Adversarial Learning and Voronoi Tessellations: A Stereological Approach for Microstructure Generation

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Abstract

Understanding structure-property relationships in materials requires detailed knowledge of three-dimensional microstructures. However, comprehensive 3D characterization remains a significant bottleneck in materials science. 3D imaging techniques like FIB-SEM can be destructive and time-consuming, while X-ray tomography may damage sensitive materials. In contrast, 2D imaging is often readily accessible, non-destructive, and cost-effective, creating a need for methods that can reliably reconstruct representative 3D structures from 2D data.

Existing approaches for 3D microstructure reconstruction face several limitations. Voxel-based methods require extensive parameterization and lack physical interpretability, while statistical reconstruction techniques often struggle with complex cellular materials. Machine learning approaches, particularly generative adversarial networks (GANs), have shown promising results but typically generate structures that are difficult to interpret physically and computationally expensive to process [1].

We present a novel stereological framework that addresses these challenges by combining Voronoi tessellations with adversarial learning. Our approach leverages the natural ability of Voronoi tessellations to represent cellular microstructures through convex cells, while requiring only three parameters per grain.

The core methodology operates through adversarial training similar to GANs, but with a crucial difference: instead of generating images directly, we optimize the parameters of fuzzy encoding of a Voronoi tessellations, making the tessellation differentiable [2-3]. A discriminator network learns to distinguish between 2D cross-sections extracted from measured microstructures and those taken from 3D tessellations. The parameters of the tessellation are optimized in order to produce 2D cross-sections that are indistinguishable from measured ones by the discriminator. This adversarial training process naturally captures complex spatial correlations, grain size distributions, and morphological features present in the training data without requiring explicit definition of similarity metrics.

To enable training by means of backpropagation, we employ a softmax-based relaxation that converts the hard assignment of points to Voronoi cells into a differentiable probability distribution. This maintains the interpretability of the tessellation while allowing gradient descent-based optimization.

Our framework offers several advantages. (i) It allows for the (re-)construction of 3D cellular structures from 2D image data; (ii) it provides an enormous complexity reduction, representing complex 3D structures with just three coordinates per grain compared to thousands of voxels of state-of-the art computational stereological approaches; (iii) the analytical representation of 3D structures can be converted to any desired resolution without interpolation artifacts, making it ideal for subsequent numerical simulations.

We demonstrate the versatility of our approach across diverse material systems including metallic alloys, cellular foams, and biological tissues. Validation on synthetic data confirms the framework's ability to recover ground truth structures with high precision. Application to experimental data shows excellent agreement in statistical descriptors such

as the distributions of grain size, surface area, grain elongation and grain sphericity. Furthermore, compared to existing methods, our approach achieves superior computational time.
This talk demonstrates that by combining classical geometrical methods with modern machine learning techniques, we can achieve both computational efficiency and physical interpretability in microstructure reconstruction, opening new possibilities for materials characterization and design.

References

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