Data-Driven Approaches for the Classification of Crystallisation Outcomes from In-line Images

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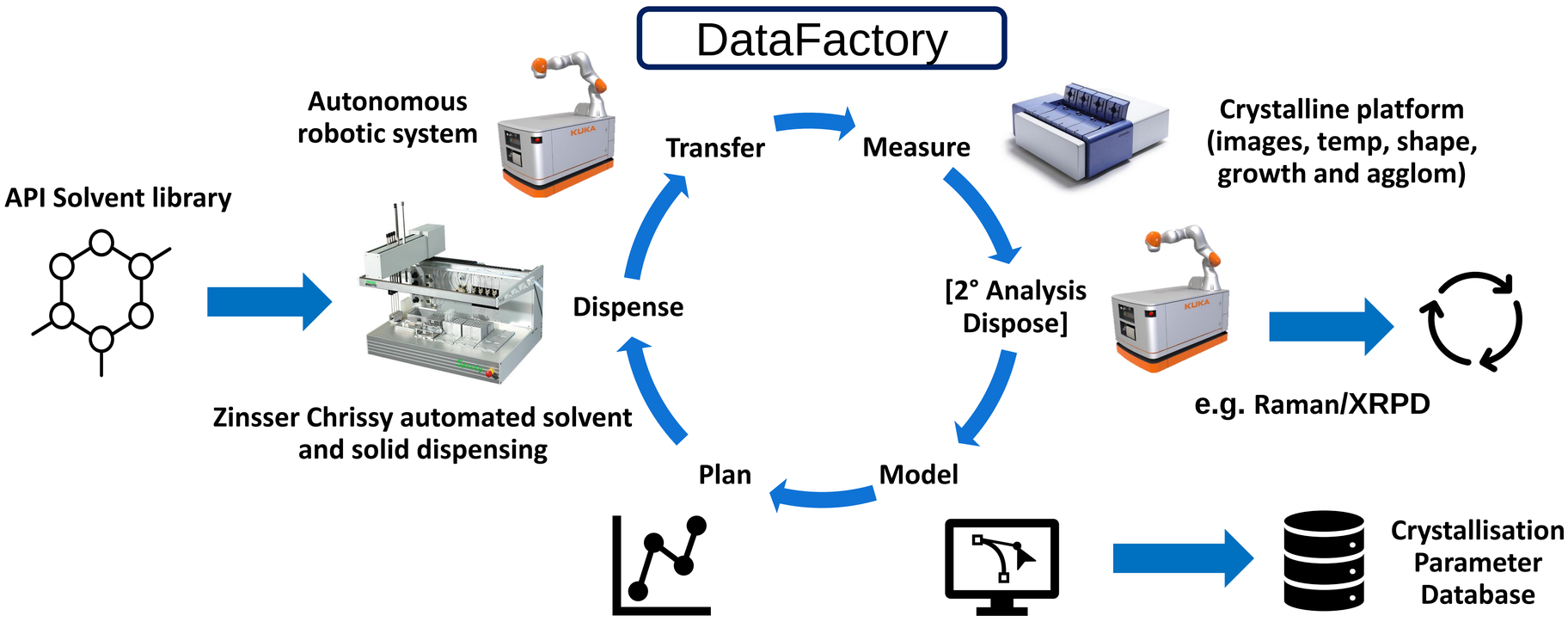
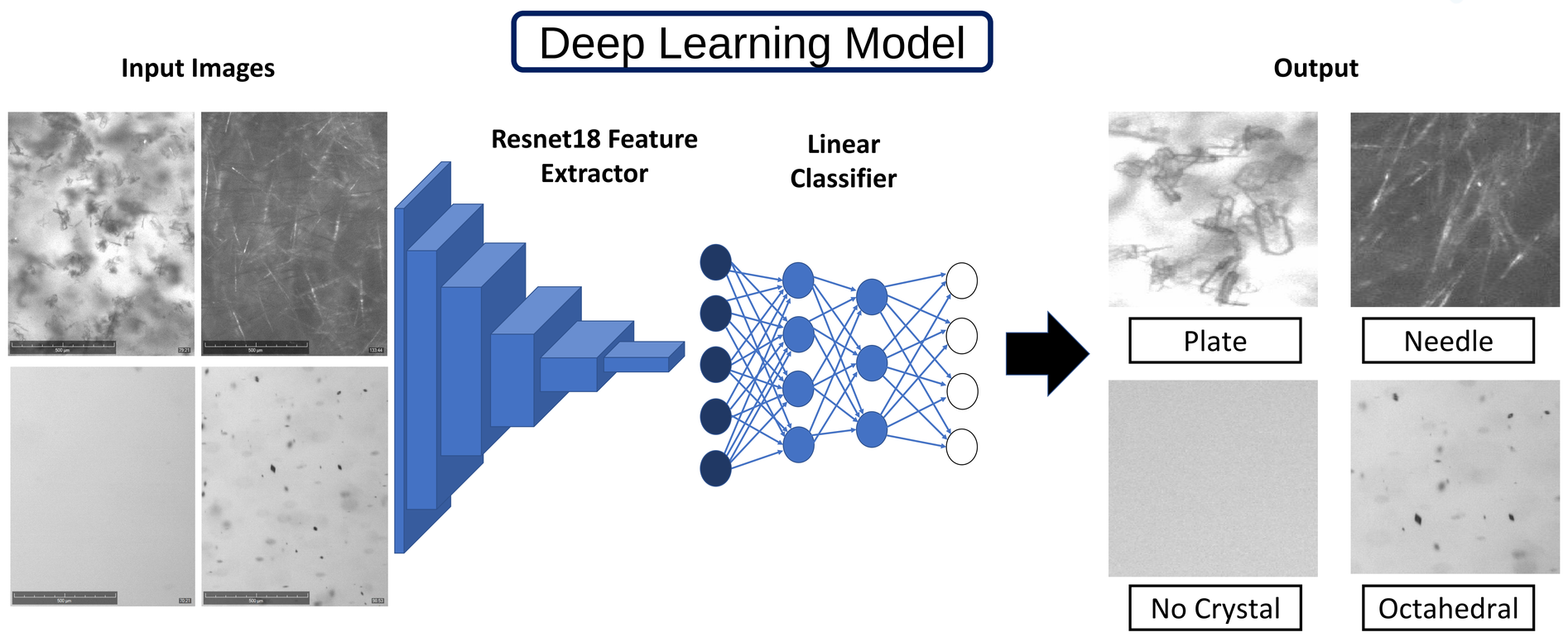


Motivation

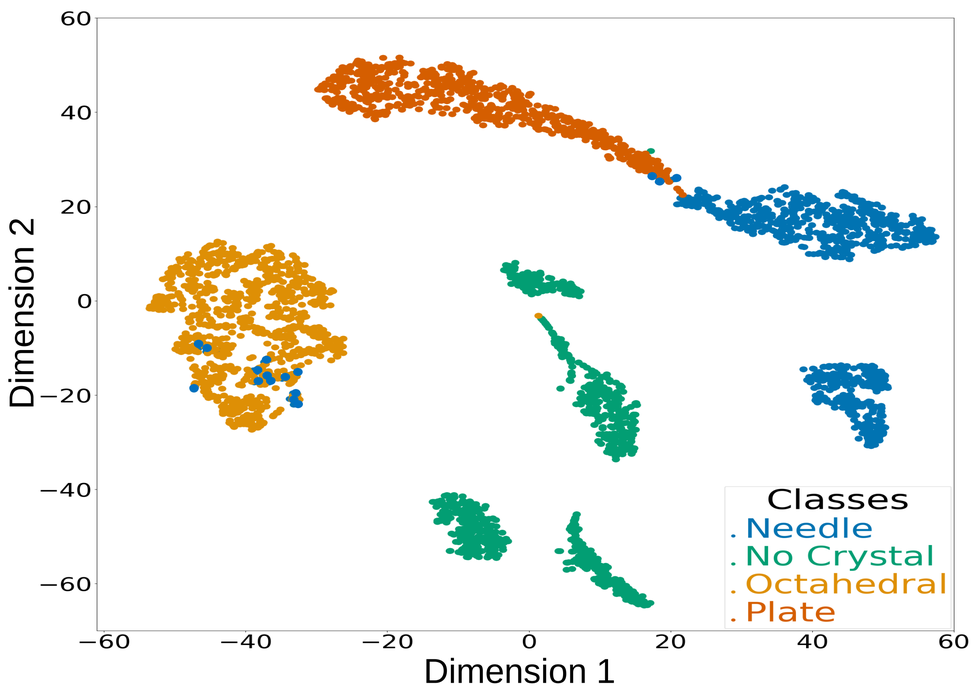
- Implementing a data-driven approach that can automate the classification of different phases of high-throughput crystallisation processes can be a powerful tool for **[1][2]**:
  - ❑ Predict the quality and consistency of the final pharmaceutical product
  - ❑ Optimise manufacturing processes
  - ❑ Reduce waste
- Advanced analytical techniques and machine learning algorithms can be leveraged to extract relevant features on crystallisation outcomes from in-line images.

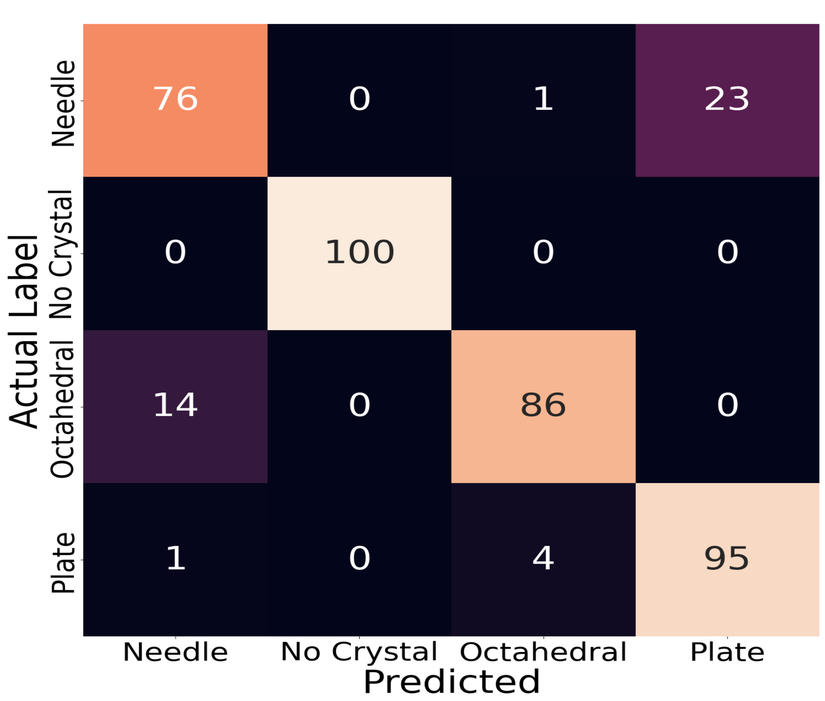
Method

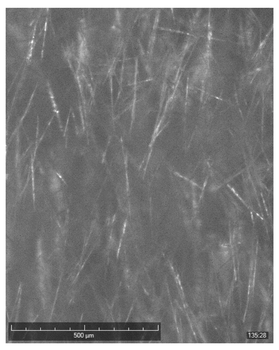
- Model comprised of pre-trained ResNet-18 feature extractor and one-layer linear classifier.
- 3164 images were used as training data (791 images per class), 788 images as validation data (197 images per class) and 400 images were used as test data (100 images per class).
- Augmentations (edge crop, image rotation and padding) applied to the training data to increase data diversity allowing improved model generalisation.

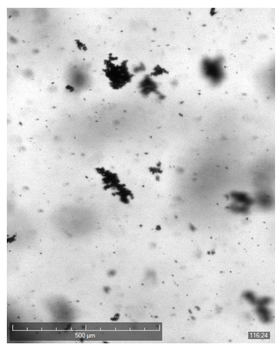


Results

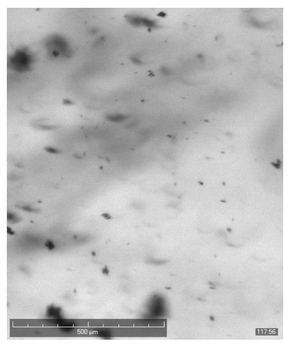


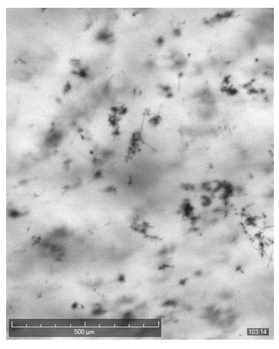



True: Needle


True: Octahedral


True: Plate


True: Octahedral
Predicted: Needle


True: Needle
Predicted: Plate

Conclusion

- The model achieves an average precision and recall greater than 85%.
- In the latent space graph, we can see features from the needle class overlap with the plate and octahedral cluster space.
- A more varied dataset and more augmentations (brightness and contrast) are necessary to further improve the classification of crystallisation outcomes.

References

[1] Borsos, A., Szilágyi, B., Agachi, P. S. & Nagy, Z. K. Real-Time Image Processing Based Online Feedback Control System for Cooling Batch Crystallization. *Org Process Res Dev* 21, 511–519 (2017).

[2] Silva, A. F. T. et al. Particle sizing measurements in pharmaceutical applications: Comparison of in-process methods versus off-line methods. Eur J Pharm Biopharm 85, 1006–1018 (2013).