Deep-learning based 3D map sharpening in cryo-electron microscopy

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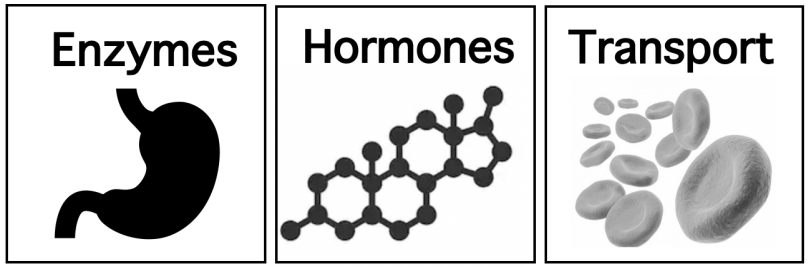
February 27, 2020

Motivation

- Proteins play a crucial role in our lives!



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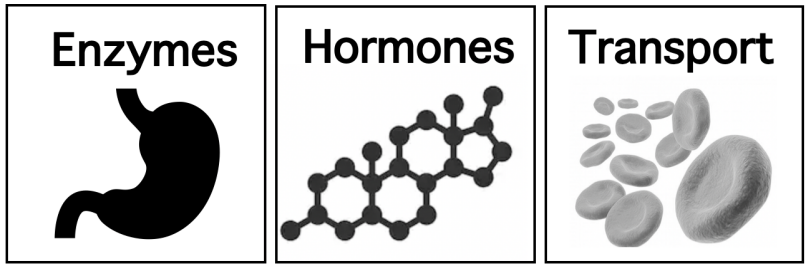

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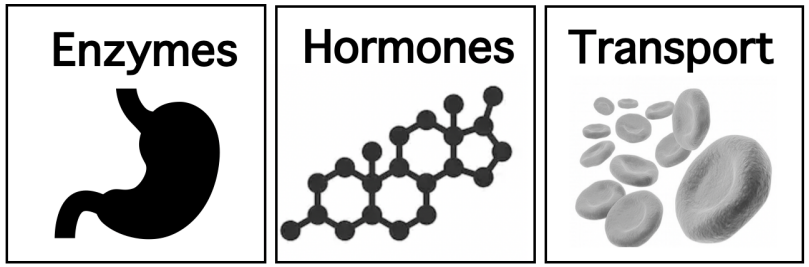

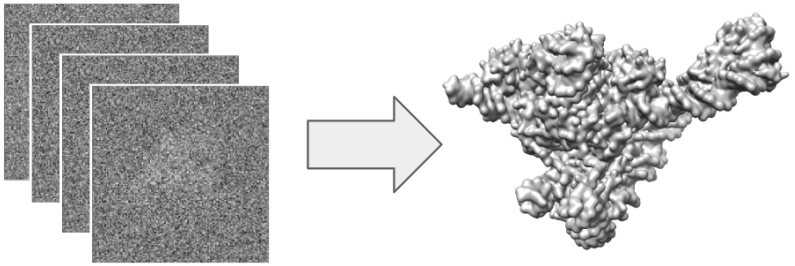

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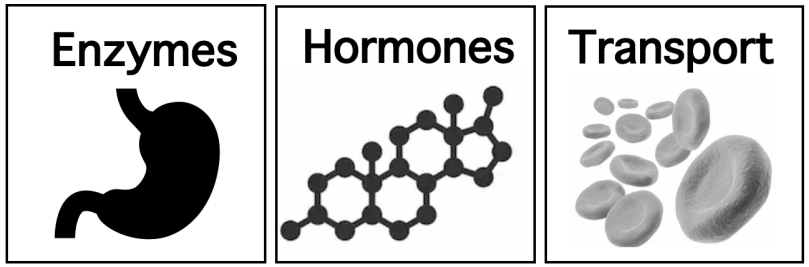

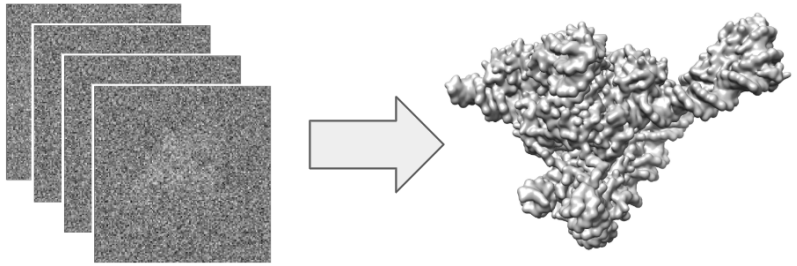

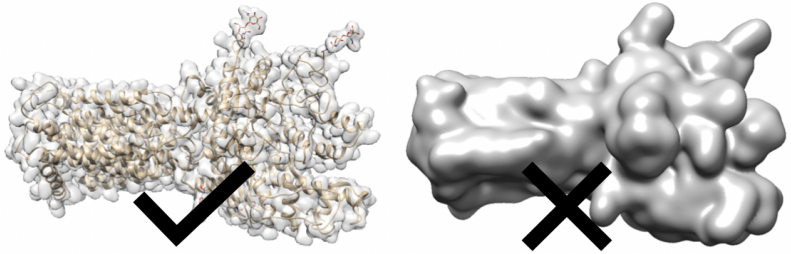

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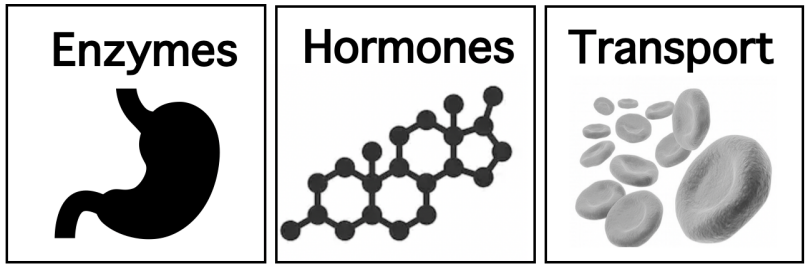

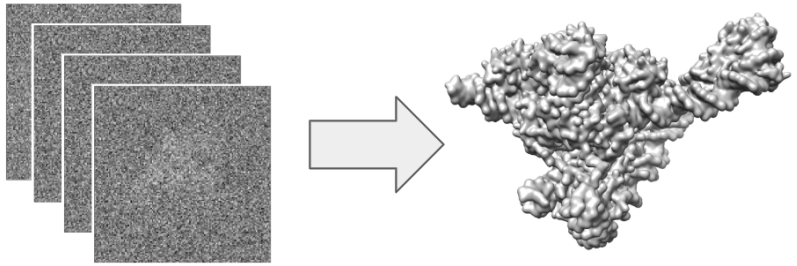

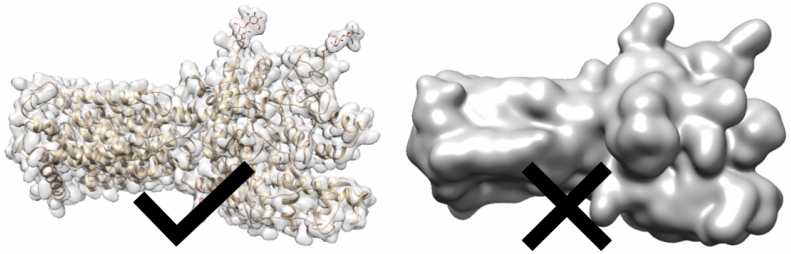

Need for methods to enhance the quality of maps

Outline

- Problem definition
- Related work
- Our approach
- Preliminary results
- Conclusion

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- Computational complexity

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- Weighting low and high frequency terms of Fourier series to maximize connectivity and surface area[1][2]

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[2] Optimal Determination of Particle Orientation, Absolute Hand, and Contrast Loss in Single-particle Electron Cryo-microscopy

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A data-driven model that maps low-res to high-res volumes.

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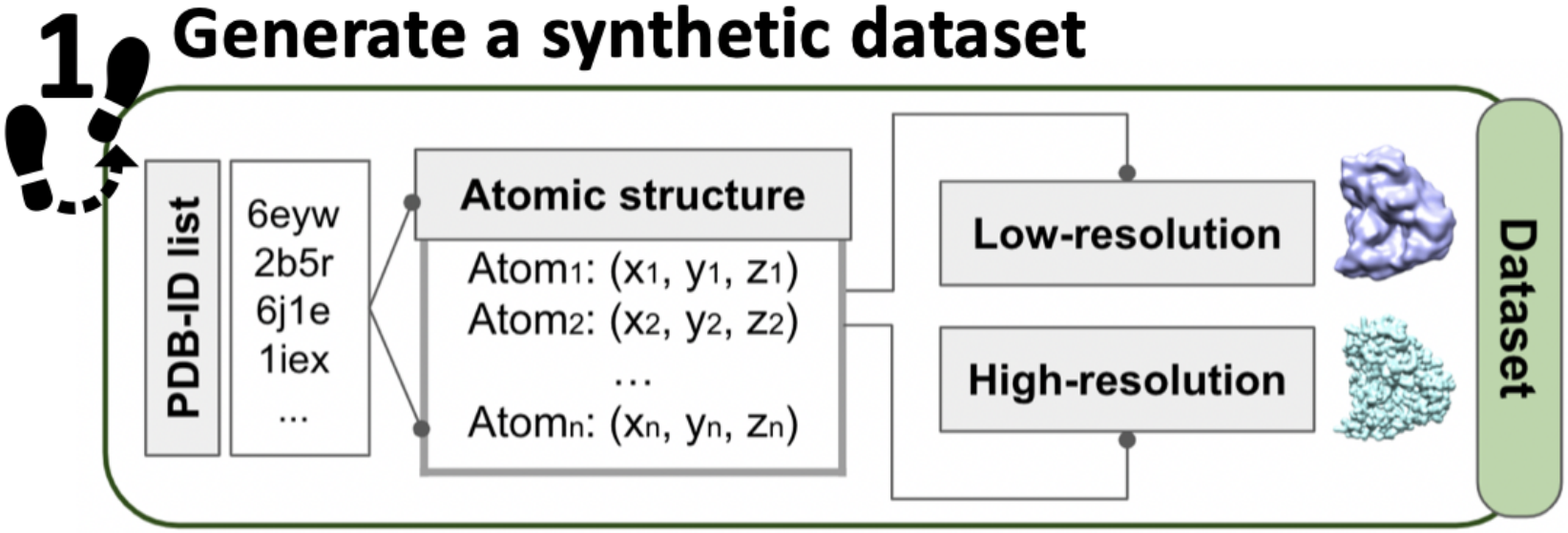

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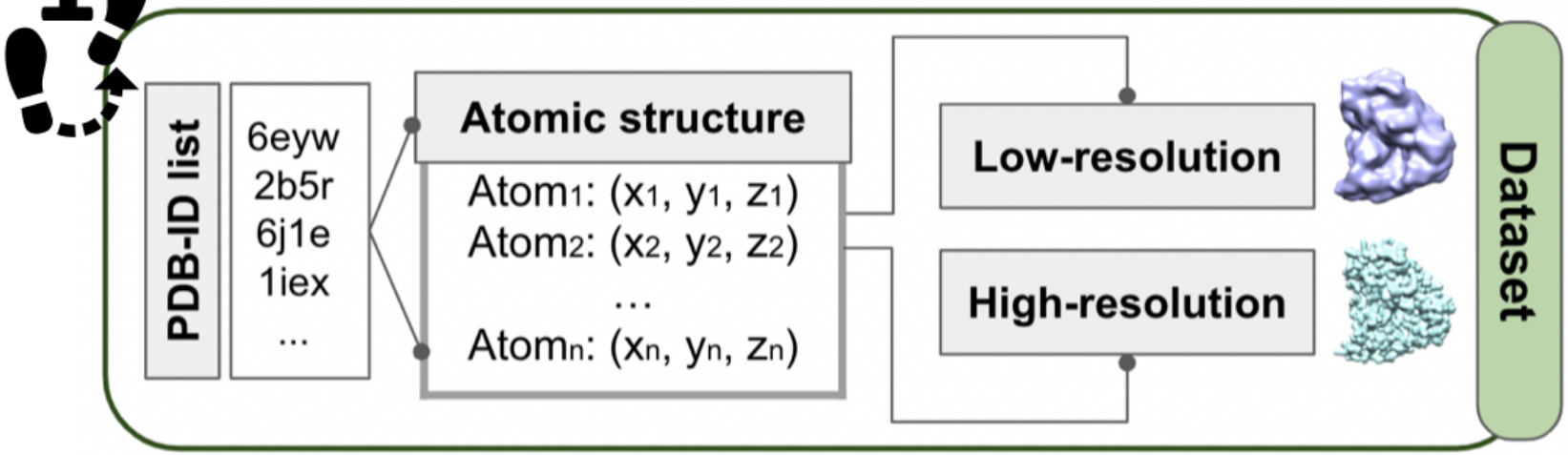
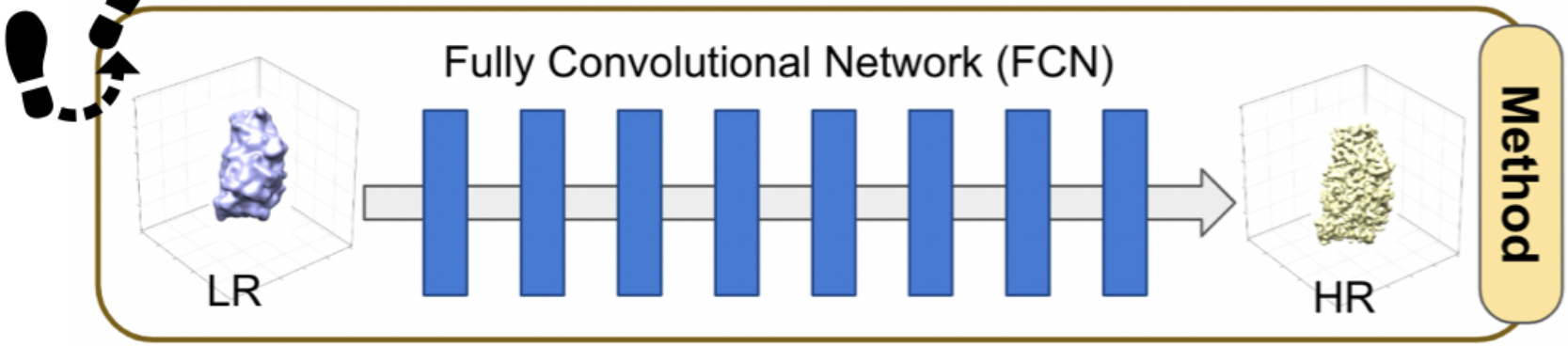


2 Train a fully convolutional net.



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Dataset

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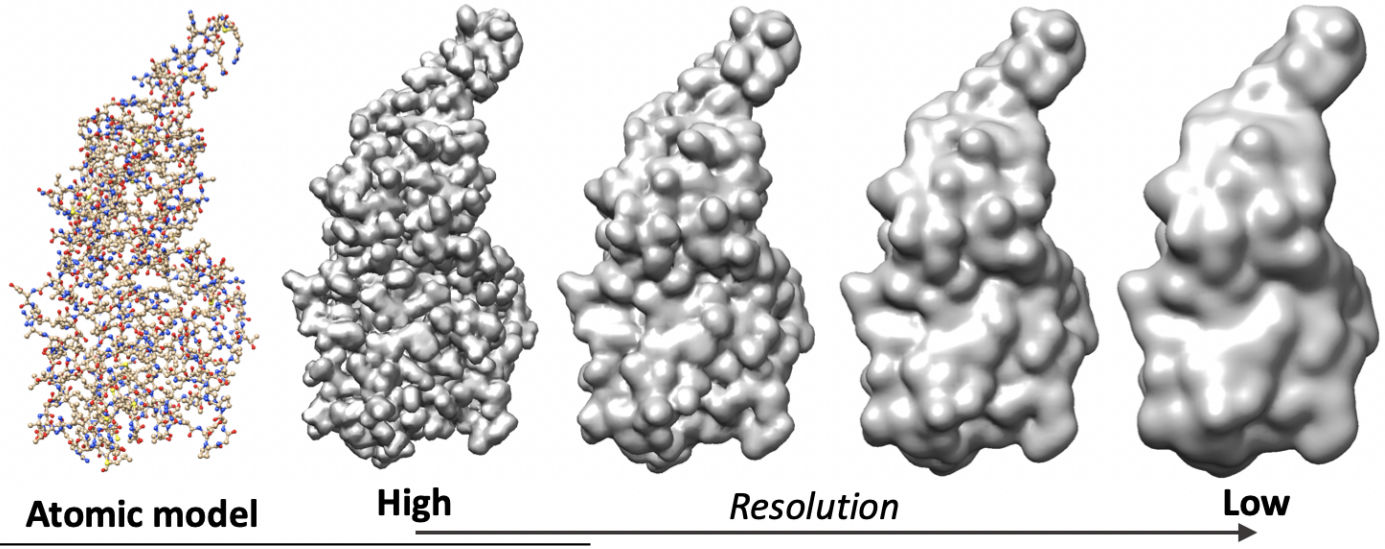
- Generate samples with different resolutions



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Network architecture

Fully convolutional architectures

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Visual results{simulated

PDB ID: 2b5r

Low-res (input)

High-res (gt.)

Ours

CC = 0:75

CC = 0:95

Visual results{experimental

EMD-7550

Kucukelbir et al, Quantifying the Local Resolution of Cryo-EM Density Maps, Nature Methods., 2014.

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- Consider other type of map degradation in experimental density maps