**Can liquid crystal phases be identified via machine learning?**

08/02/21

**Timeline for second semester**

1. Improve dataset
2. Consider more systematic uncertainty evaluation
3. Consider metrics for unbalanced datasets
4. Consider methods to tackle class imbalance
5. Implement and investigate transformer networks
6. Investigate further state of the art CNNs
7. Ambitious goal: accurate classifier of many phases

**Minimum uncertainty**

Going forward, a minimum percentage uncertainty will be assigned to model test accuracy predictions, as the square root of the total number of test set examples divided by itself.

**Transformer network implementation**

We have attempted to implement a transformer network following the paper “AN IMAGE IS WORTH 16X16 WORDS: TRANSFORMERS FOR IMAGE RECOGNITION AT SCALE”, however early testing has proved unsuccessful so far.

19/02/21

**Updated smectic 3 phase dataset**

We have now constructed an updated smectic dataset with additional samples in fluid and hexatic phases. The distribution of the new set is given below.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Fluid smectic | Hexatic | Soft crystal | Totals |
| Training | 2047 | 1338 | 600 | 3985 |
| Validation | 576 | 474 | 144 | 1194 |
| Test | 581 | 414 | 96 | 1091 |
| Totals | 3204 | 2226 | 840 | 6270 |

Since there were no new samples in the soft crystal class, it is now substantially underrepresented.

26/02/21

**Inception models for the updated set**

We now train the inception models again with the updated smectic set. This time, we perform 12 training runs. The model setups and training configurations are the same as the previous attempt at the general smectic task, aside from an increased batch size of 64. With the larger sample size of 12, the uncertainty is now taken as the standard deviation. The results are presented below.

|  |  |  |  |
| --- | --- | --- | --- |
| **Inception models, validation set accuracies** | | | |
| Training run | Number of blocks | | |
|  | 1 | 2 | 3 |
| 1 | 69.1 | 62.24 | 69.44 |
| 2 | 70.66 | 61.37 | 79.77 |
| 3 | 64.41 | 59.55 | 71.88 |
| 4 | 71.61 | 54.6 | 67.19 |
| 5 | 70.92 | 66.06 | 50.52 |
| 6 | 55.9 | 71.01 | 58.33 |
| 7 | 59.98 | 60.68 | 58.68 |
| 8 | 68.4 | 64.58 | 66.06 |
| 9 | 57.29 | 53.99 | 48 |
| 10 | 65.62 | 68.92 | 65.54 |
| 11 | 64.41 | 55.3 | 57.03 |
| 12 | 72.48 | 61.81 | 60.85 |
| Mean | 65.9 | 61.68 | 62.77 |
| Uncertainty | 5.43 | 5.19 | 8.64 |

|  |  |  |  |
| --- | --- | --- | --- |
| **Inception models, test set accuracies** | | | |
| Training run | Number of blocks | | |
|  | 1 | 2 | 3 |
| 1 | 75.83 | 62.87 | 62.68 |
| 2 | 65.53 | 66.82 | 81.34 |
| 3 | 69.94 | 83 | 85.48 |
| 4 | 74.08 | 72.52 | 84.19 |
| 5 | 71.51 | 87.13 | 47.79 |
| 6 | 62.04 | 69.85 | 64.71 |
| 7 | 68.93 | 76.93 | 65.9 |
| 8 | 76.84 | 84.93 | 87.59 |
| 9 | 71.51 | 68.57 | 53.4 |
| 10 | 66.64 | 77.3 | 76.19 |
| 11 | 60.94 | 68.38 | 57.17 |
| 12 | 67.56 | 72.06 | 83.36 |
| Mean | 69.28 | 74.2 | 70.82 |
| Uncertainty | 4.83 | 7.37 | 13.29 |

The means and uncertainties are displayed in the plot below.

Chart, box and whisker chart

Description automatically generated

The test set accuracy is noticeably higher than validation. This could imply that the test set is more similar to the training set than the validation set is. There is no notable improvement over the previous attempt at this task with the smaller dataset. We see large standard deviations suggesting low training stability.

01/03/21

**Focal Loss**

In an attempt to tackle the class imbalance issue, we retrain the best inception model from the updated smectic set using the focal loss, a type of loss function introduced by Lin et al in 2017 in the paper “Focal Loss for Dense Object Detection”. It is a modification of the standard cross-entropy that recues the loss for correctly classified examples, with a greater reduction for greater confidence in the prediction. This can help when training on an imbalanced set by ensuring the smaller classes are not “ignored” by the model. The focal loss function is

Alpha and gamma are the modulating and focussing hyperparameters respectively. We use the recommended default values of 0.25 for alpha and 2.0 for gamma, and train the 2 block inception model 12 times, with all other configurations the same as before.

|  |  |  |  |
| --- | --- | --- | --- |
| **Inception models with focal loss, validation set accuracies** | | | |
| Training run | Number of blocks | | |
|  | 1 | 2 | 3 |
| 1 | 66.06 | 57.73 | 48.35 |
| 2 | 57.55 | 76.48 | 54.08 |
| 3 | 63.02 | 48.26 | 70.23 |
| 4 | 66.58 | 53.47 | 48.09 |
| 5 | 65.97 | 65.02 | 69.27 |
| 6 | 61.46 | 56.86 | 48.18 |
| 7 | 61.63 | 58.25 | 39.93 |
| 8 | 59.64 | 71.01 | 61.28 |
| 9 | 69.62 | 55.82 | 62.93 |
| 10 | 56.42 | 48.44 | 58.85 |
| 11 | 60.5 | 64.06 | 63.54 |
| 12 | 63.11 | 53.04 | 67.1 |
| Mean | 62.63 | 59.04 | 57.65 |
| Uncertainty | 6.6 | 14.11 | 15.15 |

|  |  |  |  |
| --- | --- | --- | --- |
| **Inception models with focal loss, test set accuracies** | | | |
| Training run | Number of blocks | | |
|  | 1 | 2 | 3 |
| 1 | 68.66 | 70.5 | 53.31 |
| 2 | 73.16 | 90.44 | 56.62 |
| 3 | 82.9 | 53.22 | 81.71 |
| 4 | 69.12 | 74.08 | 53.4 |
| 5 | 70.86 | 69.76 | 59.1 |
| 6 | 63.14 | 61.4 | 53.22 |
| 7 | 70.68 | 72.33 | 37.96 |
| 8 | 76.01 | 78.68 | 70.31 |
| 9 | 60.2 | 68.57 | 57.08 |
| 10 | 66.27 | 43.11 | 56.43 |
| 11 | 65.44 | 89.43 | 78.68 |
| 12 | 71.51 | 49.72 | 80.88 |
| Mean | 69.83 | 68.44 | 61.56 |
| Uncertainty | 11.35 | 23.67 | 21.88 |

The plot of the mean accuracies is displayed on the next page.

Chart, box and whisker chart

Description automatically generated

Overall the models with focal loss perform worse than the ones without, and have much larger deviations in accuracies. This suggests that focal loss is not suitable for this task. The best single trained models, however, did perform slightly better than the normal loss best models.

The mean confusion matrices (averaged over all training repeats) are displayed below.

Chart, waterfall chart

Description automatically generatedChart, bar chart, waterfall chart

Description automatically generatedChart, bar chart, waterfall chart

Description automatically generatedChart, waterfall chart

Description automatically generatedChart, bar chart, waterfall chart

Description automatically generatedChart, waterfall chart

Description automatically generated

05/03/21

**New data sets**

We have created and split new datasets using all available images. These include (with a label in brackets):

* Cholesteric, smectic (ChSm2)
* Cholesteric, fluid smectic, hexatic smectic (ChSm3)
* Cholesteric, fluid smectic, hexatic smectic, soft crystal (ChSm4)
* Cholesteric, smectic A, C, F, I (ChSm5)
* Cholesteric, smectic A, C, F, I, soft crystal (ChSm6)
* Smectic A, C (smecticAC)
* Smectic I, F (smecticIF)

All have been split into training, validation and test with a 70:15:15 ratio.

**Batch size and learning rate on ChSm4 investigation**

We train the three layer sequential model, with 8 starting channels (doubling with each layer), for batch sizes of 16, 32 and 64, and learning rates of 1e-5, 1e-4, 1e-3, 1e-2, 1e-1. An early stopping patience of 30 is used, and the models are trained 5 times. The mean validation and test accuracies over the 5 runs for each configuration are presented in the tables below.

|  |  |  |  |
| --- | --- | --- | --- |
| **Validation mean accuracies** | | | |
| Learning rate | Batch size | | |
|  | 16 | 32 | 64 |
| 1.00E-05 | 64.85 | 62.65 | 64.49 |
| 1.00E-04 | 74.74 | 74.19 | 70.62 |
| 1.00E-03 | 72.24 | 68.96 | 71.76 |
| 1.00E-02 | 67.45 | 68.42 | 59.82 |
| 1.00E-01 | 53.52 | 58.16 | 50.77 |

|  |  |  |  |
| --- | --- | --- | --- |
| **Test mean accuracies** | | | |
| Learning rate | Batch size | | |
|  | 16 | 32 | 64 |
| 1.00E-05 | 70.56 | 67.13 | 68.61 |
| 1.00E-04 | 78.91 | 77.1 | 77.88 |
| 1.00E-03 | 82.48 | 74.86 | 76.6 |
| 1.00E-02 | 74.86 | 76.96 | 68.27 |
| 1.00E-01 | 62.23 | 64.42 | 55.48 |

From these results, we choose batch size of 16 and learning rate of 1e-4 for future training.

19/03/21

**Training sequential and inception models on the new sets**

We now train 3 and 4 layer sequential models and 1, 2 and 3 block inception models on the ChSm3, smecticAC and smecticIF sets. Starting channels of 8, 16, and 32 are tested for each of the 3 and 4 layer sequential models, and 2, 4, and 8 for the inception models. We use a batch size of 16 and learning rate of 1e-4 in all cases, and perform 10 training runs for all models. All other training configurations and augmentations are as before.

**ChSm3, sequential**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Validation accuracies** | | | | | | |
| Run | Architecture (number of layers, starting channels) | | | | | |
|  | 3, 8 | 3, 16 | 3, 32 | 4, 8 | 4, 16 | 4, 32 |
| 1 | 84.01 | 78.31 | 88.42 | 84.38 | 88.24 | 82.54 |
| 2 | 78.95 | 83.82 | 83.36 | 79.5 | 84.74 | 83 |
| 3 | 80.51 | 83.09 | 86.03 | 80.79 | 81.8 | 85.57 |
| 4 | 81.53 | 76.84 | 84.74 | 70.59 | 87.13 | 88.69 |
| 5 | 85.66 | 89.34 | 84.1 | 81.53 | 84.28 | 82.26 |
| 6 | 83.46 | 83.27 | 81.71 | 82.9 | 83.55 | 86.76 |
| 7 | 78.03 | 89.43 | 87.68 | 81.99 | 84.1 | 82.63 |
| 8 | 88.79 | 86.21 | 87.13 | 71.97 | 83 | 87.68 |
| 9 | 84.1 | 84.19 | 86.4 | 87.87 | 84.47 | 80.61 |
| 10 | 80.15 | 78.58 | 80.7 | 86.03 | 84.83 | 80.33 |
| Mean | 82.52 | 83.31 | 85.03 | 80.75 | 84.61 | 84.01 |
| Uncertainty | 3.13 | 4.15 | 2.44 | 5.3 | 1.78 | 2.81 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Test accuracies** | | | | | | |
| Run | Architecture (number of layers, starting channels) | | | | | |
|  | 3, 8 | 3, 16 | 3, 32 | 4, 8 | 4, 16 | 4, 32 |
| 1 | 81.88 | 82.68 | 83.39 | 86.07 | 84.2 | 86.43 |
| 2 | 83.75 | 87.59 | 88.84 | 78.48 | 88.84 | 86.34 |
| 3 | 83.84 | 82.05 | 88.3 | 86.87 | 89.46 | 85.89 |
| 4 | 82.23 | 71.16 | 87.5 | 81.52 | 84.29 | 83.39 |
| 5 | 85.62 | 88.48 | 83.3 | 79.11 | 85.45 | 84.46 |
| 6 | 83.75 | 85.27 | 84.02 | 82.32 | 87.32 | 85.98 |
| 7 | 80.18 | 86.52 | 85.89 | 86.25 | 86.61 | 87.32 |
| 8 | 88.57 | 89.02 | 88.84 | 79.82 | 84.38 | 87.32 |
| 9 | 86.7 | 86.96 | 88.21 | 83.93 | 85.09 | 83.57 |
| 10 | 79.46 | 85.54 | 82.5 | 87.14 | 83.93 | 83.57 |
| Mean | 83.6 | 84.53 | 86.08 | 83.15 | 85.96 | 85.43 |
| Uncertainty | 2.69 | 4.95 | 2.42 | 3.18 | 1.91 | 1.47 |

Chart, box and whisker chart

Description automatically generated

Fairly good performance with 86.08% mean test accuracy for the best architecture. Test accuracies overall higher than validation.

Chart, bar chart, waterfall chart

Description automatically generated

The mean confusion matrix for the best shows that the inaccuracies are mostly due to confusion of the smectic classes.

**ChSm3, inception**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Validation accuracies** | | | | | | | | | |
| Run | Architecture (number of blocks, starting channels) | | | | | | | | |
|  | 1, 2 | 1, 4 | 1, 8 | 2, 2 | 2, 4 | 2, 8 | 3, 2 | 3, 4 | 3, 8 |
| 1 | 75.37 | 72.43 | 77.85 | 70.31 | 72.43 | 70.59 | 77.3 | 85.11 | 83.92 |
| 2 | 84.83 | 71.97 | 85.66 | 76.38 | 76.47 | 86.03 | 79.32 | 76.47 | 81.62 |
| 3 | 79.14 | 80.42 | 80.7 | 80.79 | 86.4 | 85.39 | 74.91 | 82.81 | 80.06 |
| 4 | 80.33 | 78.4 | 86.86 | 83.92 | 88.97 | 77.76 | 81.71 | 81.99 | 83 |
| 5 | 77.94 | 79.87 | 85.39 | 79.78 | 84.56 | 83.64 | 76.29 | 86.03 | 86.21 |
| 6 | 79.14 | 81.89 | 83 | 79.5 | 71.05 | 82.72 | 77.67 | 81.8 | 85.11 |
| 7 | 81.25 | 79.23 | 84.74 | 79.5 | 79.32 | 86.58 | 79.87 | 75.37 | 84.1 |
| 8 | 82.54 | 83.55 | 80.15 | 82.9 | 83 | 82.26 | 70.86 | 85.29 | 79.32 |
| 9 | 79.5 | 85.94 | 84.01 | 79.32 | 74.91 | 78.68 | 80.61 | 85.02 | 82.81 |
| 10 | 76.65 | 81.89 | 80.42 | 78.77 | 80.33 | 77.76 | 81.07 | 79.5 | 87.22 |
| Mean | 79.67 | 79.56 | 82.88 | 79.12 | 79.74 | 81.14 | 77.96 | 81.94 | 83.34 |
| Uncertainty | 2.63 | 4.22 | 2.8 | 3.55 | 5.72 | 4.71 | 3.15 | 3.57 | 2.4 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Test accuracies** | | | | | | | | | |
| Run | Architecture (number of blocks, starting channels) | | | | | | | | |
|  | 1, 2 | 1, 4 | 1, 8 | 2, 2 | 2, 4 | 2, 8 | 3, 2 | 3, 4 | 3, 8 |
| 1 | 80.89 | 78.57 | 79.02 | 77.77 | 85.8 | 80.09 | 82.05 | 84.91 | 89.29 |
| 2 | 76.7 | 79.55 | 82.77 | 77.23 | 76.61 | 85 | 81.25 | 84.38 | 86.25 |
| 3 | 76.25 | 82.86 | 80.89 | 75.27 | 85 | 87.59 | 71.43 | 81.96 | 80.54 |
| 4 | 69.73 | 80.62 | 90.45 | 79.91 | 86.52 | 81.43 | 83.3 | 77.95 | 80.89 |
| 5 | 78.21 | 83.04 | 85.89 | 77.68 | 87.41 | 83.84 | 77.77 | 86.52 | 82.95 |
| 6 | 77.77 | 79.64 | 84.73 | 79.29 | 78.93 | 85.98 | 82.14 | 80.89 | 85.27 |
| 7 | 74.29 | 76.61 | 85.8 | 79.46 | 83.66 | 87.23 | 75.71 | 81.25 | 85.36 |
| 8 | 77.23 | 80.62 | 86.7 | 83.13 | 81.52 | 87.32 | 68.12 | 82.68 | 81.25 |
| 9 | 73.57 | 82.95 | 84.73 | 80.98 | 81.34 | 80.45 | 77.32 | 84.55 | 80.62 |
| 10 | 81.7 | 86.61 | 84.38 | 81.34 | 78.84 | 85.36 | 86.25 | 79.55 | 79.64 |
| Mean | 76.63 | 81.11 | 84.54 | 79.21 | 82.56 | 84.43 | 78.54 | 82.46 | 83.21 |
| Uncertainty | 3.33 | 2.69 | 3 | 2.18 | 3.49 | 2.72 | 5.33 | 2.52 | 3.01 |

**Chart, box and whisker chart

Description automatically generated**

The accuracies appear to increase with the number of starting channels, whereas increasing the number of inception blocks does not seem to provide any benefit. Overall performance was worse than for sequential.

Chart, bar chart, waterfall chart

Description automatically generated

This mean confusion matrix for the best inception model again shows substantial confusion between the smectic phases, in addition to a 16% misclassification of N\* as HSm.

**SmecticAC, sequential**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Validation accuracies** | | | | | | |
| Run | Architecture (number of layers, starting channels) | | | | | |
|  | 3, 8 | 3, 16 | 3, 32 | 4, 8 | 4, 16 | 4, 32 |
| 1 | 97.29 | 94.17 | 90.42 | 94.58 | 90.83 | 95.83 |
| 2 | 88.96 | 94.38 | 93.33 | 92.71 | 94.38 | 98.12 |
| 3 | 88.75 | 92.71 | 92.5 | 88.75 | 92.5 | 94.79 |
| 4 | 90.42 | 93.96 | 94.38 | 88.75 | 93.75 | 94.17 |
| 5 | 90.62 | 94.79 | 93.75 | 92.5 | 94.38 | 92.29 |
| 6 | 88.75 | 92.71 | 92.5 | 91.04 | 92.29 | 98.12 |
| 7 | 94.38 | 88.75 | 90.62 | 90.62 | 98.12 | 99.58 |
| 8 | 88.75 | 91.46 | 91.67 | 99.37 | 92.5 | 95.21 |
| 9 | 88.75 | 88.96 | 90.42 | 88.75 | 93.75 | 94.38 |
| 10 | 94.38 | 92.5 | 95.83 | 88.75 | 93.75 | 93.33 |
| Mean | 91.1 | 92.44 | 92.54 | 91.58 | 93.63 | 95.58 |
| Uncertainty | 2.95 | 2.03 | 1.73 | 3.24 | 1.83 | 2.22 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Test accuracies** | | | | | | |
| Run | Architecture (number of layers, starting channels) | | | | | |
|  | 3, 8 | 3, 16 | 3, 32 | 4, 8 | 4, 16 | 4, 32 |
| 1 | 96.88 | 95.51 | 99.8 | 100 | 98.83 | 91.8 |
| 2 | 92.77 | 99.61 | 97.07 | 98.05 | 97.27 | 97.66 |
| 3 | 98.63 | 98.24 | 98.24 | 100 | 97.66 | 90.04 |
| 4 | 96.68 | 97.66 | 99.8 | 96.48 | 91.99 | 98.05 |
| 5 | 99.41 | 97.07 | 90.82 | 97.66 | 99.02 | 94.14 |
| 6 | 100 | 99.61 | 99.8 | 100 | 97.07 | 89.26 |
| 7 | 99.22 | 99.61 | 99.8 | 98.24 | 93.75 | 97.27 |
| 8 | 97.27 | 90.62 | 92.38 | 99.22 | 99.8 | 92.19 |
| 9 | 99.61 | 99.8 | 98.83 | 99.22 | 98.63 | 94.73 |
| 10 | 100 | 98.83 | 98.24 | 98.05 | 98.83 | 99.61 |
| Mean | 98.05 | 97.66 | 97.48 | 98.69 | 97.29 | 94.47 |
| Uncertainty | 2.13 | 2.69 | 3.08 | 1.13 | 2.38 | 3.41 |

**Chart, box and whisker chart

Description automatically generated**

The sequential models perform extremely well on the smecticAC set, with 5 out 6 models above 97% mean test accuracy. The test accuracies are substantially higher than validation.

Chart, waterfall chart

Description automatically generated

**SmecticAC, inception**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Validation accuracies** | | | | | | | | | |
| Run | Architecture (number of blocks, starting channels) | | | | | | | | |
|  | 1, 2 | 1, 4 | 1, 8 | 2, 2 | 2, 4 | 2, 8 | 3, 2 | 3, 4 | 3, 8 |
| 1 | 96.04 | 95.21 | 98.75 | 89.38 | 99.58 | 96.67 | 96.67 | 97.5 | 100 |
| 2 | 100 | 96.04 | 100 | 98.75 | 94.38 | 98.54 | 90.83 | 91.46 | 96.25 |
| 3 | 92.5 | 98.12 | 93.12 | 97.92 | 96.67 | 97.5 | 92.5 | 100 | 98.75 |
| 4 | 91.25 | 94.38 | 95.63 | 94.38 | 94.38 | 99.37 | 97.29 | 100 | 94.38 |
| 5 | 99.79 | 98.33 | 94.38 | 94.79 | 99.58 | 92.5 | 93.96 | 94.58 | 100 |
| 6 | 88.75 | 97.92 | 95 | 91.04 | 100 | 99.58 | 96.04 | 99.37 | 94.79 |
| 7 | 93.75 | 88.75 | 97.08 | 93.96 | 100 | 93.96 | 94.38 | 95.63 | 97.08 |
| 8 | 88.75 | 98.96 | 94.58 | 95.42 | 96.25 | 98.54 | 98.96 | 94.58 | 97.71 |
| 9 | 93.96 | 94.17 | 98.54 | 100 | 96.25 | 100 | 98.12 | 96.04 | 93.33 |
| 10 | 92.29 | 99.58 | 93.12 | 91.67 | 98.33 | 99.79 | 93.96 | 93.96 | 98.75 |
| Mean | 93.71 | 96.15 | 96.02 | 94.73 | 97.54 | 97.65 | 95.27 | 96.31 | 97.1 |
| Uncertainty | 3.75 | 3.07 | 2.31 | 3.27 | 2.13 | 2.44 | 2.45 | 2.71 | 2.24 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Test accuracies** | | | | | | | | | |
| Run | Architecture (number of blocks, starting channels) | | | | | | | | |
|  | 1, 2 | 1, 4 | 1, 8 | 2, 2 | 2, 4 | 2, 8 | 3, 2 | 3, 4 | 3, 8 |
| 1 | 98.05 | 99.8 | 90.23 | 100 | 87.5 | 98.63 | 91.02 | 97.85 | 99.22 |
| 2 | 98.63 | 99.02 | 95.31 | 99.02 | 99.61 | 98.63 | 93.75 | 99.61 | 98.83 |
| 3 | 100 | 99.41 | 95.12 | 99.8 | 95.7 | 93.95 | 99.8 | 99.41 | 97.27 |
| 4 | 100 | 100 | 98.05 | 100 | 98.83 | 89.65 | 99.41 | 93.95 | 99.8 |
| 5 | 85.74 | 98.05 | 98.44 | 99.8 | 93.75 | 95.31 | 99.22 | 99.61 | 94.53 |
| 6 | 99.02 | 91.99 | 99.8 | 96.88 | 84.96 | 99.02 | 99.8 | 85.55 | 99.61 |
| 7 | 99.02 | 98.44 | 92.38 | 97.27 | 99.8 | 93.16 | 97.85 | 99.61 | 95.12 |
| 8 | 100 | 96.88 | 99.41 | 99.8 | 95.12 | 86.33 | 97.07 | 99.8 | 99.22 |
| 9 | 97.66 | 98.05 | 89.65 | 99.8 | 93.55 | 94.53 | 98.83 | 98.83 | 99.8 |
| 10 | 98.83 | 93.75 | 94.14 | 99.02 | 85.35 | 90.23 | 95.51 | 97.85 | 96.88 |
| Mean | 97.7 | 97.54 | 95.25 | 99.14 | 93.42 | 93.95 | 97.23 | 97.21 | 98.03 |
| Uncertainty | 4.06 | 2.53 | 3.49 | 1.09 | 5.37 | 4.03 | 2.8 | 4.23 | 1.87 |

**Chart, box and whisker chart

Description automatically generated**

The inception models also perform very well, with the best model achieving 99.14% mean test accuracy.

Chart, waterfall chart

Description automatically generated

**SmecticIF, sequential**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Validation accuracies** | | | | | | |
| Run | Architecture (number of layers, starting channels) | | | | | |
|  | 3, 8 | 3, 16 | 3, 32 | 4, 8 | 4, 16 | 4, 32 |
| 1 | 82.67 | 68.75 | 72.73 | 79.55 | 80.4 | 73.86 |
| 2 | 82.67 | 76.99 | 87.22 | 76.42 | 75.28 | 82.95 |
| 3 | 78.69 | 72.44 | 66.48 | 96.59 | 71.31 | 87.78 |
| 4 | 68.75 | 75.85 | 76.14 | 81.25 | 74.72 | 77.56 |
| 5 | 78.69 | 60.23 | 75.28 | 82.39 | 81.53 | 81.82 |
| 6 | 76.42 | 84.66 | 77.84 | 74.43 | 89.77 | 78.98 |
| 7 | 83.52 | 83.24 | 76.7 | 92.33 | 78.41 | 79.26 |
| 8 | 76.14 | 82.39 | 80.97 | 76.99 | 82.95 | 86.08 |
| 9 | 78.69 | 70.45 | 72.16 | 81.53 | 63.07 | 90.34 |
| 10 | 56.82 | 81.53 | 87.78 | 87.5 | 77.84 | 65.06 |
| Mean | 76.31 | 75.65 | 77.33 | 82.9 | 77.53 | 80.37 |
| Uncertainty | 7.66 | 7.37 | 6.26 | 6.8 | 6.82 | 6.95 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Test accuracies** | | | | | | |
| Run | Architecture (number of layers, starting channels) | | | | | |
|  | 3, 8 | 3, 16 | 3, 32 | 4, 8 | 4, 16 | 4, 32 |
| 1 | 51.63 | 46.74 | 77.99 | 68.75 | 69.57 | 71.74 |
| 2 | 69.84 | 69.29 | 54.62 | 63.59 | 77.72 | 68.75 |
| 3 | 67.93 | 86.96 | 64.95 | 49.46 | 60.6 | 65.76 |
| 4 | 57.88 | 73.1 | 68.48 | 59.24 | 46.47 | 64.13 |
| 5 | 75 | 65.76 | 73.91 | 37.5 | 52.99 | 54.35 |
| 6 | 61.41 | 57.07 | 63.32 | 57.34 | 53.26 | 60.33 |
| 7 | 72.28 | 64.4 | 70.11 | 56.25 | 66.58 | 38.86 |
| 8 | 53.53 | 70.11 | 67.12 | 74.46 | 55.71 | 53.8 |
| 9 | 64.67 | 79.89 | 73.64 | 61.96 | 61.68 | 65.22 |
| 10 | 70.65 | 65.76 | 56.79 | 39.95 | 70.11 | 50.54 |
| Mean | 64.48 | 67.91 | 67.09 | 56.85 | 61.47 | 59.35 |
| Uncertainty | 7.67 | 10.62 | 7.07 | 11.15 | 9.1 | 9.46 |

**Chart, box and whisker chart

Description automatically generated**

We see worse results for the smecticIF set. The validation accuracies fall in the range of 70-80%, with even lower test accuracies, with the best at 67.91%.

Chart, waterfall chart

Description automatically generated

**SmecticIF, inception**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Validation accuracies** | | | | | | | | | |
| Run | Architecture (number of blocks, starting channels) | | | | | | | | |
|  | 1, 2 | 1, 4 | 1, 8 | 2, 2 | 2, 4 | 2, 8 | 3, 2 | 3, 4 | 3, 8 |
| 1 | 68.47 | 82.67 | 80.97 | 82.67 | 83.52 | 79.26 | 86.08 | 86.93 | 92.9 |
| 2 | 74.43 | 71.88 | 85.8 | 80.97 | 89.49 | 83.24 | 76.14 | 71.59 | 90.34 |
| 3 | 53.98 | 76.14 | 74.72 | 54.55 | 54.55 | 76.42 | 86.36 | 75.85 | 83.81 |
| 4 | 76.99 | 92.05 | 84.94 | 78.98 | 76.99 | 96.59 | 92.61 | 77.84 | 90.06 |
| 5 | 90.34 | 86.65 | 94.6 | 72.73 | 63.64 | 77.84 | 88.92 | 73.3 | 87.5 |
| 6 | 46.02 | 73.58 | 84.09 | 93.18 | 89.49 | 82.39 | 79.26 | 90.91 | 80.97 |
| 7 | 45.17 | 93.75 | 98.01 | 70.17 | 81.53 | 94.03 | 69.03 | 92.05 | 81.82 |
| 8 | 82.39 | 91.19 | 92.9 | 75 | 83.24 | 84.38 | 83.81 | 73.01 | 95.74 |
| 9 | 66.76 | 86.65 | 95.17 | 84.38 | 57.39 | 89.77 | 90.62 | 54.83 | 98.58 |
| 10 | 84.94 | 85.23 | 80.68 | 89.77 | 86.36 | 92.9 | 79.26 | 88.35 | 88.92 |
| Mean | 68.95 | 83.98 | 87.19 | 78.24 | 76.62 | 85.68 | 83.21 | 78.47 | 89.06 |
| Uncertainty | 15.2 | 7.39 | 7.22 | 10.44 | 12.52 | 6.82 | 6.9 | 10.85 | 5.48 |

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Test accuracies** | | | | | | | | | |
| Run | Architecture (number of blocks, starting channels) | | | | | | | | |
|  | 1, 2 | 1, 4 | 1, 8 | 2, 2 | 2, 4 | 2, 8 | 3, 2 | 3, 4 | 3, 8 |
| 1 | 63.32 | 64.67 | 57.61 | 63.32 | 52.45 | 58.15 | 53.8 | 43.48 | 46.2 |
| 2 | 76.9 | 57.07 | 58.42 | 57.61 | 65.22 | 59.51 | 38.86 | 60.05 | 43.21 |
| 3 | 57.61 | 63.86 | 66.85 | 56.25 | 56.52 | 61.41 | 58.42 | 56.79 | 57.61 |
| 4 | 48.91 | 66.58 | 52.45 | 50.82 | 48.37 | 60.87 | 52.99 | 63.32 | 42.66 |
| 5 | 44.57 | 64.13 | 50.54 | 60.87 | 58.7 | 64.67 | 55.98 | 56.79 | 44.29 |
| 6 | 44.02 | 46.47 | 64.95 | 41.85 | 41.85 | 65.49 | 71.74 | 43.48 | 61.96 |
| 7 | 72.01 | 49.18 | 52.17 | 67.66 | 57.88 | 47.28 | 45.92 | 54.62 | 60.05 |
| 8 | 50.27 | 51.36 | 49.18 | 42.12 | 56.52 | 38.86 | 58.42 | 33.7 | 46.47 |
| 9 | 72.55 | 59.24 | 48.64 | 54.08 | 66.03 | 60.33 | 54.35 | 56.52 | 38.04 |
| 10 | 67.66 | 58.42 | 49.73 | 48.91 | 59.78 | 53.26 | 50.54 | 47.83 | 54.89 |
| Mean | 59.78 | 58.1 | 55.05 | 54.35 | 56.33 | 56.98 | 54.1 | 51.66 | 49.54 |
| Uncertainty | 11.72 | 6.69 | 6.28 | 8.14 | 6.94 | 7.88 | 8.16 | 8.73 | 7.91 |

**Chart, box and whisker chart

Description automatically generated**

The inception models perform even worse on the test set than the sequential models.

Chart, waterfall chart

Description automatically generated

Further investigation or expansion of the smecticIF dataset is needed.

29/03/21

**ChACHex**

Due to the difficulty in differentiating the smectic I and F phases, we have constructed another new dataset called ChACHex that includes cholesteric, smectic A, C, and hexatic smectic. With all the standard configurations and again 10 repeats, we train 3, 4, and 5 layer sequential models with starting channels of 4, 8, 16 and 32, and 1, 2, and 3 block inception models with starting channels of 2, 4, 8, and 16. The results are given below.

**Sequential**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sequential, validation accuracies** | | | | | | | | | | | | |
| Run | Architecture (number of layers, starting channels) | | | | | | | | | | | |
|  | 3, 4 | 3, 8 | 3, 16 | 3, 32 | 4, 4 | 4, 8 | 4, 16 | 4, 32 | 5, 4 | 5, 8 | 5, 16 | 5, 32 |
| 1 | 70.77 | 78.58 | 81.8 | 83 | 69.49 | 76.47 | 79.32 | 78.31 | 73.71 | 77.02 | 80.51 | 66.91 |
| 2 | 75.37 | 76.01 | 79.69 | 80.06 | 66.27 | 74.08 | 77.57 | 82.35 | 71.14 | 77.94 | 78.49 | 72.61 |
| 3 | 79.04 | 82.72 | 80.51 | 74.26 | 79.87 | 75.46 | 81.8 | 79.6 | 76.56 | 73.25 | 72.61 | 80.97 |
| 4 | 84.1 | 74.45 | 82.63 | 83 | 73.9 | 82.17 | 84.56 | 81.16 | 75.92 | 76.1 | 76.19 | 75.64 |
| 5 | 75.55 | 84.38 | 80.7 | 84.38 | 73.71 | 77.67 | 83.09 | 80.06 | 76.01 | 76.29 | 77.3 | 79.04 |
| 6 | 70.5 | 87.78 | 75.37 | 77.76 | 76.29 | 84.28 | 79.32 | 83.55 | 74.63 | 83.09 | 78.31 | 76.19 |
| 7 | 76.01 | 79.14 | 79.32 | 78.68 | 77.02 | 77.67 | 75 | 83.73 | 76.1 | 79.32 | 76.47 | 69.49 |
| 8 | 79.78 | 79.87 | 73.53 | 82.35 | 80.33 | 78.31 | 83.09 | 77.85 | 75.37 | 76.65 | 76.38 | 82.81 |
| 9 | 74.08 | 74.26 | 84.93 | 79.5 | 63.14 | 82.72 | 82.44 | 74.08 | 78.12 | 73.9 | 73.81 | 70.77 |
| 10 | 80.15 | 80.42 | 79.6 | 75.18 | 76.29 | 80.15 | 79.5 | 80.33 | 73.44 | 80.79 | 76.1 | 81.8 |
| Mean | 76.53 | 79.76 | 79.81 | 79.82 | 73.63 | 78.9 | 80.57 | 80.1 | 75.1 | 77.44 | 76.62 | 75.62 |
| Uncertainty | 4.07 | 4.11 | 3.14 | 3.25 | 5.39 | 3.17 | 2.79 | 2.76 | 1.86 | 2.84 | 2.16 | 5.26 |

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Sequential, test accuracies** | | | | | | | | | | | | |
| Run | Architecture (number of layers, starting channels) | | | | | | | | | | | |
|  | 3, 4 | 3, 8 | 3, 16 | 3, 32 | 4, 4 | 4, 8 | 4, 16 | 4, 32 | 5, 4 | 5, 8 | 5, 16 | 5, 32 |
| 1 | 79.64 | 85.62 | 87.14 | 84.55 | 68.04 | 81.61 | 83.3 | 85.8 | 78.21 | 83.04 | 86.87 | 79.55 |
| 2 | 77.14 | 83.04 | 86.07 | 81.34 | 79.82 | 85.45 | 82.86 | 86.61 | 76.34 | 83.66 | 83.93 | 77.86 |
| 3 | 77.77 | 89.2 | 85.09 | 81.79 | 86.34 | 71.34 | 84.55 | 85 | 70.63 | 84.55 | 75.89 | 78.48 |
| 4 | 79.29 | 82.86 | 89.2 | 82.77 | 74.37 | 88.13 | 87.59 | 88.04 | 81.25 | 84.29 | 87.14 | 85.45 |
| 5 | 73.57 | 83.39 | 85.54 | 88.13 | 78.12 | 82.23 | 84.2 | 85.27 | 80.45 | 79.46 | 78.39 | 83.57 |
| 6 | 71.52 | 86.25 | 83.13 | 82.32 | 73.66 | 83.66 | 80.98 | 87.77 | 66.25 | 82.05 | 85.09 | 79.11 |
| 7 | 79.82 | 83.75 | 84.64 | 83.04 | 76.79 | 85.18 | 79.46 | 86.96 | 78.75 | 83.04 | 82.59 | 79.55 |
| 8 | 82.95 | 80.09 | 84.82 | 88.13 | 78.04 | 83.93 | 87.05 | 84.73 | 74.37 | 82.77 | 83.3 | 80.27 |
| 9 | 76.79 | 83.3 | 86.79 | 87.59 | 61.34 | 90.09 | 87.77 | 83.66 | 75.36 | 78.21 | 81.96 | 78.12 |
| 10 | 79.46 | 82.95 | 82.5 | 90.71 | 79.64 | 85.27 | 85.36 | 87.32 | 78.66 | 77.86 | 85.8 | 83.04 |
| Mean | 77.79 | 84.04 | 85.49 | 85.04 | 75.62 | 83.69 | 84.31 | 86.12 | 76.03 | 81.89 | 83.1 | 80.5 |
| Uncertainty | 3.13 | 2.33 | 1.85 | 3.14 | 6.55 | 4.77 | 2.63 | 1.37 | 4.4 | 2.35 | 3.44 | 2.47 |

Chart, box and whisker chart

Description automatically generated

Overall the sequential models perform well, with the best being the 4 layers, 32 starting channels architecture at 86.12% test accuracy. The models again perform better on the test set than the validation set.

Chart, bar chart

Description automatically generated

From the mean confusion matrix, the main source of inaccuracy appears to be from misidentification of smectic C as hexatic, at 25%. There is also a 10% confusion rate of cholesteric as hexatic.

**Inception**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Inception, validation accuracies** | | | | | | | | | | | | |
| Run | Architecture (number of blocks, starting channels) | | | | | | | | | | | |
|  | 1, 2 | 1, 4 | 1, 8 | 1, 16 | 2, 2 | 2, 4 | 2, 8 | 2, 16 | 3, 2 | 3, 4 | 3, 8 | 3, 16 |
| 1 | 79.78 | 78.31 | 71.78 | 80.88 | 80.79 | 85.57 | 80.42 | 79.6 | 75.37 | 79.6 | 85.11 | 62.13 |
| 2 | 68.93 | 80.79 | 80.79 | 80.97 | 73.07 | 77.39 | 75.09 | 84.65 | 81.62 | 72.43 | 76.1 | 80.97 |
| 3 | 83.64 | 75.83 | 76.93 | 79.32 | 72.43 | 71.14 | 65.26 | 83.73 | 77.02 | 77.02 | 82.26 | 81.07 |
| 4 | 75.18 | 76.84 | 81.07 | 83.82 | 77.02 | 74.36 | 75 | 76.19 | 73.16 | 79.04 | 80.15 | 71.88 |
| 5 | 71.88 | 73.07 | 73.99 | 82.08 | 80.88 | 76.29 | 78.68 | 80.33 | 82.44 | 78.12 | 79.23 | 71.14 |
| 6 | 74.45 | 77.94 | 80.33 | 74.36 | 69.85 | 85.11 | 80.7 | 80.51 | 78.12 | 81.99 | 80.15 | 80.51 |
| 7 | 76.19 | 79.96 | 73.81 | 78.03 | 77.94 | 81.89 | 80.15 | 75.55 | 77.94 | 79.04 | 85.39 | 75.46 |
| 8 | 77.21 | 83.36 | 82.35 | 78.31 | 77.11 | 77.21 | 82.44 | 73.53 | 74.26 | 77.85 | 76.93 | 83.09 |
| 9 | 77.02 | 82.72 | 79.5 | 78.58 | 73.44 | 77.3 | 83.82 | 77.94 | 77.48 | 77.3 | 80.42 | 80.61 |
| 10 | 79.23 | 85.75 | 81.25 | 85.85 | 71.78 | 79.69 | 77.94 | 84.93 | 79.96 | 72.89 | 84.28 | 82.72 |
| Mean | 76.35 | 79.46 | 78.18 | 80.22 | 75.43 | 78.59 | 77.95 | 79.7 | 73.86 | 77.53 | 81 | 76.96 |
| Uncertainty | 3.93 | 3.63 | 3.57 | 3.09 | 3.65 | 4.33 | 5.02 | 3.74 | 2.94 | 2.78 | 3.07 | 6.41 |

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Inception, test accuracies** | | | | | | | | | | | | |
| Run | Architecture (number of blocks, starting channels) | | | | | | | | | | | |
|  | 1, 2 | 1, 4 | 1, 8 | 1, 16 | 2, 2 | 2, 4 | 2, 8 | 2, 16 | 3, 2 | 3, 4 | 3, 8 | 3, 16 |
| 1 | 88.13 | 79.55 | 75.54 | 81.07 | 80.89 | 83.13 | 88.75 | 81.43 | 79.91 | 82.05 | 79.02 | 77.14 |
| 2 | 72.59 | 89.38 | 83.21 | 82.05 | 75.45 | 83.93 | 80.27 | 84.46 | 86.96 | 77.23 | 80 | 83.93 |
| 3 | 77.86 | 77.14 | 78.39 | 85.09 | 73.57 | 76.43 | 80.45 | 85.54 | 81.25 | 83.84 | 80.45 | 83.57 |
| 4 | 82.05 | 81.34 | 84.29 | 89.38 | 82.23 | 82.14 | 85.36 | 88.21 | 80.27 | 80.98 | 78.93 | 78.04 |
| 5 | 71.25 | 73.12 | 80.89 | 90.27 | 85.18 | 80.8 | 81.7 | 84.73 | 79.46 | 78.75 | 78.57 | 75.71 |
| 6 | 75.89 | 85.8 | 81.88 | 74.55 | 80.54 | 86.96 | 81.88 | 87.32 | 86.52 | 82.5 | 85.71 | 83.13 |
| 7 | 72.59 | 79.46 | 72.32 | 80.89 | 79.02 | 82.5 | 80.62 | 80.54 | 82.68 | 81.88 | 84.73 | 82.5 |
| 8 | 74.55 | 81.16 | 82.14 | 79.64 | 79.55 | 85.45 | 81.34 | 83.48 | 70.18 | 73.75 | 81.61 | 85.89 |
| 9 | 74.29 | 80.45 | 83.04 | 85.89 | 77.14 | 81.79 | 89.38 | 87.23 | 74.11 | 81.07 | 84.11 | 83.39 |
| 10 | 81.07 | 84.29 | 82.14 | 85.62 | 67.5 | 77.32 | 86.16 | 88.75 | 81.34 | 85.62 | 86.52 | 79.55 |
| Mean | 77.03 | 81.17 | 80.38 | 83.45 | 78.11 | 82.04 | 83.59 | 85.17 | 76.81 | 80.77 | 81.96 | 81.29 |
| Uncertainty | 5.03 | 4.31 | 3.63 | 4.5 | 4.74 | 3.1 | 3.33 | 2.65 | 4.7 | 3.24 | 2.88 | 3.23 |

Chart, box and whisker chart

Description automatically generated

The inception models perform worse overall than the sequential ones. The best model was the 2 block, 16 starting channels architecture with 85.17% test accuracy.

Chart, bar chart

Description automatically generated

The mean confusion matrix for the best inception model is very similar to that of the best sequential model.