

Open-Source 3-D Membrane Reconstruction from a Single 2-D FIB-SEM Micrograph

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Abstract

Porous membranes are versatile material structures with many important applications in fields such as water treatment, energy storage, and biomedical devices [1]. Focused ion beam scanning electron microscopy (FIB-SEM) can provide very high imaging resolution compared to other imaging techniques, however FIB-SEM could damage soft membranes during scanning and require advanced instruments and preparations, meaning producing many FIB-SEM images is not feasible for studying 3D porous membrane structures [1]. The concept of using machine learning in MATLAB to reconstruct 3D structure with a single FIB-SEM image was explored earlier with encouraging results [1]. The aim of this study is to adapt the previous study to Python and apply various improvements to the previous study.

Methodology

The initial data for this study contained a .tif file containing 400 FIB-SEM images of a Viresolve® Pro membrane from MilliporeSigma [2], each image is 1024 x 899 pixels, and each image is taken with spacing of 3nm between each other.

The methodology of this study was split into four steps

- Step 1: process initial FIB-SEM images into binary 0 (pore) and 1 (solid) images
- Step 2: use different parameters to generate a 1024 x 899 x 400 matrix containing only binary 0 and 1 entries as the 3D reconstruction of the porous structure
- Step 3: compare one random FIB-SEM image and one random slice of 3D reconstruction and use Bayesian optimization to propose new parameter values for step 2 to minimize the difference between original and reconstructed images
- Step 4: evaluate properties of the final 3D porous structure reconstruction

Results

We reconstructed the 3D image 3 times, and ran Bayesian optimization over 50 iterations. Our results show a strong match in structure but some variation in specific metrics.

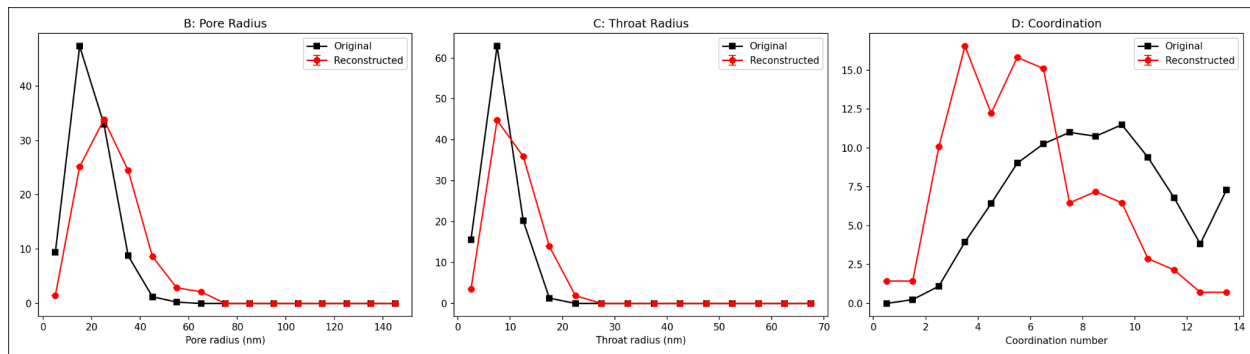
Figure 1: *Performance metrics between original and reconstructed structures*

Structure	Mean Body (nm)	Mean Throat (nm)	Mean Coord	Porosity (total)	Tortuosity	Perm (LMH/ psi)

			Number (-)			
Original structure	28.59	15.00	5.95	0.74	1.16	0.01
Average of 3 reconstructions (95% CI)	43.4 ± 4.4	35.24 ± 12.8	6.3 ± 0.9	0.8 ± 0.2	1.1 ± 0.2	0.63 ± 0.33
Error (%)	51.7	134.7	5.2	10.5	2.5	62.8

- **Coordination and Tortuosity.** The coordination number (average connections per pore) was heavily accurate, with only a 5.95% error and a small variation in outputs (± 0.9). Tortuosity was also accurate at 1.1 ± 0.2 vs. 1.16 (2.5% error).
- **Sizing.** Pore and throat sizes were larger in our model. The body radius had a high error of 51.7% and was 43.4 ± 4.4 nm compared to the original 28.59 nm.
- **Permeability.** As noticed with a similar architecture [1], the predicted permeability predicted a higher, and noisy output for permeability.

Figure 2: Comparing original and reconstructed pore, throat, and coordination distributions



Qualitatively, the structural properties (body radius, throat radius, and coordination number) show similar trends between the original FIB-SEM data and the reconstructed images. Quantitatively however, metrics still show a high error rate (over 50%) in these properties.

Conclusion

We open-sourced a Python implementation of the 2D-to-3D membrane reconstruction method from [1]. While deep learning models like SliceGAN [3] are popular, this method is preferred in scenarios requiring physically interpretable models and no training data. Improvements to our method include using multiple slices at varying depths to better match the original membrane, or the 3D generation method can be varied.

References

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