

Porous materials: spatial models of 3D geometries with specific global connectivity structures & new methods for capturing the connectivity

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Porous materials are widely used in industry, e.g., as packaging materials; in hygiene products; for pharmaceutical applications such as controlled drug release; and as electrodes controlling electrochemical processes in fuel cells and re-chargeable batteries. The properties of these materials (flow, diffusion and/or electrical conductivity) are determined by the 3D geometry of the pores. It is becoming more and more common to use 3D microscopy data of the material and models informed by that data when developing new materials. With this data, there is a need for new spatial statistical models that capture the features of the 3D geometry that are most relevant for the materials properties.

In this talk I will show new methods for capturing the global connectivity of a porous material which are based on computing shortest (geodesic) paths through the 3D geometry. This type of global connectivity is highly correlated with the materials properties. An example is poor connectivity in battery electrodes, caused by pore heterogeneity, which can lead to quick degradation and even battery failure. Methods for capturing global connectivity, geodesic tortuosity and geodesic channels, have been implemented in a freely available software Mist which will soon be available to download from <https://mist.math.chalmers.se>

I will also show a new method of constructing spatial statistical models with specific global connectivity properties. The method is based on constructing a pore network representation of the 3D geometry and thinning the network by removing links based on a resistance network simulation of diffusion/electrical conductivity. Links in the network are removed iteratively based on how much of the simulated mass transport (diffusion) that goes through the link.

References

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Semiparametric point process modeling of blinking artifacts in photoactivated localization microscopy

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Photoactivated localization microscopy (PALM) is a powerful imaging technique for characterization of protein organization in biological cells. Due to the stochastic blinking of fluorescent probes, and camera discretization effects, each protein gives rise to a cluster of artificial observations. These blinking artifacts are an obstacle for quantitative analysis of PALM data, and tools for their correction are in high demand. We develop the Independent Blinking Cluster point process (IBC_{pp}) family of models, and present results on the mark correlation function. We then construct the semiparametric PALM-IBC_{pp} model for PALM data, and describe a procedure for estimation of blinking cluster parameters. We apply the model to real PALM data, and on simulated data, and consider the performance of the estimation procedures. Porous materials are widely used in industry, e.g., as packaging materials; in hygiene products; for pharmaceutical applications such as controlled drug release; and as electrodes controlling electrochemical processes in fuel cells and re-chargeable batteries. The properties of these materials (flow, diffusion and/or electrical conductivity) are determined by the 3D geometry of the pores. It is becoming more and more common to use 3D microscopy data of the material and models informed by that data when developing new materials. With this data, there is a need for new spatial statistical models that capture the features of the 3D geometry that are most relevant for the materials properties.

Point patterns on linear networks: a focus on intensity estimation

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The last decade witnessed an extraordinary increase in scientific interest in the analysis of network-related spatial point patterns, which is partly caused by their strongly expanded availability. Examples of such data may include the locations of traffic accidents or street crimes that only happen on/along a network of lines and their spatial distribution greatly depends on the inhomogeneous structure of the underlying network. Hence, there is a need of restricting the support of the underlying point process over the corresponding network structure to set and define a more realistic scenario. However, the analysis of point processes on linear networks has been extremely challenging due to the geometrical complexities of the network. In this talk, after highlighting some related common mathematical/computational challenges, a review of different (non)adaptive and non-parametric intensity estimators for point processes on linear networks, together with their benefits and drawbacks, will be presented. We finally demonstrate applications to traffic accident and criminology.