Identifying Insolubles in Ice Core Data

Applied Machine Learning Final Project

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Introduction to the problem and the dataset

The datasets

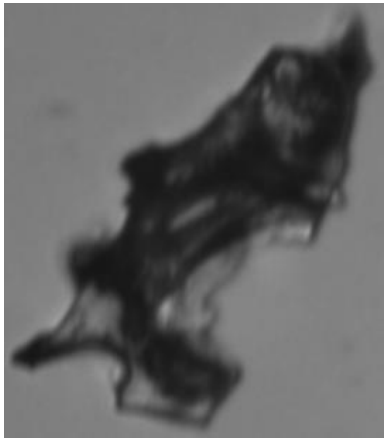
- Real
  - Greenland ice core data (GRIP)
  - 4 ice cores
  - 14-17,000 years old
  - Supplied by Niccolò Maffezzoli
  - 3,085,063 images
  - Not labelled

- Synthetic
  - 136,022 images
  - 6 classes

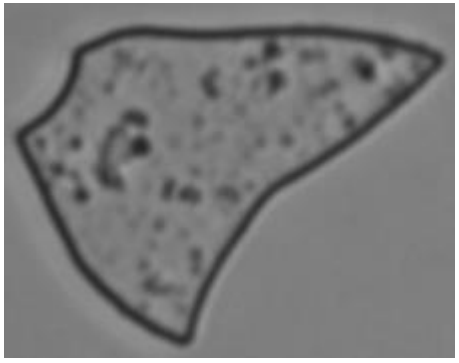
Classes

Ash (55.2%)

Grimsvotn (10.8%)

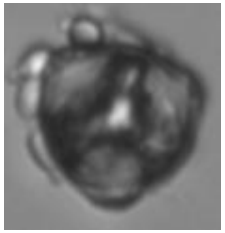


Campanian (44.4%)

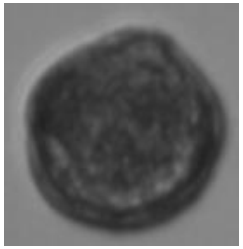


Pollen (22.3%)

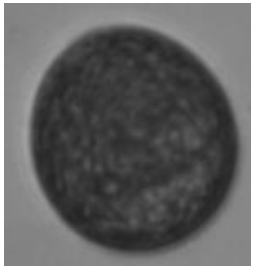
Corylus (5.8%)



Qrobur (8.1%)



Qsuber (8.4%)



Dust (22.6%)

Introduction to the problem

- Classification:
  1. Three-class classification
  2. Six-class classification
  3. Classification of the three pollen types
- Utilizing both meta-data and images
- Real data:
  - Separate "interesting" particle types from dust ("background")

Methods

- CNNs with dense network classifier
  - Keras
  - PyTorch
- Classification using metadata and images
  - LightGBM
  - Keras NN
- Unsupervised learning: UMAP

CNNs with dense network classifier

Pre-processing, data augmentation, setup | CNNs

- Balancing dataset or not?
- Pre-processing: Resizing (1x128x128) and normalization
- Augmentation:
  - Random Crop, Flip and Gaussian Blur
- Early Stopping

Architectures | CNNs

PyTorch:

A1:
Conv(11x11)
MaxPool(2x2)
Conv(5x5)
MaxPool(2x2)
Flatten
Dense
Dense
|
Output

A2:
Conv(11x11)
MaxPool(2x2)
Conv(5x5)
MaxPool(2x2)
Flatten
Dense
BatchNorm
DropOut
Dense
|
Output

A3:
Conv(11x11)
MaxPool(2x2)
Conv(5x5)
MaxPool(2x2)
Conv(3x3)
MaxPool(2x2)
Flatten
Dense
BatchNorm
DropOut
Dense
|
Output

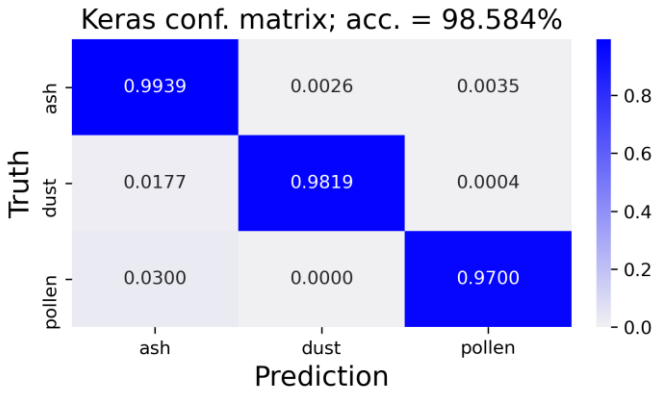
A4:
Conv(11x11)
MaxPool(2x2)
Conv(5x5)
MaxPool(2x2)
Conv(3x3)
MaxPool(2x2)
Conv(3x3)
MaxPool(2x2)
Flatten
Dense
BatchNorm
DropOut
Dense
|
Output

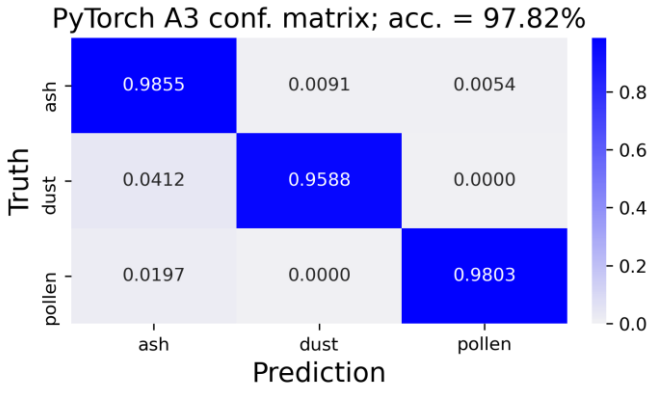
Keras:

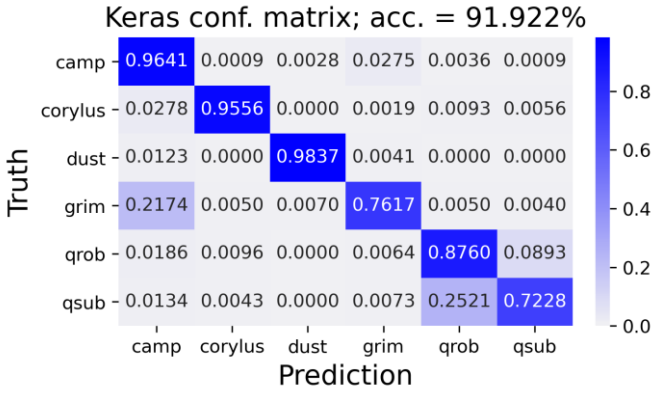
K1:
Conv(3x3)
MaxPool(2x2)
Conv(3x3)
MaxPool(2x2)
Conv(3x3)
MaxPool(2x2)
Conv(3x3)
MaxPool(2x2)
Flatten
Dense
Dense
|
Output

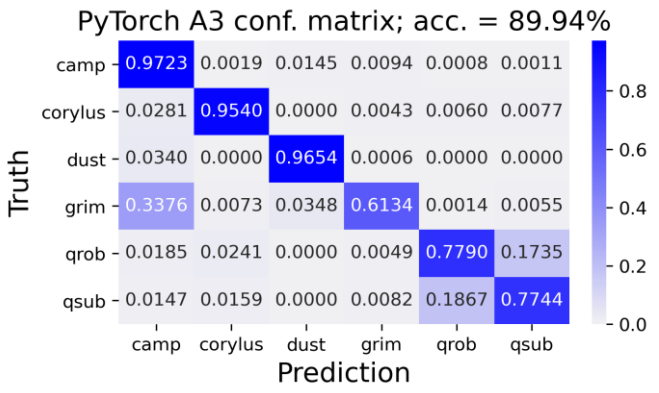
Results | CNNs

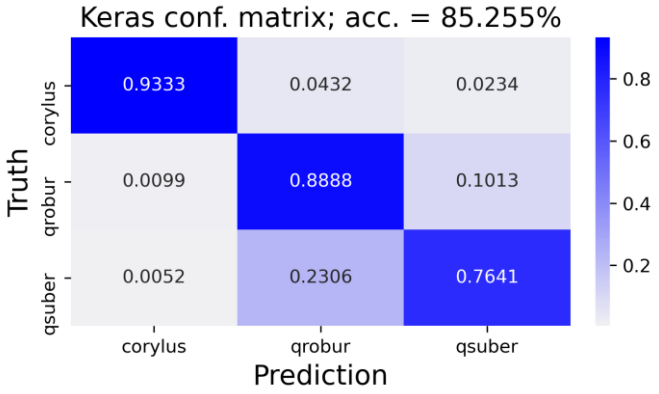
- Three-class classification
- Six-class classification
- Pollen classification

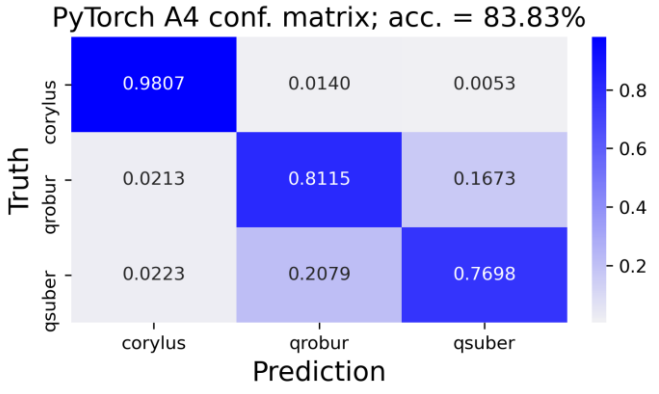










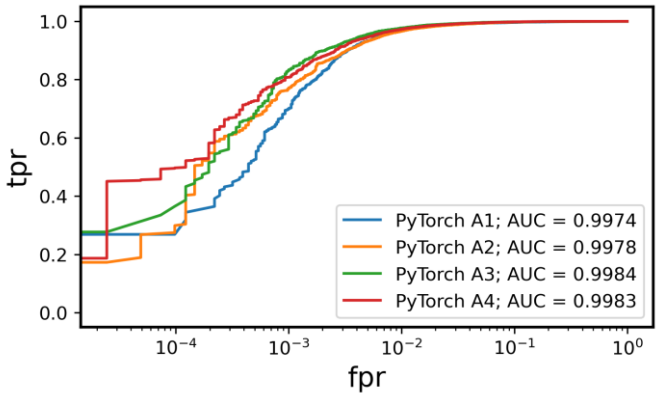


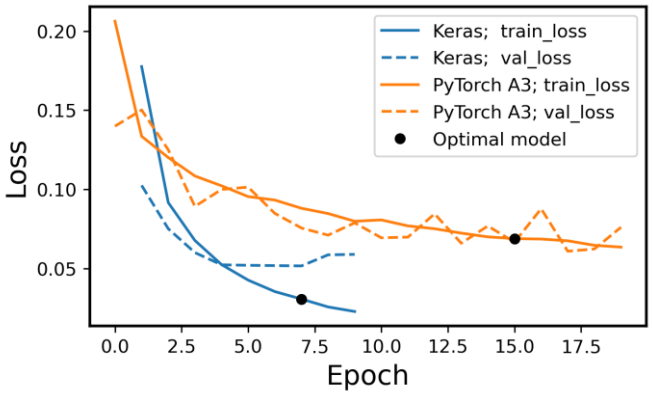
Results | CNNs

ROC curves

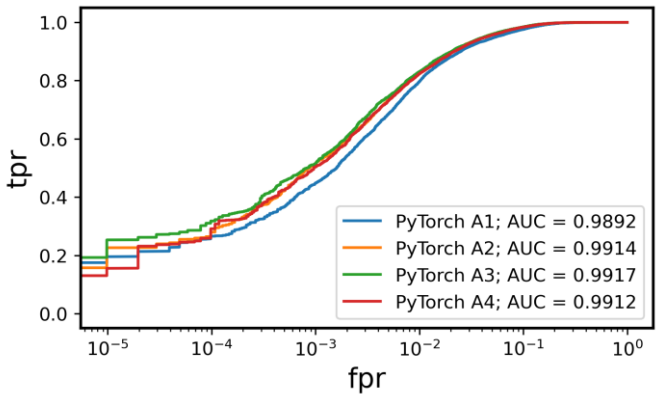
Train and Val. Loss

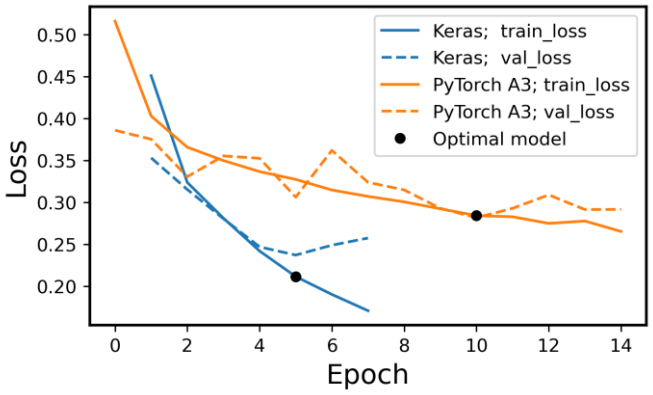
- Three class classification



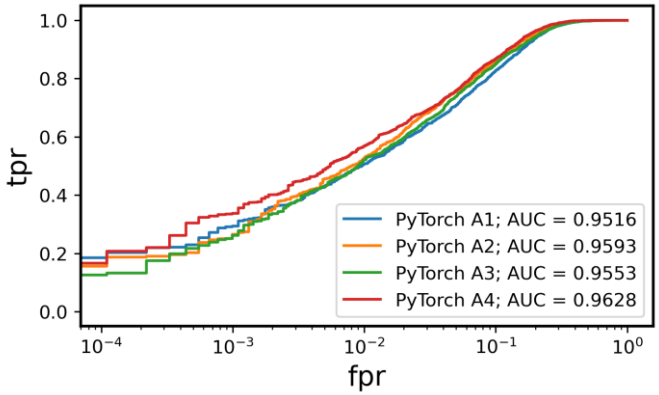


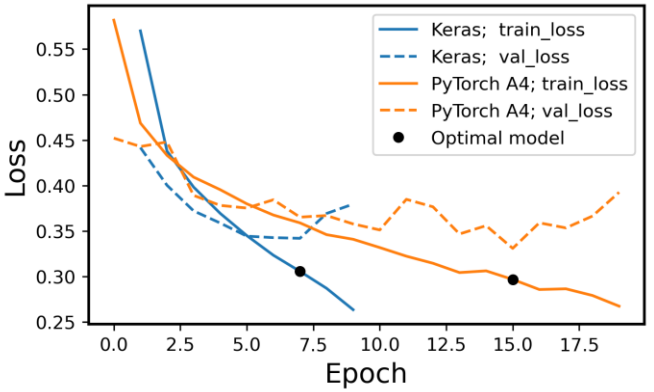
- Six class classification





- Pollen classification





Results | CNNs

- Three class classification

PyTorch A3
Actual consumption for 20 epoch(s):
Time: 0:30:46
Energy: 0.028414 kWh
CO2eq: 8.359634 g
This is equivalent to: 0.069432 km travelled by car

- Six class classification

PyTorch A3
Actual consumption for 14 epoch(s):
Time: 0:24:04
Energy: 0.021607 kWh
CO2eq: 6.357014 g
This is equivalent to: 0.052799 km travelled by car

- Pollen classification

PyTorch A4
Actual consumption for 20 epoch(s):
Time: 0:07:28
Energy: 0.006822 kWh
CO2eq: 2.007057 g
This is equivalent to: 0.016670 km travelled by car

Results | CNNs

- Three-class c

- S c

- Pollen classification

PyTorch A3
Actual consumption for 20 epoch(s):

by car

by car

PyTorch A4
Actual consumption for 20 epoch(s):
Time: 0:07:28
Energy: 0.006822 kWh
CO2eq: 2.007057 g
This is equivalent to: 0.016670 km travelled by car

Approx. total consumption:

8 g/class. • 3 class. • 3 persons
• 30 runs = **2.16 kg**
or **18 km** travelled by car!

Classification using metadata and images

Pre-processing | Metadata and images

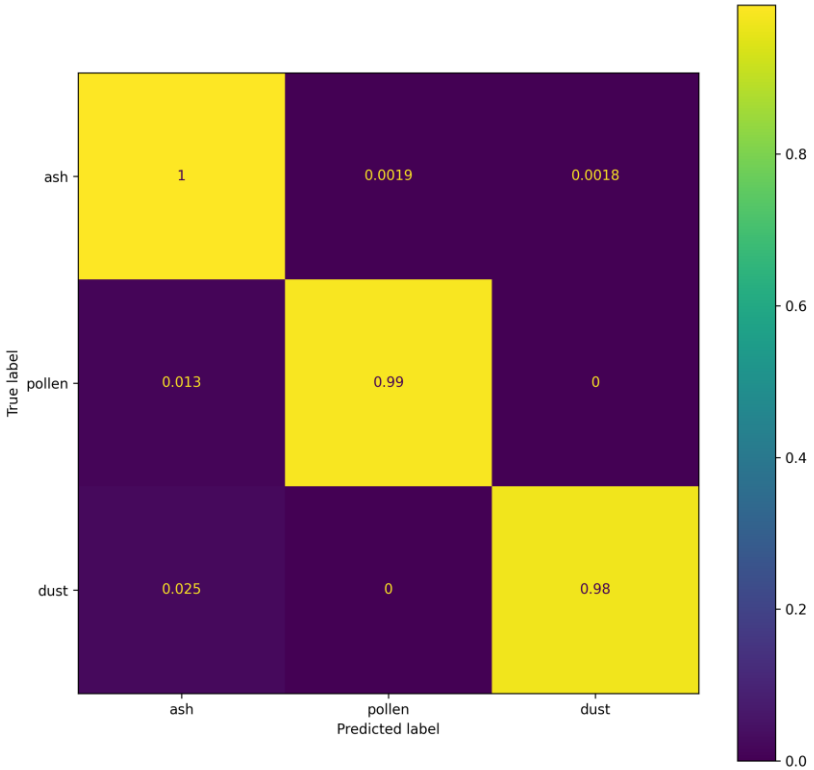
- LightGBM (Tree-based)
  - No pre-processing required
  - Simply include only the relevant features
  - Label according to the classification required

- IsolationForest
  - Train only on the 'normal' class (Dust)
  - Fits a decision boundary that determines the support of what is normal.
  - Predict anomaly scores for unseen data. More negative scores indicate more anomalous. I.e. Interesting!

Classification: MetaData and Transfer Learning LightGBM

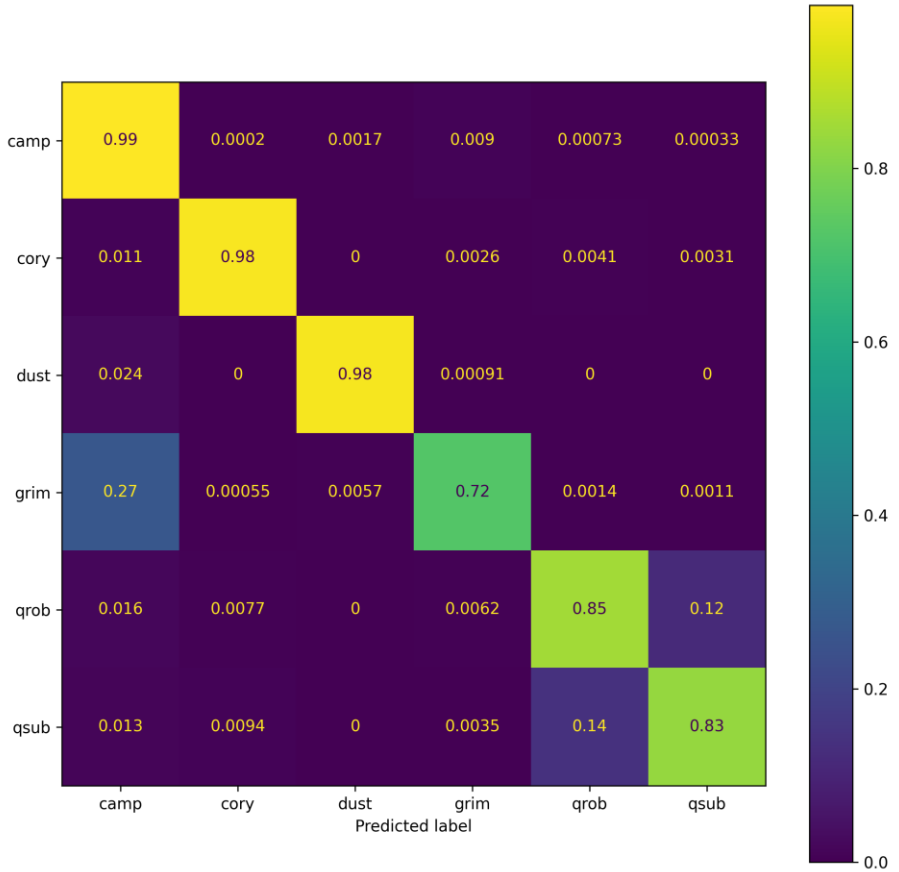
3 class accuracy: 0.99

Confusion Matrix: 3 Class



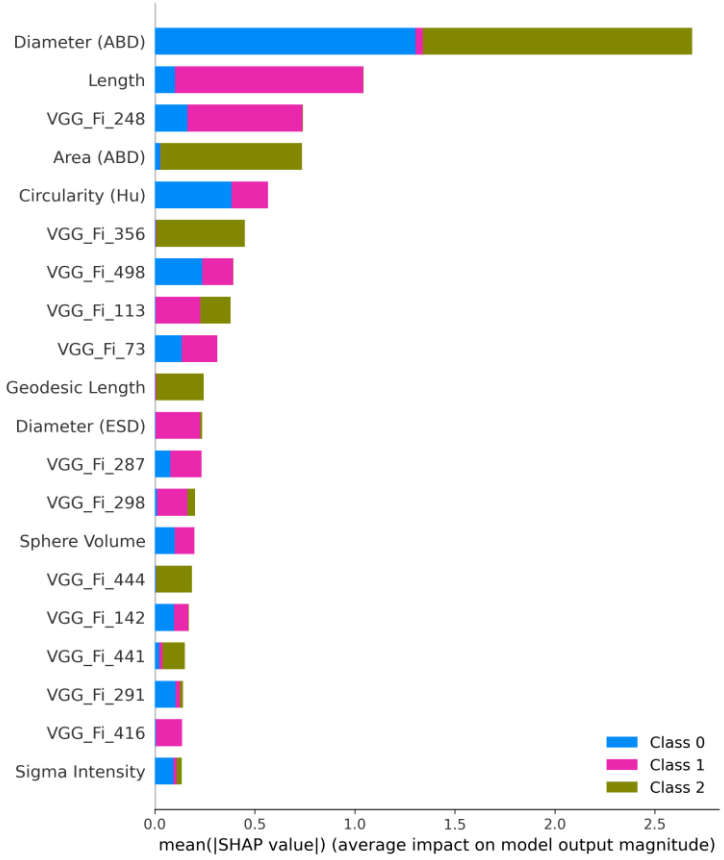
6 class accuracy: 0.92

Confusion Matrix: 6 Class

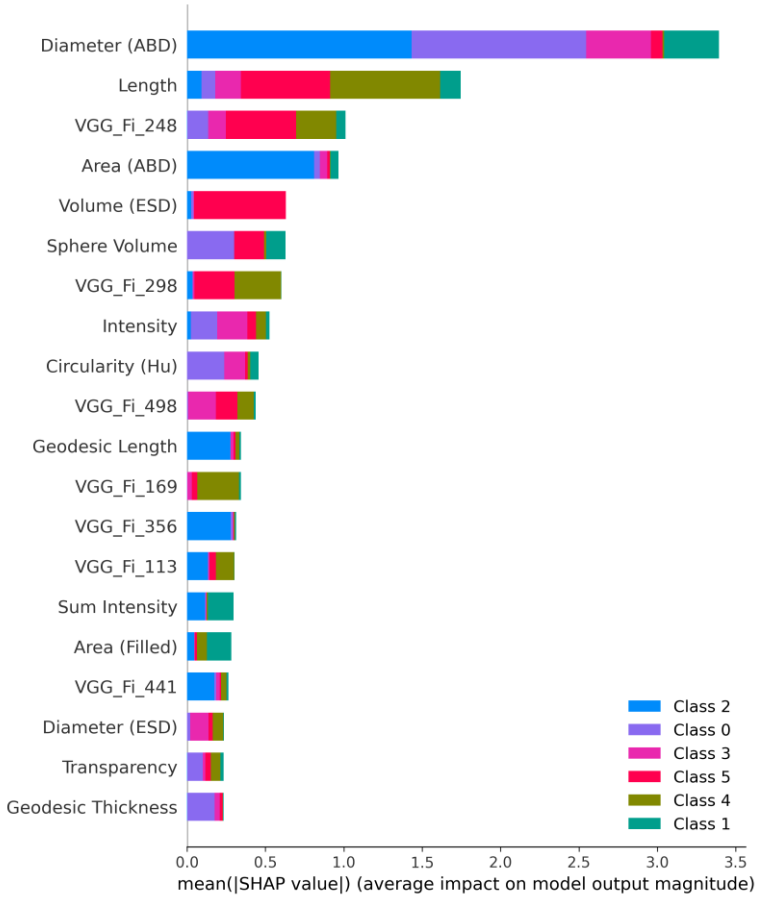


Classification: MetaData and Transfer Learning LightGBM

Shap values: 3 Class

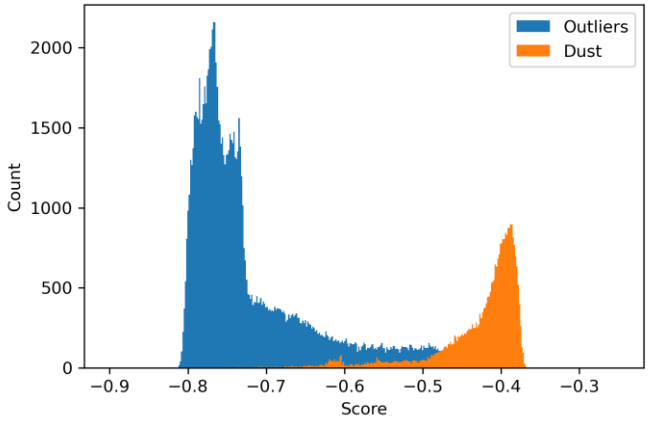


Shap values: 6 Class

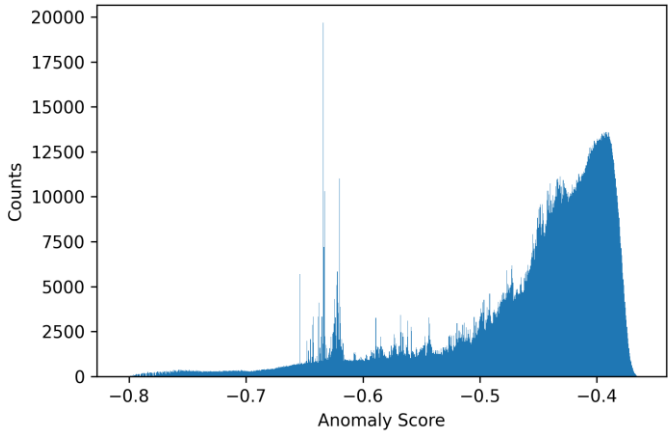


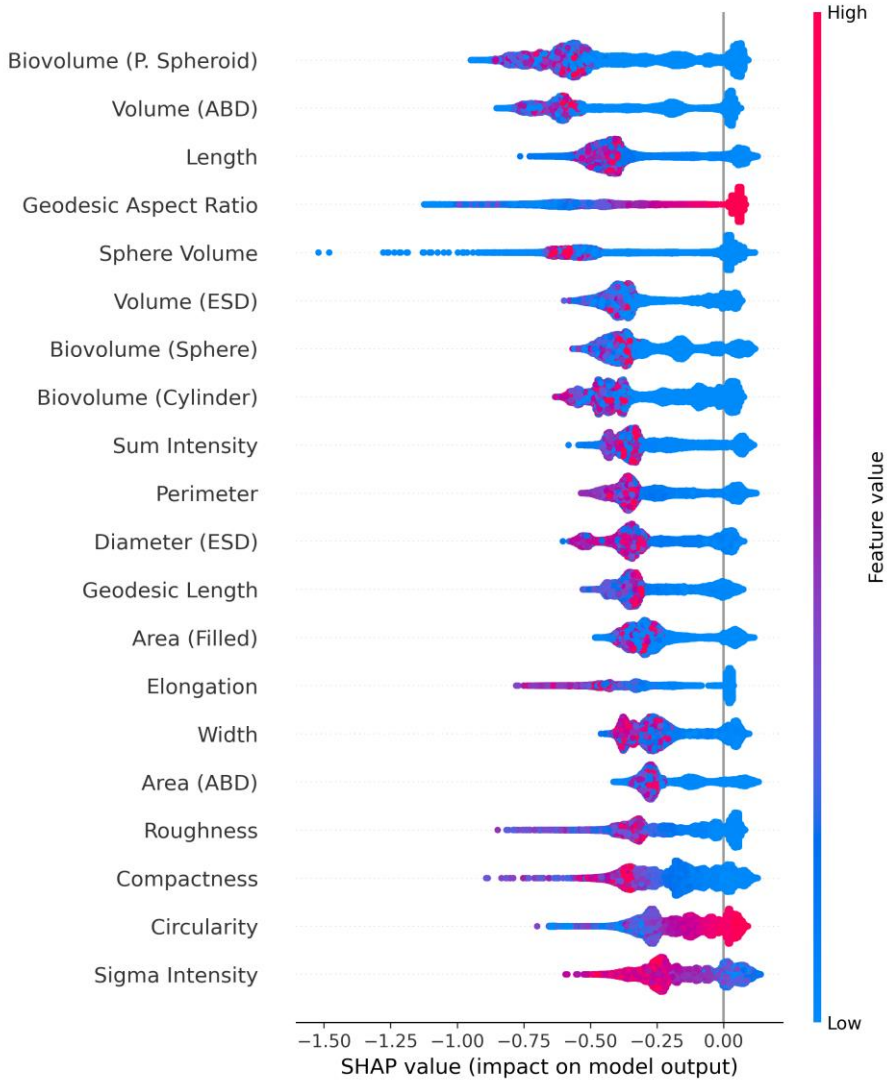
Results | Metadata and images

Isolation Forest Scores Synthetic



Isolation Forest Scores All Ice Data



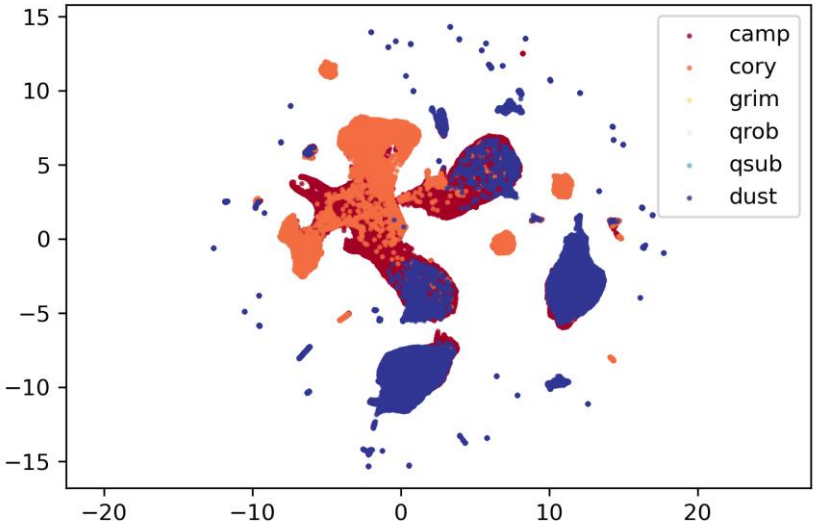


Unsupervised learning (UMAP)

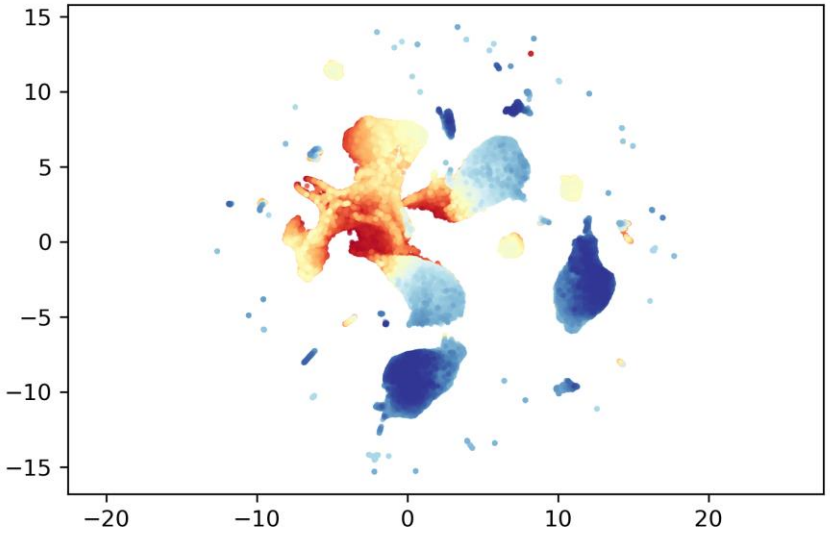
Results | Unsupervised learning (UMAP)

- Synthetic data

UMAP Synthetic Data: Class



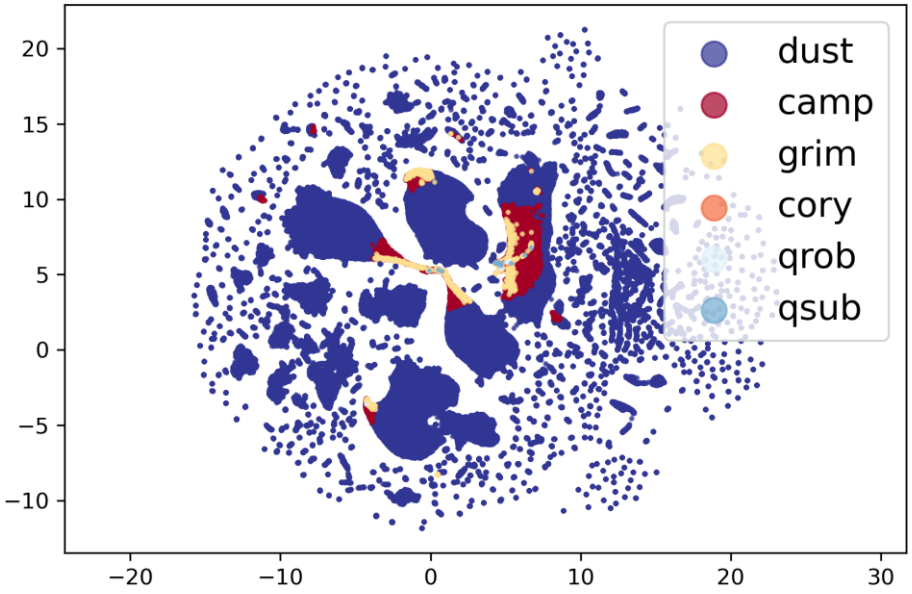
UMAP Synthetic Data: Anomaly



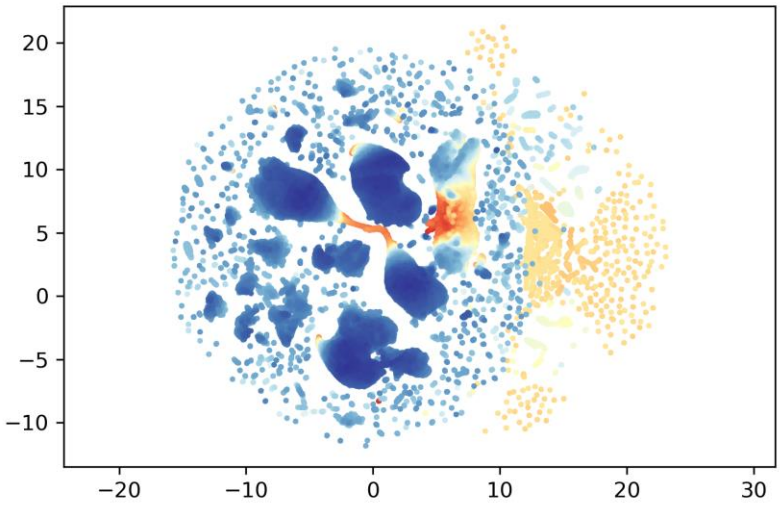
Results | Unsupervised learning (UMAP)

- Real ice data

UMAP 15% Total Ice Data:
Colored by Predicted Class



UMAP 15% Total Ice Data:
Colored by Anomaly Score



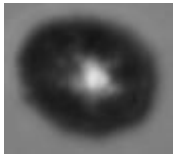
Future work

- Investigate more elaborate CNN architectures
- Experimenting more with data-augmentation
- Automated HP optimisation
- Auto encoders
- One-shot learning

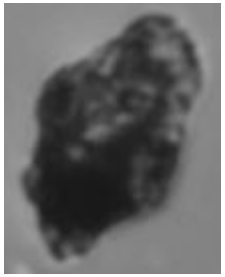
Conclusion

- Synthetic ice core insolubles identified to a relatively high degree: up to 99%
- Utilising meta-data only; very efficient
- Anomalies detected in both synthetic data and real data
- Structures in the real ice core data were found using unsupervised learning.

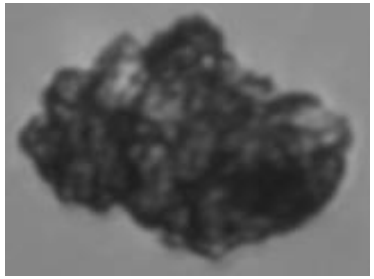
Six interesting anomalous images from GRIP



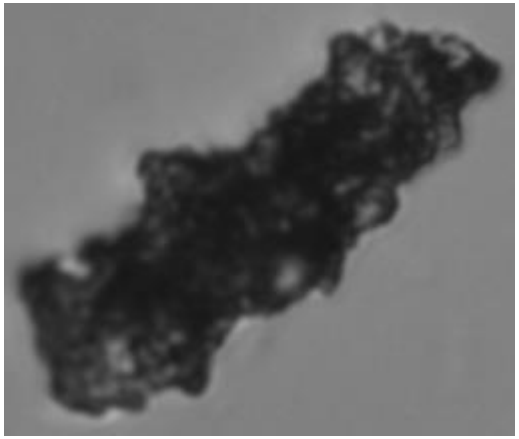
GRIP_3046_40_55_1_2787



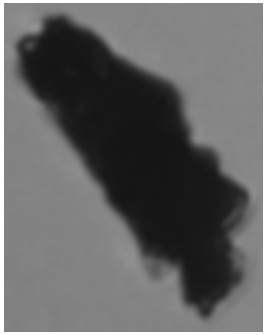
GRIP_3136_0_20_1_828



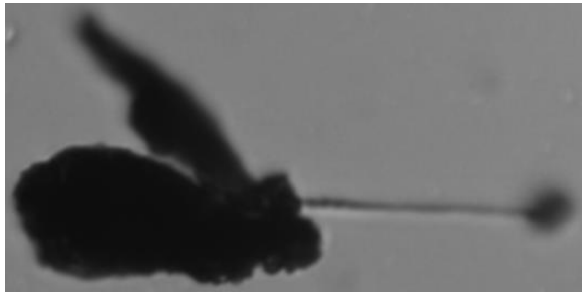
GRIP_3046_40_55_1_12275



GRIP_3136_0_20_1_823



GRIP_3136_0_20_1_830



GRIP_3136_0_20_1_805

References

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- Koushik, Jayanth. "Understanding convolutional neural networks." *arXiv preprint arXiv:1605.09081* (2016).
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- LeCun, Yann, et al. "Gradient-based learning applied to document recognition." *Proceedings of the IEEE* 86.11 (1998): 2278-2324.

Reference

- Kuo, C-C. Jay. "Understanding convolutional neural networks with a mathematical model." *Journal of Visual Communication and Image Representation* 41 (2016): 406-413.
- Aizman, Alex, Gavin Maltby, and Thomas Breuel. "High Performance I/O For Large Scale Deep Learning." *2019 IEEE International Conference on Big Data (Big Data)*. IEEE, 2019.

Appendix A.2

Pre-processing, data augmentation, setup | CNNs

```
TRAIN_TRANSFORM = tv_transforms.Compose([
    tv_transforms.RandomApply([
        tv_transforms.RandomCrop(80, pad_if_needed=True)],
        p=0.10),
    tv_transforms.Resize([IMAGE_WIDTH, IMAGE_HEIGHT],
        interpolation=tv_transforms.InterpolationMode.BILINEAR),
    tv_transforms.Normalize(mean=[60], std=[30], inplace=True),
    tv_transforms.RandomHorizontalFlip(p=0.10),
    tv_transforms.RandomVerticalFlip(p=0.10),
    tv_transforms.RandomApply([tv_transforms.GaussianBlur(5)], p=0.10)
])
```

Appendix A.2

Pre-processing, data augmentation, setup | CNNs

- Evaluation (val: 15%, test: 15%)
- Loss:
  - PyTorch: CrossEntropyLoss
  - Keras: SparseCategorialCrossEntropyLoss
- Optimizer: Adam
- Learning rate:
  - PyTorch: 0.001
  - Keras: 0.0008

Appendix B.1 | PyTorch architectures

Architecture 1

```
----------------------------------------------------------------
   Layer (type)               Output Shape         Param #
================================================================
      Conv2d-1         [-1, 8, 118, 118]             976
     MaxPool2d-2          [-1, 8, 59, 59]               0
      Conv2d-3         [-1, 16, 55, 55]           3,216
     MaxPool2d-4         [-1, 16, 27, 27]               0
      Linear-5              [-1, 108]           1,259,820
      Linear-6                [-1, 6]                 654
================================================================
Total params: 1,264,666
Trainable params: 1,264,666
Non-trainable params: 0
Input size (MB): 0.06
Forward/backward pass size (MB): 1.52
Params size (MB): 4.82
Estimated Total Size (MB): 6.41
----------------------------------------------------------------
```

Appendix B.2 | PyTorch architectures

Architecture 2

```
----------------------------------------------------------------
      Layer (type)               Output Shape         Param #
================================================================
          Conv2d-1         [-1, 8, 118, 118]             976
       MaxPool2d-2           [-1, 8, 59, 59]               0
          Conv2d-3          [-1, 16, 55, 55]           3,216
       MaxPool2d-4          [-1, 16, 27, 27]               0
          Linear-5                [-1, 108]       1,259,820
     BatchNorm1d-6                [-1, 108]             216
          Dropout-7                [-1, 108]               0
          Linear-8                  [-1, 6]             654
================================================================
Total params: 1,264,882
Trainable params: 1,264,882
Non-trainable params: 0
Input size (MB): 0.06
Forward/backward pass size (MB): 1.52
Params size (MB): 4.83
Estimated Total Size (MB): 6.41
----------------------------------------------------------------
```

Appendix B.3 | PyTorch architectures

Architecture 3

Layer (type)	Output Shape	Param #
Conv2d-1	[-1, 8, 118, 118]	976
MaxPool2d-2	[-1, 8, 59, 59]	0
Conv2d-3	[-1, 16, 55, 55]	3,216
MaxPool2d-4	[-1, 16, 27, 27]	0
Conv2d-5	[-1, 32, 25, 25]	4,640
MaxPool2d-6	[-1, 32, 12, 12]	0
Linear-7	[-1, 64]	294,976
BatchNorm1d-8	[-1, 64]	128
Dropout-9	[-1, 64]	0
Linear-10	[-1, 6]	390

Total params: 304,326
Trainable params: 304,326
Non-trainable params: 0

Input size (MB): 0.06
Forward/backward pass size (MB): 1.71
Params size (MB): 1.16
Estimated Total Size (MB): 2.93

Appendix B.4 | PyTorch architectures

Architecture 4

```
----------------------------------------------------------------
      Layer (type)               Output Shape         Param #
================================================================
          Conv2d-1         [-1, 8, 118, 118]             976
       MaxPool2d-2           [-1, 8, 59, 59]               0
          Conv2d-3          [-1, 16, 55, 55]           3,216
       MaxPool2d-4          [-1, 16, 27, 27]               0
          Conv2d-5          [-1, 32, 25, 25]           4,640
       MaxPool2d-6          [-1, 32, 12, 12]               0
          Conv2d-7          [-1, 64, 10, 10]          18,496
       MaxPool2d-8           [-1, 64, 5, 5]               0
          Linear-9                 [-1, 40]          64,040
     BatchNorm1d-10                 [-1, 40]              80
         Dropout-11                 [-1, 40]               0
         Linear-12                  [-1, 3]             123
================================================================
Total params: 91,571
Trainable params: 91,571
Non-trainable params: 0
Input size (MB): 0.06
Forward/backward pass size (MB): 1.77
Params size (MB): 0.35
Estimated Total Size (MB): 2.18
```

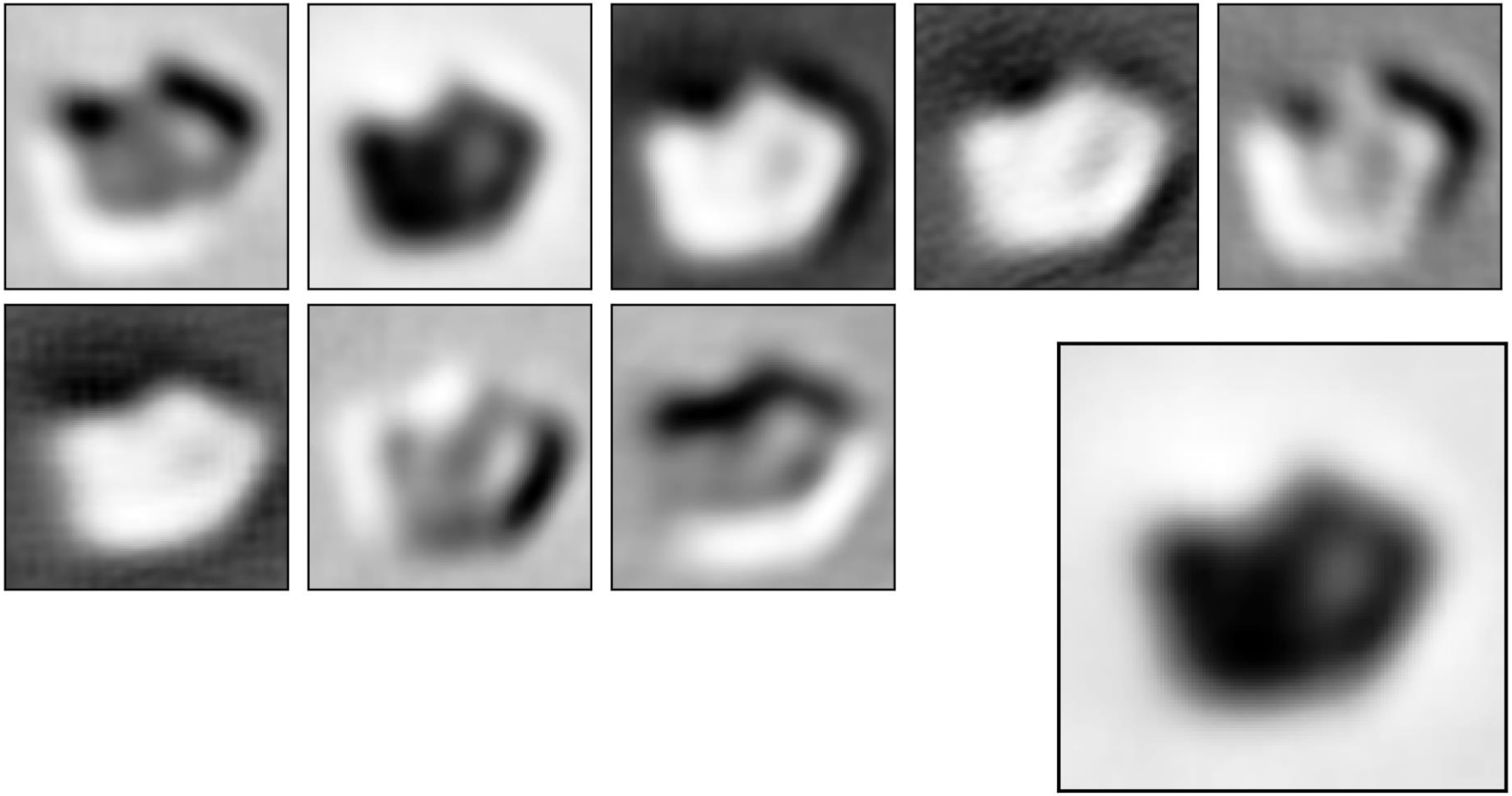
Appendix B.5 | Keras architecture

Layer (type)	Output Shape	Param #
rescaling (Rescaling)	(None, 128, 128, 1)	0
conv2d (Conv2D)	(None, 126, 126, 8)	80
max_pooling2d (MaxPooling2D)	(None, 63, 63, 8)	0
conv2d_1 (Conv2D)	(None, 61, 61, 16)	1168
max_pooling2d_1 (MaxPooling2	(None, 30, 30, 16)	0
conv2d_2 (Conv2D)	(None, 28, 28, 32)	4640
max_pooling2d_2 (MaxPooling2	(None, 14, 14, 32)	0
conv2d_3 (Conv2D)	(None, 12, 12, 64)	18496
max_pooling2d_3 (MaxPooling2	(None, 6, 6, 64)	0
flatten (Flatten)	(None, 2304)	0
dense (Dense)	(None, 128)	295040
dense_1 (Dense)	(None, 3)	387

Total params: 319,811
Trainable params: 319,811
Non-trainable params: 0

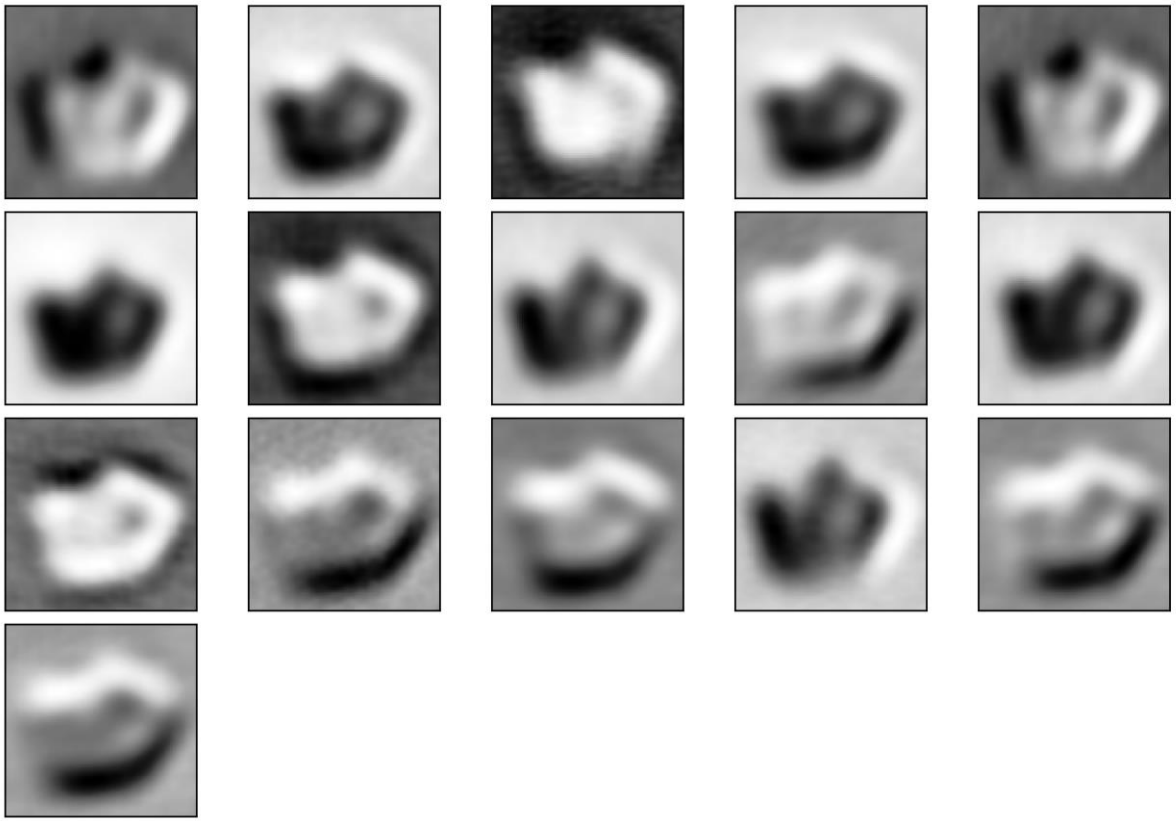
Appendix C.1 | Feature maps

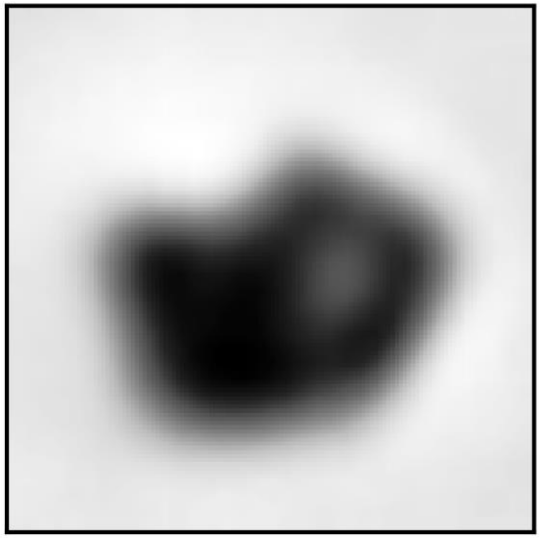
- PyTorch A3 on 6 class problem, Conv2d-1



Appendix C.2 | Feature maps

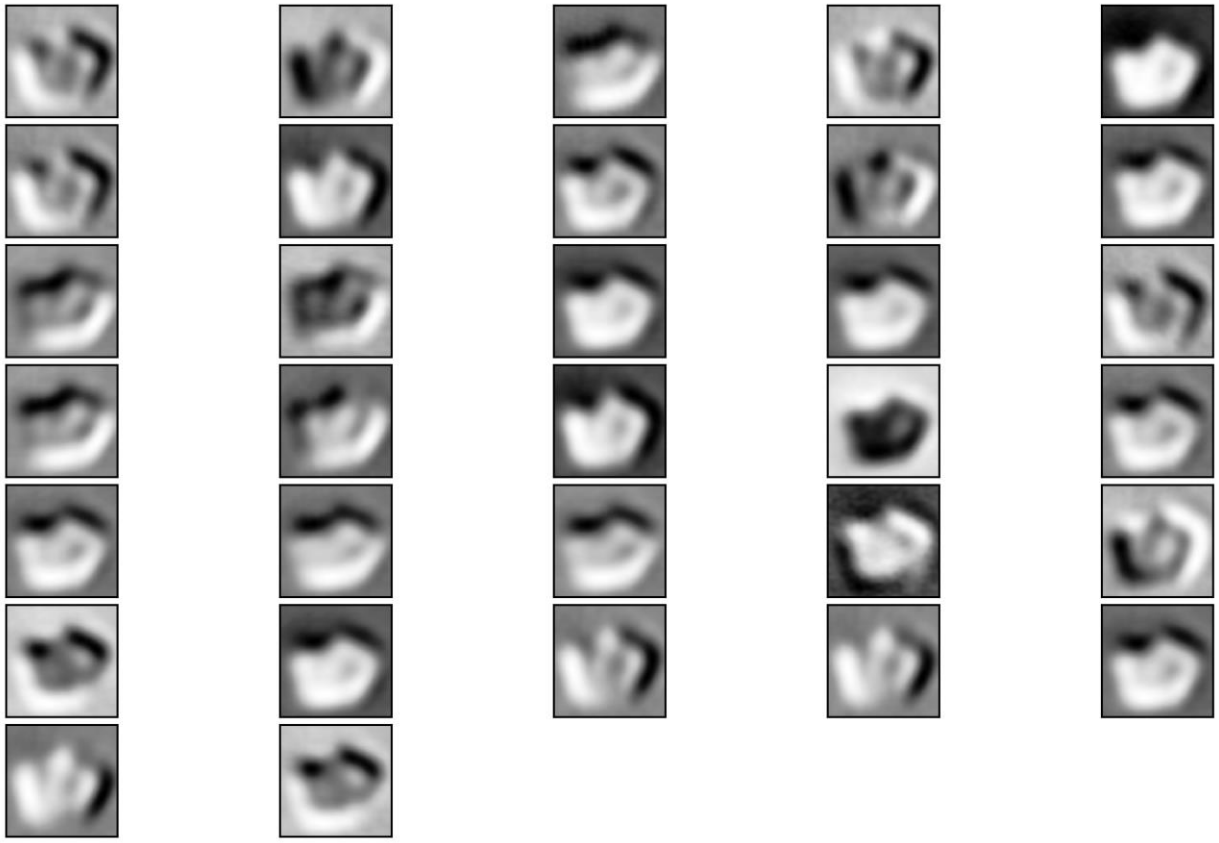
- PyTorch A3 on 6 class problem, Conv2d-2

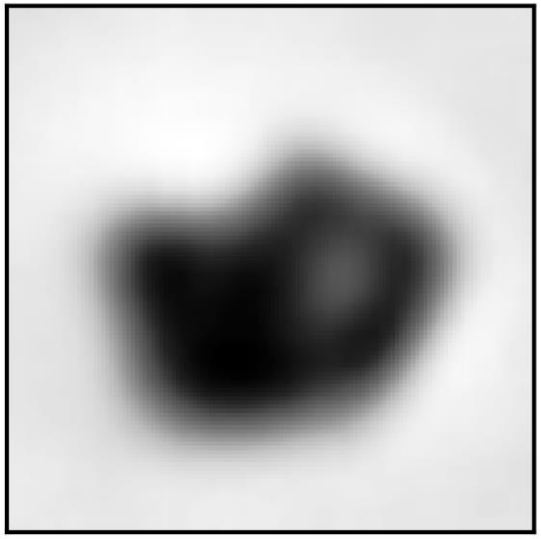




Appendix C.3 | Feature maps

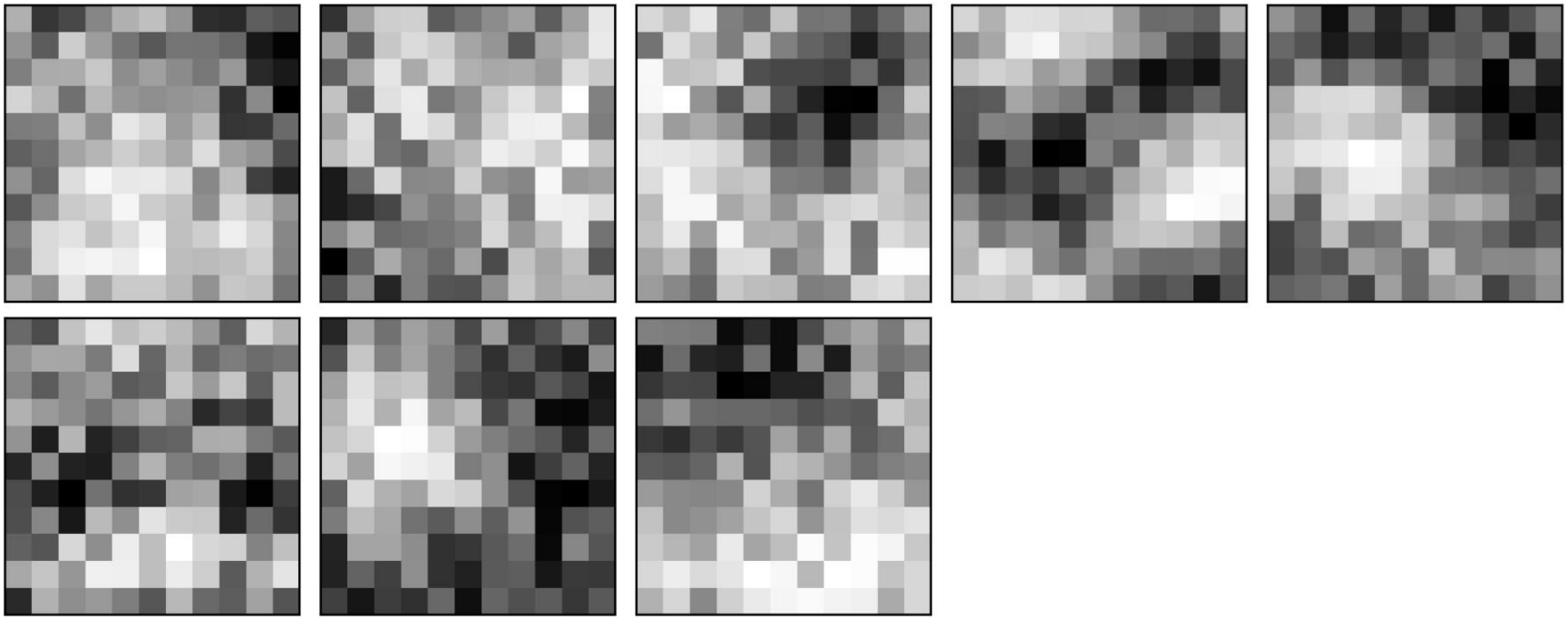
- PyTorch A3 on 6 class problem, Conv2d-3





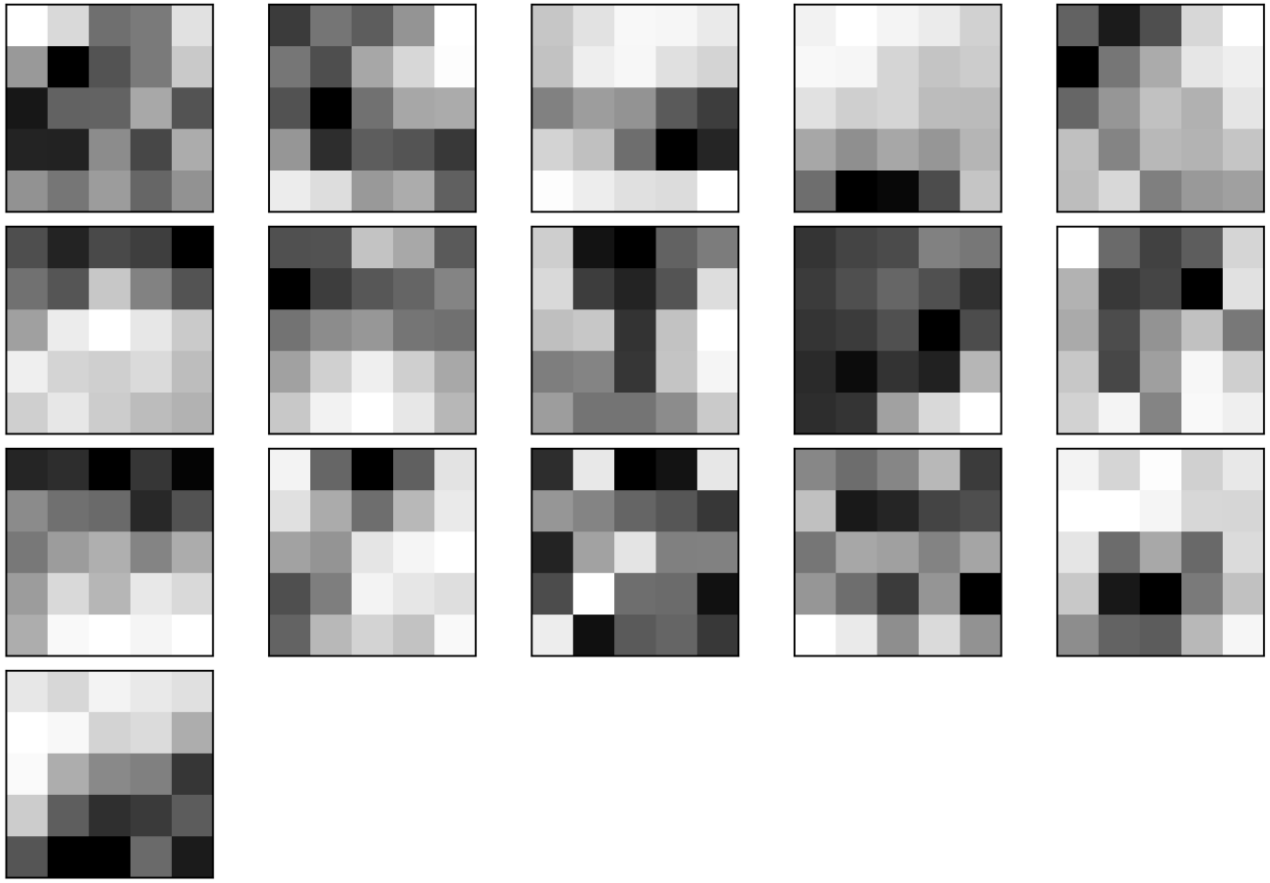
Appendix D.1 | Filters

- PyTorch A3 on 6 class problem, Conv2d-1



Appendix D.2 | Filters

- PyTorch A3 on 6 class problem, Conv2d-2

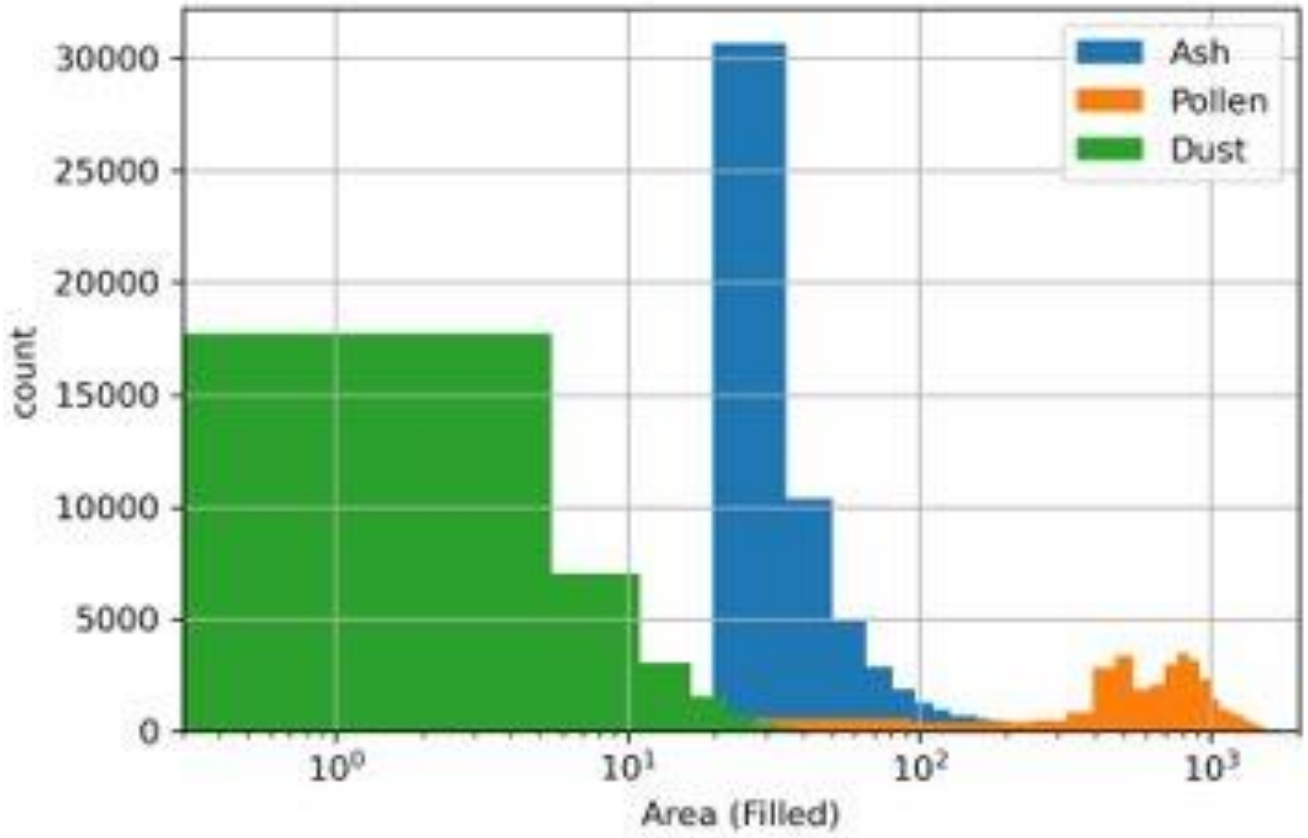


Appendix D.3 | Filters

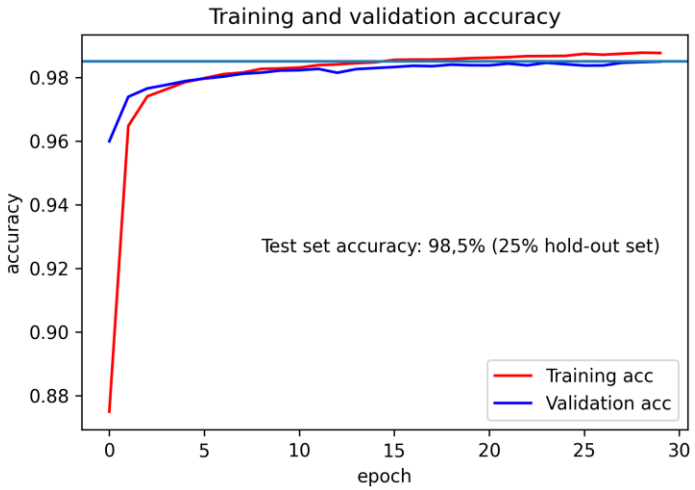
- PyTorch A3 on 6 class problem, Conv2d-3

Appendix E | Synthetic data size distributions

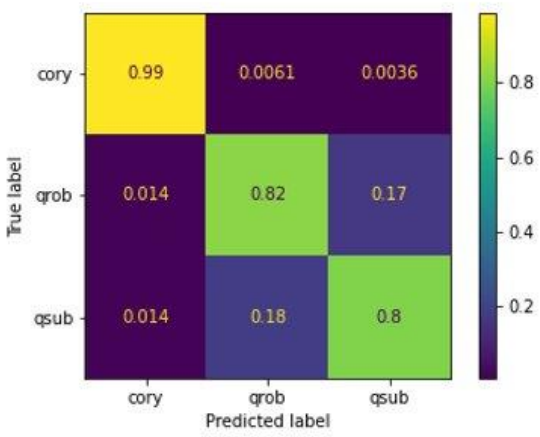
UMAP ICE Data: fit_transform ICE

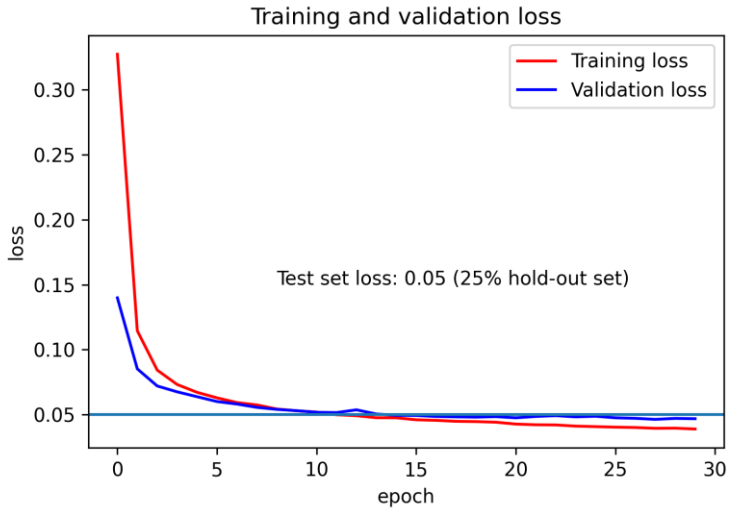


Appendix F | Classification: Transfer Learning Only Keras Dense Feedforward NN Classifier



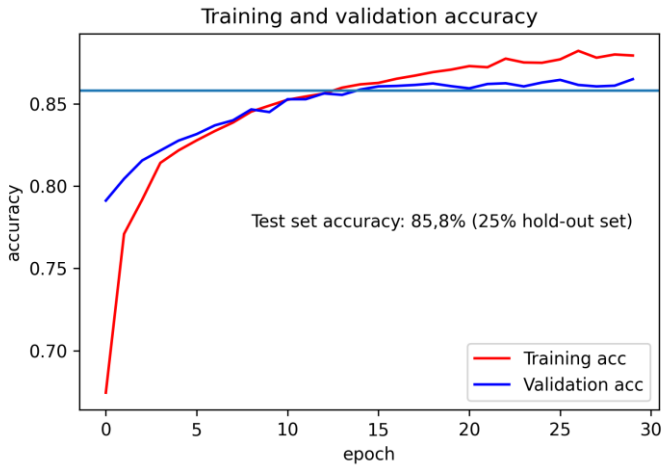
3 Class

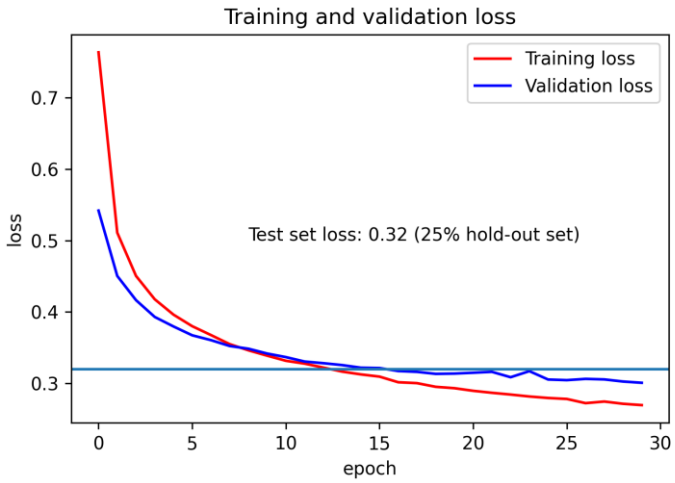




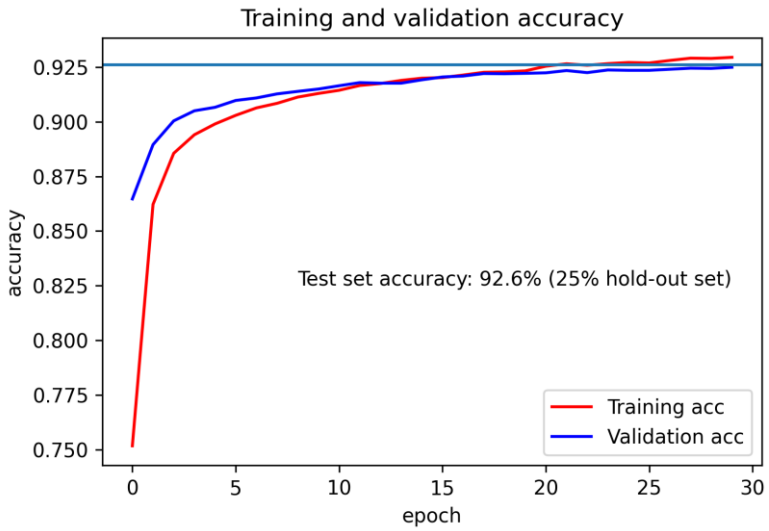
Appendix H | Classification: Transfer Learning Only Keras Dense Feedforward NN Classifier

Pollen Only

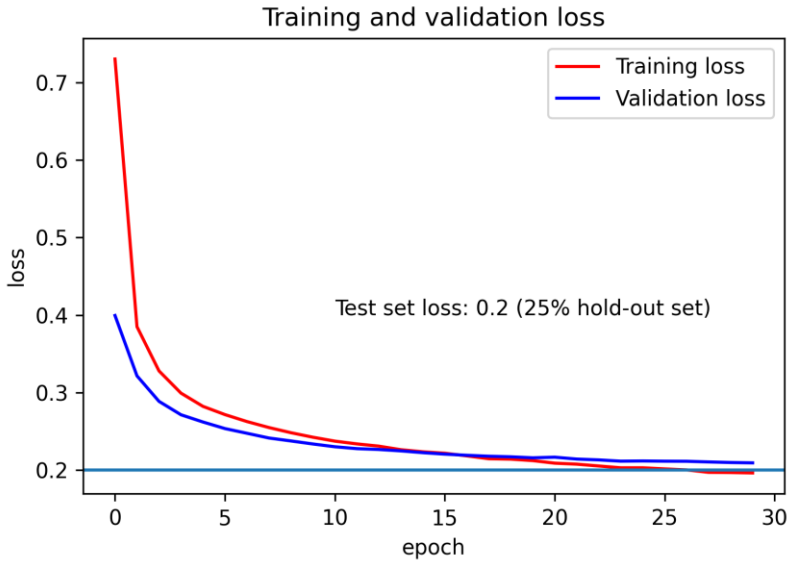




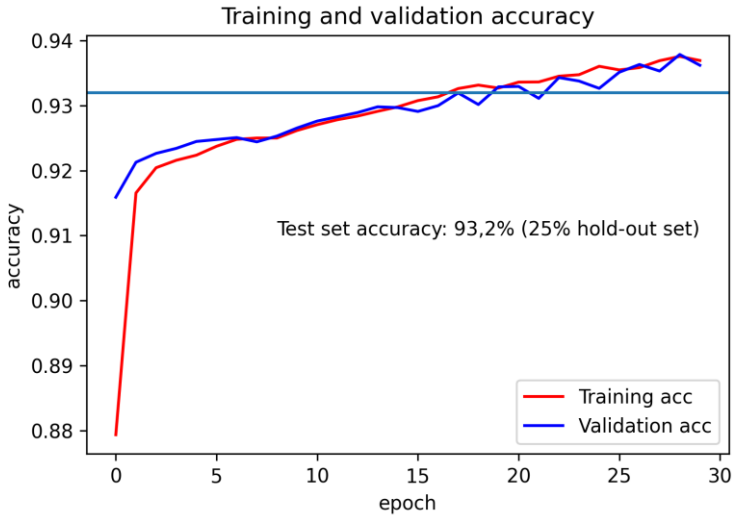
Appendix G | Classification: MetaData and Transfer Learning Keras Dense Feedforward NN Classifier



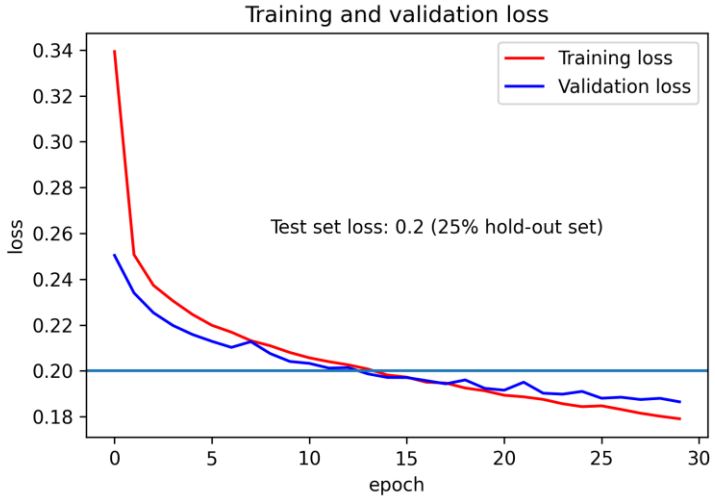
6 class classification



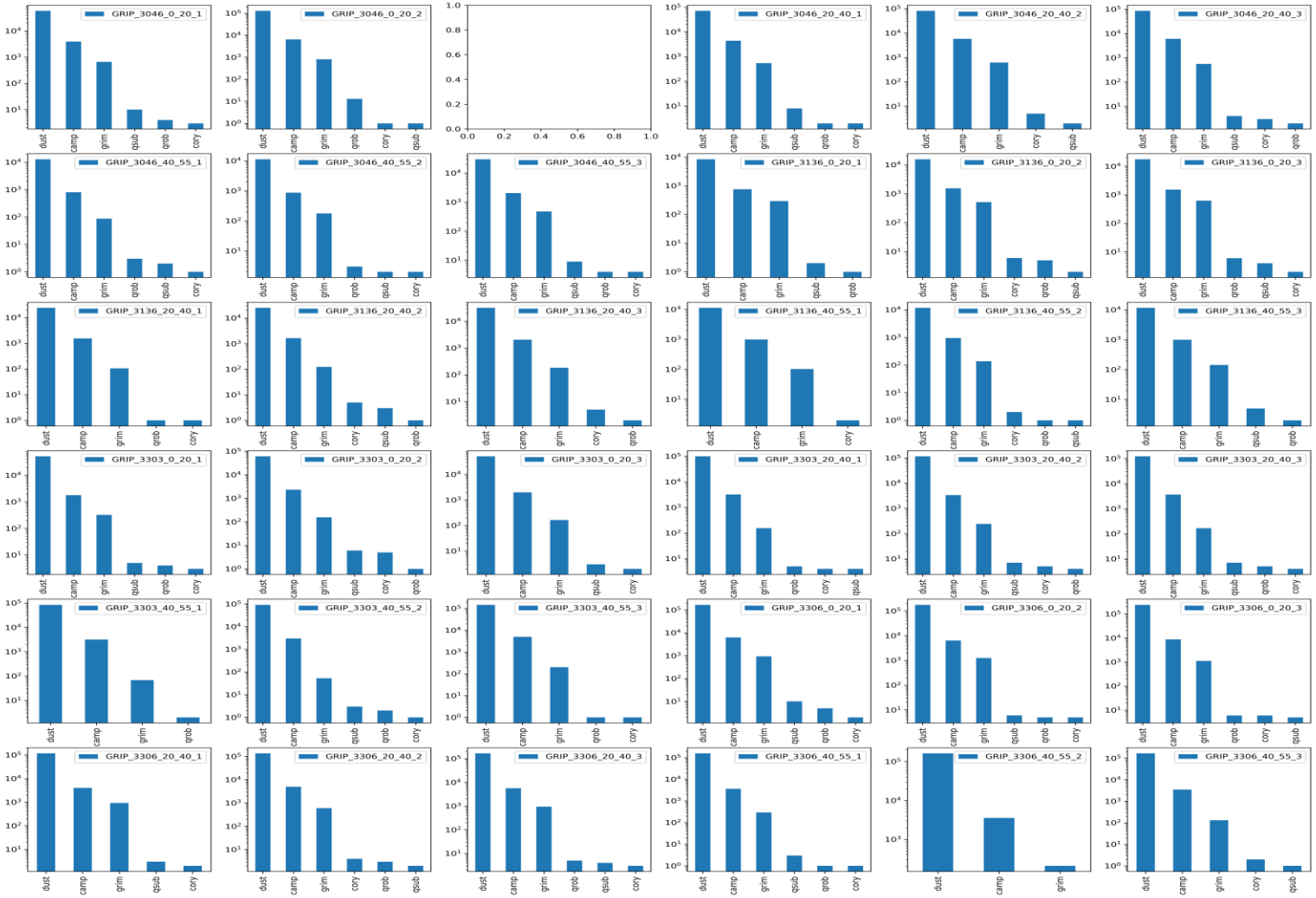
Appendix I | Classification: Transfer Learning Only Keras Dense Feedforward NN Classifier



Ash Only



Appendix I.1 | Predicted Class Distributions for real ICE data set by sample, segment, and repeated measurement



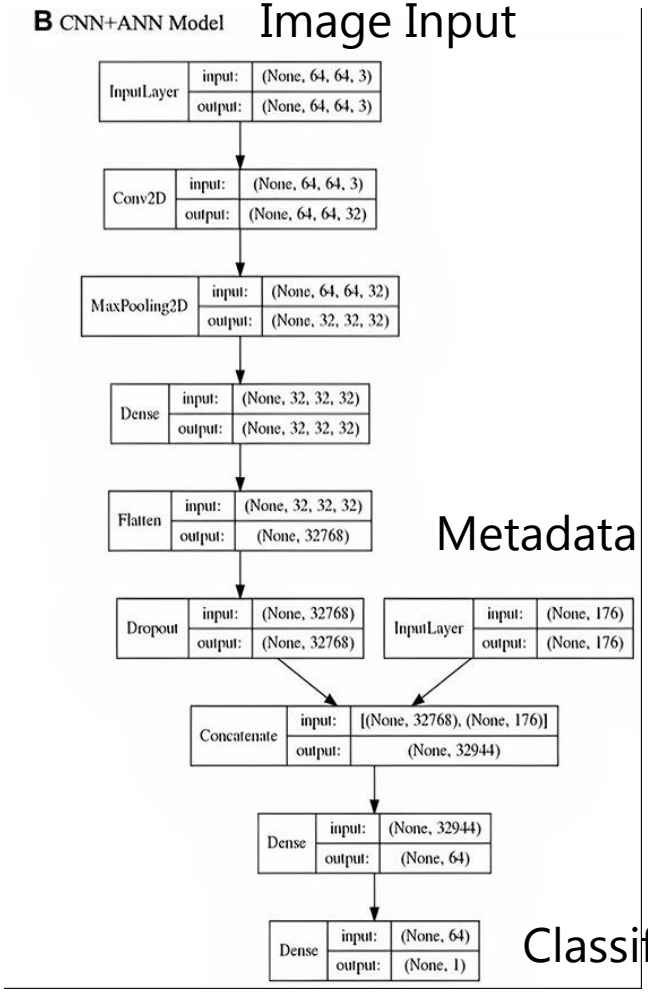
Appendix J | Also investigated

- Autoencoders – vanilla, convolutional, variational
  - Autoencoders may be used as anomaly detection
  - Convolutional autoencoders are appropriate for use with Images
  - Variational autoencoders may be used for a rich form of data augmentation

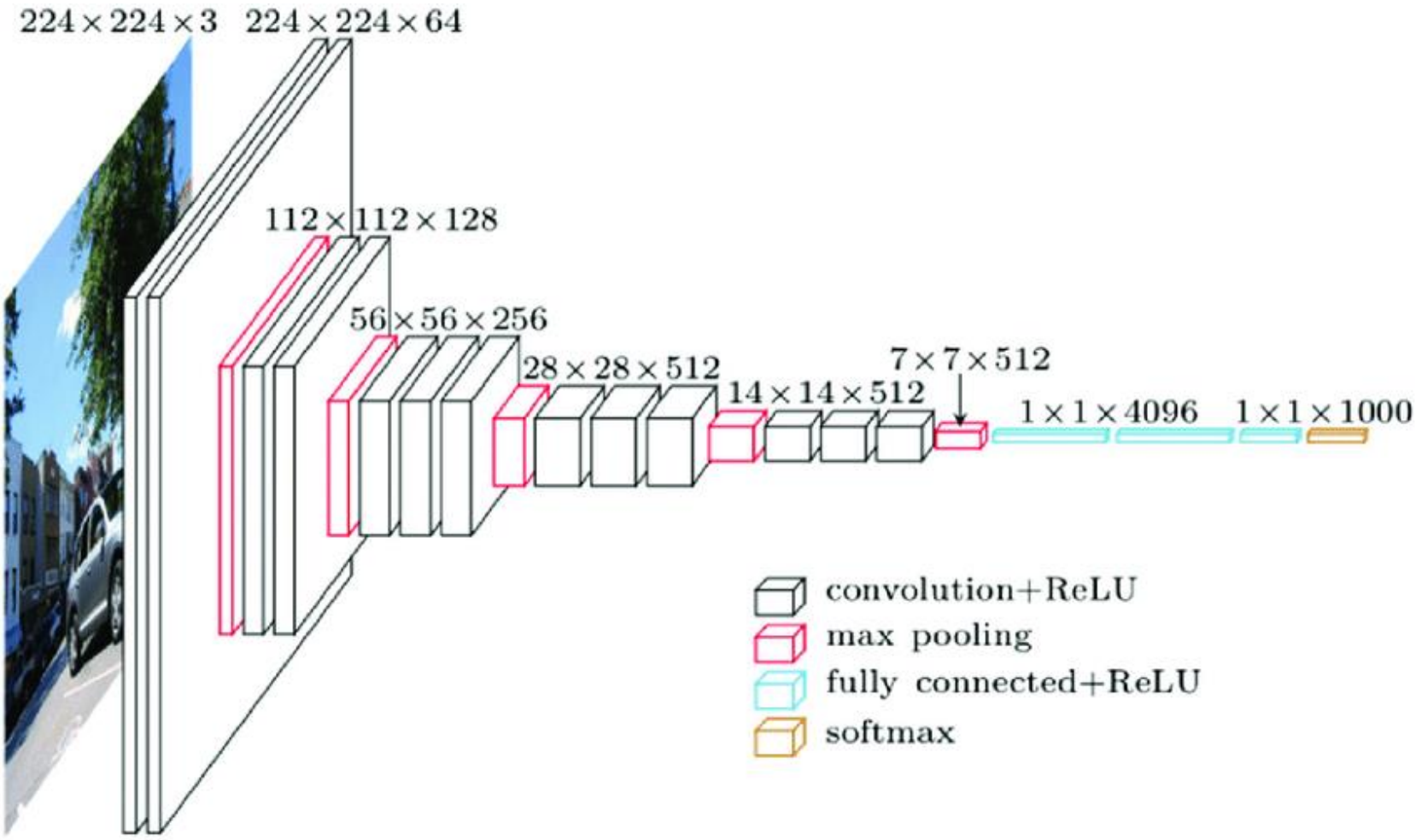
- Zero, one, few, and many shot learning
  - Use a siamese network to train on pairs of classes allowing classification to be performed on a similarity metric to high accuracy with very few if any labelled classes!

Appendix K | Schematic combining image data with metadata

Ningrum, Dina Nur Anggraini, et al. "Deep Learning Classifier with Patient's Metadata of Dermoscopic Images in Malignant Melanoma Detection." *Journal of Multidisciplinary Healthcare* 14 (2021): 877.



Appendix L | VGG Architecture



Appendix M | Isolation Forest: Separating Power