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Review report on the PhD thesis
„Modeling and statistics of random tessellations with applications to the study of microstructure of polycrystallic materials“
by Filip Seitl

Models from stochastic geometry have been widely established to simulate virtual materials' microstructure geometries. For cellular or polycrystalline materials, random tessellations are the model class of choice. In his thesis, Filip Seitl considers Laguerre tessellation models for the grain system in polycrystalline materials. He formulates new modelling approaches based on Gibbs-Laguerre tessellations and provides a two-step model which reproduces dependencies of generator locations and radii.

The thesis starts with an introduction where the motivation of the work is outlined. The contributions of the candidate are summarized and the organization of the manuscript is discussed.

Chapter 1, also under the headline "Motivation", introduces Laguerre tessellations as well as the datasets to be used in the thesis. These are two samples of polycrystalline materials, a nickel titanium (NiTi) and an aluminium alloy. For the former, Laguerre generators are taken from another study where a cross-entropy reconstruction is applied to a 3D X-ray diffraction microscopy measurement. For the latter, a sample is imaged in 3D by synchrotron tomography. A Laguerre tessellation approximation is also obtained by the cross-entropy method. For both sets of generators, Mr Seitl checks stationarity and computes distributions and correlations of several characteristics of the Laguerre tessellations.

In the second chapter, the theoretical background of the methods developed in the thesis is presented. This includes the definition of tessellations, in particular the Voronoi and the

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Laguerre tessellation, as well as their main properties and geometric characteristics. Additionally, hypergraphs are introduced as a tool for representing the tessellation geometry. The second half of the chapter is devoted to (marked) point processes which serve as generators for random tessellation models. The Poisson point process and Gibbs point processes are introduced as main model classes. Some established summary statistics for stationary point processes are described together with their estimators. Finally, simulation methods and some statistical tools used in the thesis are summarized.

The scientific results of the thesis are presented in Chapters 3 and 4. Chapter 3 deals with Gibbs-Laguerre tessellations, a generalization of Gibbs-Voronoi tessellations to the Laguerre case. First, an energy function is introduced which is based on summing potentials of several orders. Hard core potentials represent examples of first order potentials. Second order potentials are used to control properties of neighbouring cells. These potentials are similar to those used for modelling hardcore and pairwise interaction point processes, respectively. An alternative option is given by the so-called reconstructing potentials which are of order n. These aim at reconstructing moments or empirical distributions of cell characteristics of the tessellation. The potential is given by a discrepancy function comparing the value/distribution for the data with the desired one.
Subsequently, conditions for the existence of Gibbs-Laguerre tessellations are established. The proof uses the hypergraph structure and is based on showing the conditions of an existence theorem from Dereudre et al. (2012). Parameter estimation by maximum pseudolikelihood and estimation of the hardcore parameters are shortly discussed.

In the second part of the chapter, some applications are presented. The first task deals with the simulation of model realizations that fit an observed cell structure. The classical parametric approach would imply to formulate a model whose parameters are then estimated from the data. Due to problems with this type of estimation, Mr Seitl favours a reconstruction approach based on a potential of order n. This is a rather non-standard interpretation of fitting Gibbs models which is more similar to reconstruction approaches based on stochastic optimization that can be found in the literature.
In a first experiment, the moments of selected cell characteristics should be fit, in a second experiment, full empirical distributions are considered. In both cases, the number of facets per cell or the cell volume are used as characteristics of interest. A third model combines both characteristics. It seems that the aluminium alloy data is used as an example. However, the given mean number of facets does not fit the value given in Table 1.4.
The model parameter θ is no longer estimated but chosen heuristically similar to a regularization parameter in variational approaches. The influence of its choice is illustrated in some experiments. The number of iterations of the algorithm is based on a stopping criterion rather than fixing it a priori.
It turns out that the models fitting the different characteristics have a very different cell intensity. For my taste, this point could be discussed in more detail as fitting the intensity (which is automatically achieved when including the mean volume) might be considered a minimal requirement for a good fit.

The reconstruction approach is then compared to the greedy algorithm introduced by Cormen et al. 2009, which is one out of several reconstruction algorithms that can be found in the literature. Here, a theoretical comparison of the reconstruction approach based on Gibbs models with these other approaches would have been of interest. Which assumptions have to

be made? Which objective functions are used? What are the runtimes? How difficult is the parametrization of the approaches?
Finally, the moment fitting approach is used to simulate tessellation models with rather extreme moments for the mean number of facets per cell, namely mean values of 12 and 18. Mark correlation statistics for the resulting generator systems are estimated and compared.
In a second simulation study, the pairwise interaction model based on the neighbour volume ratio is used as a means to generate models with varying regularity of the cell shapes.

While the Gibbs models discussed in Chapter 3 are based on simultaneous modelling of generator locations and weights, a sequential approach is introduced in Chapter 4. That is, initially the generator locations are modelled by a pairwise interaction Gibbs point process. In a second step, the radii are modelled conditioning on the locations. The latter is required as the hypothesis of independent marking is rejected by a permutation test for both data sets under consideration.
In this context, the problem of choosing the bandwidth when estimating the pair correlation function by a kernel estimator is discussed. In particular, the recommendation given by Illian et al. and the default used in the R-package spatstat are found to be inappropriate for the given data.
The proposed modelling approach is applied to the NiTi alloy data set. Model selection based on global envelope tests and evaluation of the maximal log pseudolikelihood is discussed.

The results of the thesis are then summarized in a conclusion section. The appendix contains further information on pseudo-periodic configurations used in the proof of existence of the Gibbs models. It also summarizes the results of additional simulation studies, namely a reconstruction model fit based on the sphericity and a comparison of Gibbs Laguerre tessellations with Poisson Laguerre tessellations. The values of the pseudolikelihood functions obtained in the profile pseudolikelihood approach for the two-step model from Chapter 4 are also given. Finally, software tools for the simulation of Voronoi and Laguerre tessellations are listed. In particular, there is a reference to a github repository containing the code for the methods developed in the thesis.

With his thesis, Mr Seitl contributes to the field of stochastic modelling of materials microstructures. The thesis considers both theoretical and application aspects. As a result of Chapter 3, Gibbs-Laguerre tessellations become available as a powerful class of tessellation models. The modelling approach from Chapter 4 provides an elegant way of including dependence of generator locations and radii in the model. The application focusses on modelling of polycrystalline materials. However, the methods provided here are also of interest for other classes of cellular materials such as foams. It should be noted that all practical studies in the thesis are carried out in 3D, whereas restricting to 2D is still very common in spatial statistics. In particular, implementations of established statistics such as the mark correlation function are often only available in 2D such that Mr Seitl had to reimplement them for the 3D case.

In total, the thesis is well written. Simulation studies are designed in a sound way and the conclusions are comprehensible. However, partially a different organization of the text might have improved the readability. In particular, Chapter 3 is relatively long such that a subdivision into a theory and an application chapter might have been considered. Additionally, Mr Seitl frequently refers to future parts of the text which hampers the understanding as required formulas are not yet available.

The main results of the thesis have been published in four papers in statistics journals (two for each of the Chapters 3 and 4). Additionally, Mr Seitl has coauthored three journal publications dealing with the characterization of polycrystalline microstructures. This clearly documents Mr Seitl's ability to carry out creative scientific work. Hence, I recommend acceptance of the thesis.

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