https://arxiv.org/abs/2201.03545

¹⁸https://arxiv.org/abs/2301.00808

¹⁹https://arxiv.org/abs/2104.00298

²⁰https://arxiv.org/abs/2304.07193

Training Flexibility. The classifier accepts parameters to control:

- Whether to use pretrained weights
- Whether the backbone was trained on ImageNet-22K (via in_22k)
- Whether to freeze the backbone and only fine-tune the head (for linear probing)

The model is used in both standard and fairness-aware training setups. To add a new backbone, one must define a custom create_model_x function inside src/models/model_x.py, and extend the model selection logic in src/models/melanoma_classifier.py to include the corresponding model_name.

The logic can be summarized as the following pseudocode:

```
Algorithm 1 Backbone Selection in MelanomaClassifier
```

```
1: function MelanomaClassifier(model_name, num_classes, pretrained, in_22k, freeze)
      if model name contains "convnext " then
          Load ConvNeXt backbone
3:
          Replace head with Linear(num_features, num_classes)
4:
      else if model name contains "efficientnet" then
5:
          Load EfficientNetV2 with specified parameters
6:
      else if model name contains "convnextv2" then
7:
          Load ConvNeXtV2 with specified parameters
8:
      else if model name contains "dinov2" then
9:
          Load DINOv2 backbone
10:
          Append Linear(num_features, num_classes) to CLS output
11:
12:
      else
          Raise error: Unsupported model
13:
14:
      end if
      return wrapped model
15:
16: end function
```

2.4.3 Criterion design

Inside src/models/losses/criterion.py, we define several custom loss functions: OhemCrossEntropy, RecallCrossEntropy, DomainIndependentLoss, DomainDiscriminativeLoss, and FocalLoss, along with support for InverseFrequencyWeighting.

The choice of loss function and whether to enable inverse frequency weighting is controlled via command-line arguments, making it easy to experiment with different training objectives. This modular design also allows us usage of domain-aware and domain-independent strategies during training and evaluation. Again, to add a criterion, one should add a class that inherits nn.Module with forward method and add a command line argument, and the code would work for both binary and domain aware classification.

2.4.4 Sampler design

Inside src/models/losses/sampler.py, we define two custom data samplers: BalancedBatchSampler and UnderSampler. These are built by subclassing PyTorch's Sampler class and are used to mitigate class imbalance during training.

BalancedBatchSampler. This sampler ensures that all classes are equally represented within each batch. It works by oversampling underrepresented classes to match the size of the majority class.

UnderSampler. This sampler performs dataset-level under-sampling by keeping all samples from the minority class and randomly sampling a fraction (controlled via under_sample_rate) of samples from majority classes.

Modularity. Both samplers operate independently of any specific dataset class, but expect the dataset to either expose a get_labels() method or return labels in the form (image, label, group) from __getitem__.

Samplers can be plugged directly into the PyTorch DataLoader via the sampler= argument, replacing the default shuffle behavior.

2.4.5 Metric and optimizer setup

Metric calculation differs depending on whether a standard binary classifier is trained or a domain-aware classifier is used. In the latter case, the model produces a num_classes * num_groups output, which must be reduced to num_classes before evaluation. Metrics can be seamlessly extended to support both training paradigms, and we define several prediction-handling functions in src/evaluation/metrics.py.

The optimizer is created using a utility from src/models/optim_factory.py, adapted from Facebook's official ConvNeXt repository.

2.4.6 Development workflow

We used GitHub for version control and code management. To maintain consistent code style, we configured pre-commit hooks for automatic import sorting and code formatting using isort and black. These tools are included as optional development dependencies in requirements_dev.txt on the main branch.

In addition, we defined a pyproject.toml file to centralize formatting rules for both tool, which is automatically applied when the tools are executed via the command line or through the pre-commit.

Throughout development, we maintained a feature-branch workflow, with separate branches for individual features or experiments.

2.4.7 Training and infrastructure

Training was conducted on a remote GPU server, which we accessed via SSH. Each training session was initiated through a shell script that passed command-line arguments to our main Python training script. To ensure uninterrupted execution, we used tmux, a terminal multiplexer that allows terminal sessions to be detached and reattached. This made it possible to run long sequences of experiments and monitor them as needed.

To monitor training progress, we implemented a custom logging system that recorded:

- Per-batch and per-epoch training time
- Learning rate and minimal learning rate
- Loss values and per-class accuracy

• Weight decay and memory consumption

Command-line arguments were also saved, and the system supported per-epoch checkpointing, as well as saving the best-performing model based on a target metric such as F1-score or recall for the malignant class. Evaluation results were logged per epoch into a training.log file, which allowed us to track model performance across runs.

We also supported mixed-precision training using PyTorch's Automatic Mixed Precision (AMP), which can be enabled with the <code>-use_amp</code> true flag. The training pipeline supports both single-GPU and multi-GPU setups via <code>torch.distributed.launch</code>, and we extended it with multi-node SLURM support using <code>submitit</code>, as provided by the official ConvNeXt repository.

Experiments were executed on a cluster of 8 NVIDIA L4 GPUs, each with 24GB of memory. We stored the following outputs for each run:

- events.out.tfevents.* (TensorBoard logs)
- config.json (command-line configuration)
- training.log (epoch-level metrics)
- checkpoint_epoch_X.pth and best_checkpoint.pth

2.4.8 ONNX and TorchScript support

To ensure compatibility with various deployment environments and inference frameworks, we support model export in both **TorchScript** and **ONNX** formats.

TorchScript. TorchScript is an intermediate representation of a PyTorch model that can be run independently of Python. We provide the function convert_to_torchscript for this:

```
def convert_to_torchscript(model, input_tensor, output_path):
    model.eval()
    scripted_model = torch.jit.trace(model, input_tensor)
    scripted_model.save(output_path)
```

Listing 2.2: TorchScript conversion

Link: https://pytorch.org/docs/stable/jit.html

ONNX. ONNX (Open Neural Network Exchange) is an open format built to represent machine learning models. Export is done via the export_model_to_onnx function:

Listing 2.3: ONNX export

Link: https://onnx.ai/

Supporting both formats allows portability and speed during deployment, regardless of the serving infrastructure, which is quite important for our task.

We used onnx and onnxruntime for model inference. We wanted to remove the need for users to know anything about our codebase when using our models. We will discuss this in details in Chapter 5,

Environment Setup

We ensured our code works reliably by using Conda environments. We separated dependencies into: device-specific packages (e.g., torch, torchaudio), development dependencies (e.g., isort, black), and core library requirements.

This approach was further extended using Docker to containerize our code. We created two Dockerfiles, one for GPU and one for CPU execution, depending on the availability of a CUDA-capable device. This separation of concerns was motivated by the fact that, as a two-member team with different hardware, we wanted to avoid creating custom Dockerfiles for each user. The only user-specific setting that needs to be changed is the CUDA version.

Our environment can be created by:

- 1. Using Conda and the environment.yaml dependency file.
- 2. Using Conda and following the instructions in INSTALL.md.
- 3. Building a GPU or CPU Docker image.
- 4. Pulling the prebuilt GPU or CPU Docker image from Docker Hub.

In the following sections, we provide detailed instructions on setting up the environment.

3.1 Conda install using environment YAML file

On the main branch of the code, in the root directory, you can find the environment.yml file. The only prerequisite is to have Conda installed, and the environment can be recreated with a single line of code. However, within that YAML file, the user must specify the correct versions of dependencies based on the CUDA and cuDNN versions being used.

```
conda env create -f environment.yml
```

Listing 3.1: Creating Conda environment from environment.yml

3.2 Conda install following the instructions from INSTALL.md

For a more controlled approach, follow these instructions:

```
# Create and activate Conda environment
conda create -n melanoma python=3.10 -y
conda activate melanoma
```

```
# Install dependencies from requirements file

pip install -r requirements.txt

# For CPU-only installation of PyTorch and related libraries:

pip install \

torch==2.2.0+cpu \

torchaudio==2.2.0+cpu \

torchaudio==2.2.0+cpu \

f https://download.pytorch.org/whl/cpu/torch_stable.html
```

Listing 3.2: Environment setup using Conda and pip

Note: If you are using a GPU, make sure to install the appropriate version of PyTorch that matches your CUDA version. You can find the correct installation command for your system on the official PyTorch website.

3.3 Docker installation

To build and run the project using Docker, follow the instructions below depending on whether you are using a CPU or a GPU.

CPU Setup

Place yourself in the project's root directory and run the following commands:

```
# Build the Docker image using the CPU Dockerfile
docker build -t melanoma -f docker/Dockerfile_cpu .

# Run the Docker container interactively
docker run -it melanoma
```

Listing 3.3: Build and run Docker container (CPU version)

GPU Setup

If you have a CUDA-compatible GPU and NVIDIA Docker runtime installed, use the GPU-specific Dockerfile:

```
# Build the Docker image using the GPU Dockerfile
docker build -t melanoma -f docker/Dockerfile .

# Run the Docker container interactively
docker run -it --gpus all melanoma
```

Listing 3.4: Build and run Docker container (GPU version)

3.4 Pull prebuilt image from Docker Hub

If you prefer not to build the image locally, you can pull the latest version from Docker Hub. We pushed already built images there, both for CPU and GPU devices.

3.4.1 GPU docker image from Docker Hub (preferred)

```
# Pull the GPU image from Docker Hub
docker pull haralovicmarko/melanoma_gpu:latest

# Run with GPU support
docker run -it --gpus all haralovicmarko_gpu/melanoma_cpu:latest

# Run with GPU support and mounted directories (again for weights and images dir)

docker run -it --gpus all \
-v /path/to/local/data:/melanoma-classification/data \
-v /path/to/local/weights:/melanoma-classification/weights \
haralovicmarko/melanoma_gpu:latest
```

Listing 3.5: Pull and run the Docker GPU enabled image from Docker Hub

3.4.2 CPU docker image from Docker Hub

```
# Pull the CPU image from Docker Hub
docker pull haralovicmarko/melanoma_cpu:latest

# Run the container (CPU version)
docker run -it haralovicmarko/melanoma_cpu:latest

# Run the container (CPU version) with mounted dir (of images and weights for example)
docker run -it \
-v /path/to/local/data:/melanoma-classification/data \
-v /path/to/local/weights:/melanoma-classification/weights \
haralovicmarko/melanoma_cpu:latest
```

Listing 3.6: Pull and run the Docker CPU enabled image from Docker Hub

3.5 Summary

Preferably, use the GPU Docker image to run the code. It is bulletproof and works across platforms. If you encounter any difficulties, we recommend building the environment from the provided environment.yaml file.

Codebase usage

Our codebase is designed to be controlled via command-line arguments. An argument parser captures all user-provided parameters and initializes relevant classes and components accordingly. The main training entry point is melanoma_train.py, which supports both training and evaluation on CPU, single GPU, multi-GPU, and SLURM-based distributed setups using submitit.

In addition, we provide a dedicated evaluation script, melanoma_eval.py, which includes its own argument parser and can be used independently for model evaluation.

To improve flexibility, we extended the system to support YAML configuration files. Instead of specifying all parameters via command-line arguments, users can pass a <code>-config</code> flag with a path to a YAML file. This file is automatically parsed, and its values override the defaults defined in the argument parser.

In the following sections, we provide:

- a description of key arguments,
- a sample bash script for running training and evaluation,
- an example configuration file,
- usage of torch.distributed for multi-GPU setups, and
- guidelines on writing custom YAML configuration files.

4.1 Key CLI arguments

Our training and evaluation scripts are fully configurable through command-line arguments. Below we highlight some of the most important options for customizing the training pipeline:

Dataset

- --skin_color_csv (default: None)
 Path to the CSV containing image metadata.
 --data_path (default: ./isic2020_challenge)
 Path to the images folder.
- Model configuration

- --num_classes (default: 2) Number of output classes for classification. - --num_groups (default: 1) Number of skin tone groups. (default: True) - --pretrained Load pretrained weights (automatically handled). - --freeze_model (default: False) Freeze model backbone for linear probing. - --input_size (default: 224) Input resolution of training images. Loss function - --ohem (default: False) Use Online Hard Example Mining loss. (default: False) - --ifw Apply inverse frequency weighting. - --recall_ce (default: False) Use recall-weighted Cross Entropy loss. - --focal_loss (default: False) Use Focal loss for class imbalance. - --domain_independent_loss (default: False) Ignore group info in loss function. - --domain_discriminative_loss (default: False) Separate classes across domain groups. Sampling and class balancing - --oversample_malignant (default: False) Oversample malignant lesions during training. (default: False) - --undersample_benign Undersample benign lesions during training. (default: -1) - --undersample_benign_ratio Ratio for undersampling benign cases. Preprocessing options (default: False) - --cielab Convert input images to CIELAB color space. - --skin_former (default: False) Apply skin tone shifting transformation. - --segment_out_skin (default: False) Use skin segmentation to mask background. - --conditional_accuracy (default: False) Report per-group conditional accuracy.

Training setup

```
    --use_amp
        Use PyTorch AMP for mixed precision.
    --config
        Path to YAML configuration file.
    (default: False)
        (default: None)
```

These are the most important arguments. All available arguments can be found in the argument parser defined in src/utils/argparser.py.

4.2 Example bash script

To simplify training execution, we used bash scripts to run our experiments. Here we provide example bash scripts for both CPU and multi-GPU setups.

4.2.1 CPU setup

This is a bash script designed to run linear probing using pretrained DinoV2 ViT-s/14 on resolution 224x224, with 2 classes, using recall based cross entropy and inverse frequency weighting.

```
python melanoma_train.py \
     --data_path "./isic2020_challenge" \
     --skin_color_csv ".isic2020_challenge/ISIC_2020_full.csv" \
     --model dinov2_vit_small \
     --batch_size 8 \
     --epochs 10 \
     --device cpu \
     --freeze_model True \
     --input_size 224 \
    --num_classes 2 \
10
    --pretrained True \
11
     --log_dir "./melanoma_logs" \
     --warmup_epochs 0 \
13
     --use_amp False \
14
     --lr 0.01 \
     --weight_decay 0.0001 \
17
     --update_freq 1 \
     --ifw \
18
     --recall_ce
```

Listing 4.1: Example CPU Training Script

4.2.2 Multi-GPU setup

For distributed training using multiple GPUs, the following script leverages torch.distributed.launch. It automatically detects the environment and configures the device accordingly, and perform same linear probing on the features extracted by DinoV2 ViT-s/14.

```
#!/bin/bash

python -m torch.distributed.launch \
    --nproc_per_node=4 \
    --master_port=29500 \
    --use_env \
```

```
melanoma_train.py \
     --data_path "./isic2020_challenge" \
     --skin_color_csv "./isic2020_challenge/ISIC_2020_full.csv" \
     --model dinov2_vit_small \
10
     --batch_size 32 \setminus
     --epochs 10 \
12
     --device "cuda" \
13
     --freeze_model True \
14
15
     --input_size 224 \
     --num_classes 2 \
16
     --num_workers 4 \
17
     --pretrained True \
18
     --log_dir "./melanoma_logs" \
     --warmup_epochs 0 \
20
     --use_amp False \
21
     --lr 0.01 \
22
     --weight_decay 0.0001 \
23
     --mixup 0.0 \
24
25
     --update_freq 1 \
     --ifw \
     --recall_ce \
     --distributed
```

Listing 4.2: Example Multi-GPU Training Script

These scripts can be easily adapted by changing model architecture, dataset paths, or enabling additional options such as skin tone preprocessing or different loss functions.

4.2.3 Evaluation script

To evaluate a trained model checkpoint, we use the same melanoma_train.py entry point with the -test flag. Below is an example bash command to run evaluation on a saved model.

```
python melanoma_train.py \
    --data_path "./isic2020_challenge" \
    --skin_color_csv "./isic2020_challenge/ISIC_2020_full.csv" \
    --model dinov2_vit_small \
    --batch_size 8 \
    --device $DEVICE \
    --input_size 224 \
    --num_classes 2 \
    --checkpoint <PATH_TO_CHECKPOINT > \
    --ifw \
    --test
```

Listing 4.3: Example Evaluation Script

This script loads the specified checkpoint and evaluates it on the validation split. Results such as loss, accuracy, and per-group metrics will be logged and saved to the output directory. The use of the <code>-ifw</code> flag ensures evaluation loss is consistent with the training configuration.

4.3 Running with configuration files

In addition to command-line arguments, our training pipeline supports YAML-based configuration files for improved reproducibility and cleaner experiment setup.

Usage

To run the training script using a YAML configuration file, pass the file path using the -config argument:

```
python melanoma_train.py \
    --config "configs/dino_vit_small.yaml" \
    --data_path "./isic2020_challenge" \
    --skin_color_csv "./isic2020_challenge/ISIC_2020_full.csv" \
    --device $DEVICE \
    --num_workers 4 \
    --log_dir "./melanoma_logs" \
```

Listing 4.4: Run training using a config file

The -config file can define any argument accepted by the parser. Command-line arguments provided alongside the config file will override values defined in the YAML file.

Example YAML Configuration

Below is an example of a complete YAML configuration file (e.g., configs/dino_vit_small.yaml):

```
data_path: "./isic2020_challenge"
2 skin_color_csv: "./isic2020_challenge/ISIC_2020_full.csv"
model: "dinov2_vit_small"
4 batch_size: 8
5 epochs: 10
6 input_size: 224
7 num_classes: 2
8 num_workers: 4
9 pretrained: true
10 log_dir: "./melanoma_logs"
warmup_epochs: 0
12 use_amp: false
13 lr: 0.01
14 mixup: 0.0
15 update_freq: 1
16 ifw: true
weight_decay: 0.0001
output_dir: "./melanoma_classifier_output"
```

Listing 4.5: YAML config file example

This approach makes it easy to manage multiple experimental configurations and share setups. Configs can be found inside folder ./configs on the main branch.

Inference

5.1 Inference script

To enable seamless usage of our models during inference, we converted all of our best-performing models into both ONNX and TorchScript formats using the corresponding converters. For deployment and runtime inference, we opted to use the ONNX format in combination with ONNX Runtime.

The inference script is located at:

melanoma_classification/predict.py

Usage: It can be run using this commands:

Listing 5.1: Run ONNX-based inference

Our submission automatically loads the image width and height, as well as the ONNX checkpoint of our best model. For this to be possible, please place the best_model_domain_discriminative.onnx model inside the /weights folder. The model is available at the following links:

- https://huggingface.co/Mhara/melanoma_classification/resolve/main/weights/best_model_domain_discriminative.onnx?download=true
- https://drive.google.com/file/d/1gswtct5I6AIkGUgLYI1_V-pM4tGthzaO/view? usp=sharing

To run the model on a folder of images and obtain results, the user must execute the following command:

```
cd melanoma-classification

python predict.py \
    --image_folder /path/to/images/folder \
    --output_csv /path/where/to/save/predictions.csv
```

Listing 5.2: LUMEN submssion inference command

The resulting CSV will contain the following columns:

- image_name
- target

5.2 Model conversion to onnx

First, navigate to the project root directory:

cd melanoma-classification

Then, run the script as follows:

```
cd melanoma-classification

python -m src.scripts.export_model \
    --checkpoint_path /path/to/model_checkpoint.pth \
    --model_class MelanomaClassifier \
    --output_dir /path/where/converted/models/are/saved
```

Listing 5.3: Convert model checkpoint to ONNX/TorchScript

Inference progress will be logged, and the resulting predictions should appear

5.3 Hugging Face Inference and Model Access

There are several ways to download and use the melanoma classification models from Hugging Face:

5.3.1 Option 1: Using the transformers library

First, install the transformers library if you have not already:

```
pip install transformers
```

Listing 5.4: Install Hugging Face Transformers

Then, load the model and feature extractor:

```
from transformers import AutoModelForImageClassification,
   AutoFeatureExtractor

# Load the model
model_name = "Mhara/melanoma_classification"
model = AutoModelForImageClassification.from_pretrained(model_name)
feature_extractor = AutoFeatureExtractor.from_pretrained(model_name)
)
```

Listing 5.5: Load model and feature extractor from Hugging Face

5.3.2 Option 2: Download a specific file from the Hugging Face Hub

You can download a specific file (such as a model checkpoint) directly:

```
from huggingface_hub import hf_hub_download

model_path = hf_hub_download(
    repo_id="Mhara/melanoma_classification",
    filename="weights/model_0_best.pth",
    repo_type="model"
)

print(f"Model downloaded to: {model_path}")
```

Listing 5.6: Download specific model weight file

5.3.3 Option 3: Manual download via website or Git clone

You can also manually download the files:

- Visit https://huggingface.co/Mhara/melanoma_classification/tree/main/weights
- Click on the specific model file you want to download.
- On the file page, click the download button in the top-right corner.

Alternatively, to download the entire repository:

```
# Install Git LFS
git lfs install
git clone https://huggingface.co/Mhara/melanoma_classification
```

Listing 5.7: Clone the model repository with Git LFS

After cloning, you can access all the model checkpoints locally.

Reproducibility Guide

To reproduce our results, start by cloning the repository:

https://github.com/MarkoHaralovic/melanoma-classification

Place yourself in the root directory of the cloned repository before running any commands.

6.1 System setup

- Hardware used: Most experiments were run on 8 NVIDIA Tesla L4 GPUs. However, we also conducted single-GPU experiments, whose results are reported.
- Environment setup: Chapter 3 provides detailed instructions for setting up the Python environment using Conda or Docker, matching the configuration used during training and evaluation.

6.2 Exact configurations

- As shown in Chapter 4, Listing 4.5, we provide an example YAML configuration file and instructions on how to run the project using it.
- The configuration file used for our best-performing model is available in the ./configs folder and is named best_run.yaml.
- To perform evaluation, you can use the same best_run.yaml file. Simply modify it by setting test: True and provide the path to the checkpoint file via the checkpoint parameter.

6.3 Expected output directory structure

- Output files will be saved under the directory specified by the output_dir argument, either through the config file or the CLI.
- Logs are saved in a /logs subfolder and include:
 - training.log training log + summary of metrics per epoch
 - log.txt detailed training log
 - TensorBoard logs in events.out.tfevents.* format
- Checkpoint files are named checkpoint_epoch_<NUM>.pth.

• A config. json file stores all arguments used during the run for future reference.

6.4 Setup Environment and Load Weights

Use one of the methods described in Section 3 to recreate the environment.

Create a weights directory and download the model from one of the following links:

- https://huggingface.co/Mhara/melanoma_classification/tree/main/weights
- https://drive.google.com/drive/folders/1n0T7q_B23edFUnzJSuIJGLcjuP-XZr-_ ?usp=sharing

The provided paths lead to folders containing ONNX, .pth, and TorchScript checkpoints. For inference, use the ONNX or TorchScript checkpoints. For training and evaluation, use the .pth checkpoint.

6.5 Run the Code

To run the experiment and create our best model, use the following command: For training run:

```
python melanoma_train.py --config "./configs/best_run.yaml"
```

To evaluate the newly created model, edit the configuration file by setting the 'test' field to 'true'. Then, run:

For evaluation run:

For inference run