

A Framework for Cryo-EM Image Segmentation and Processing with Conditional Random Field

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Abstract

Advancements in equipment and image analysis algorithms have ignited a resolution revolution in cryogenic electron microscopy (cryo-EM), transforming structural biology. Differentiating components from the background in micrographs is a critical first step in the computational pipeline. However, this process is laborious and challenging due to low signal-to-noise ratio (SNR), contaminants, contrast variations from ice thickness differences, and densely connected particles of varying sizes. Researchers have recently used image segmentation to distinguish particles at the pixel level. However, low SNR complicates the automated generation of accurate pixel-level annotations needed for training supervised models. Such benchmarking is crucial for understanding the strengths and limitations of existing methods and for encouraging further development and validation.

To address this, we introduce a procedural framework for generating segmentation maps from cryo-EM data as ground truth labels. We further built a modular framework allowing users to select different segmentation models and loss functions. Finally, we integrate Conditional Random Fields (CRFs) with different solvers and reference maps to refine coarse predictions, producing sharp boundaries and fine-grained segmentation. The flexibility of our framework allows users to choose the optimal configuration for the target dataset. Training on limited micrographs, we achieve over 90% accuracy, recall, precision, Intersection over Union (IoU), and F1-score on synthetic data. Additionally, CRF integration enhances segmentation results and recall on experimental data. Finally, to demonstrate the efficacy of our framework, we show that our pipeline generates 3D density maps with better resolution than other existing pickers in two experimental datasets. Our framework is organized into a modular package which is available at <https://github.com/phonchi/CryoParticleSegment>.

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<https://math.ccu.edu.tw/p/404-1069-12096.php?Lang=zh-tw>