Centre for AI-Fundamentals
RAEng Google DeepMind Summer Internship Programme 2025

Project proposal

Project Title	Machine Learning of Voronoi patterns applied to physical, chemical and biological systems
Lead supervisor	Ingo Dierking
Project Description	Calculating a Voronoi pattern from seed points is a simple task. One simply lets the seed grow radially at constant speed and stops growth whenever two interfaces of growing circles meet. The reverse process, calculating the originating seed positions from an experimentally observed Voronoi pattern, is by far more demanding. Yet in many situations it is of interest to fundamentally understand where these seeds are located, while only the final Voronoi pattern is provided from experiment. Examples can be found in systems as diverse as dragonfly wings, biological cell growth, dried mud patterns, giraffe skin, leaves, bones, and the like. Systems where the knowledge of seed position is particularly helpful in order to understand the growth process and dynamics are for example found in liquid crystals and solid state materials, the melting of thin polymer films or the processing of ultrathin metal films on substrates. Applications based on structured growth, for example in photonic devices, rely on precise knowledge and control of the growth inducing seeds. We will use machine learning algorithms to predict the seeds of Voronoi patterns. The algorithms will be trained on computer generated Voronoi patterns of known, random seed distributions and corresponding patterns. The training data will be generated computationally during the first step of the project. In a second step the prediction accuracy will be quantified via a robust mechanism comparing predicted and known seed position distribution. The algorithm will be optimised by tuning the hyperparameters used in different machine learning architectures (convolutional neural networks of varying number of layers versus inception models with varying number of modules). Finally, in a third project step the complete and optimised algorithm will be applied to a broad range of material systems, such as Blue Phases in liquid crystals, melting of thin polymer films, biological structures, and

	the processing of ultra-thin metal films. For demonstration of the feasibility of the approach, exemplary images will be taken from literature. The machine learning approach will be sufficiently robust to be applied to many other systems as well, so that it is possible to gain fundamental insight about the structure formation mechanism or regularity of the patterns under investigation. This will be of significant importance for material development in many areas of science.
Summary of project objectives	To devise a machine learning algorithm that - provides the location of seeds of a Voronoi pattern - verifies the robustness and accuracy of this algorithm - demonstrates the algorithm for different experimentally observed Voronoi patterns
Learning outcomes	- To understand Voronoi patterns and their uses - To understand training, validation and testing machine learning algorithms - To critically judge the accuracy and limitations of machine learning - To apply the gained skills and knowledge to experimental examples
Work plan	(1) To generate a sufficiently large number of Voronoi patterns including knowledge of their seed positions to act as training and verification data. (2 weeks) (2) Suitable machine learning algorithms will be trained, tuned and tested by varying the number of convolutional neural network layers or inception blocks needed to get accurate results while avoiding overfitting. (3 weeks)* (3) Prediction accuracy will be determined via a robust mechanism comparing predicted and known seed positions as well as the spatial cell boundaries. (1 week)* (4) Demonstration of the practical feasibility of the machine learning algorithm on experimental sample data for a variety of real-life systems. (1 week) *WP2 and WP3 to some extent run in parallel, to provide a feedback loop.