Learning Sample Orientation Using Variational AutoEncoders

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Cryo EM & Sample Orientation

My project focused on **learning orientation** via a type of neural network called a **conditional variational autoencoder**.

Cryo EM constructs **3D models** from the shadows of the sample.

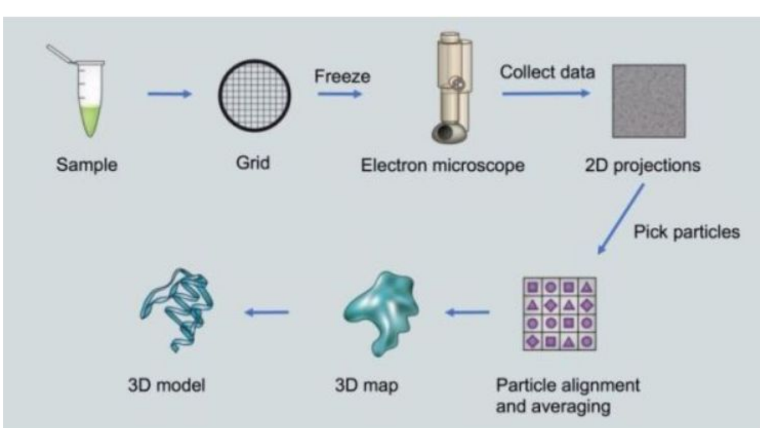
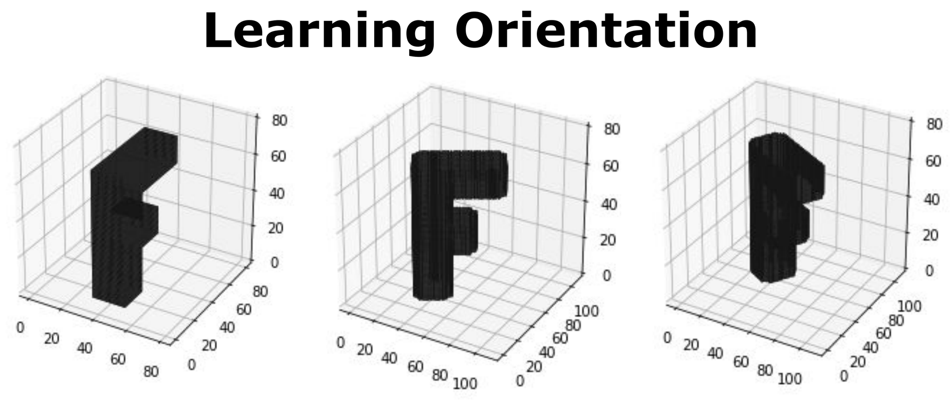
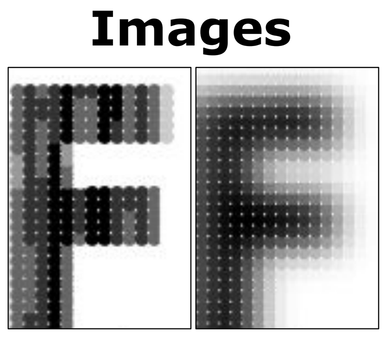


Fig. 1 Data analysis pipeline for Cryo EM
Picture Credits: Creative Biostructure, Medium, 2018

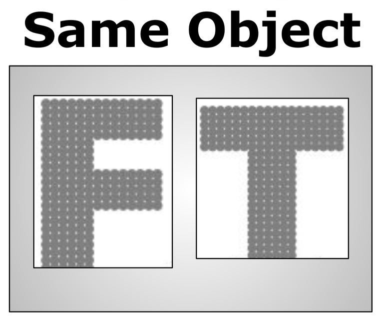
Learning Orientation



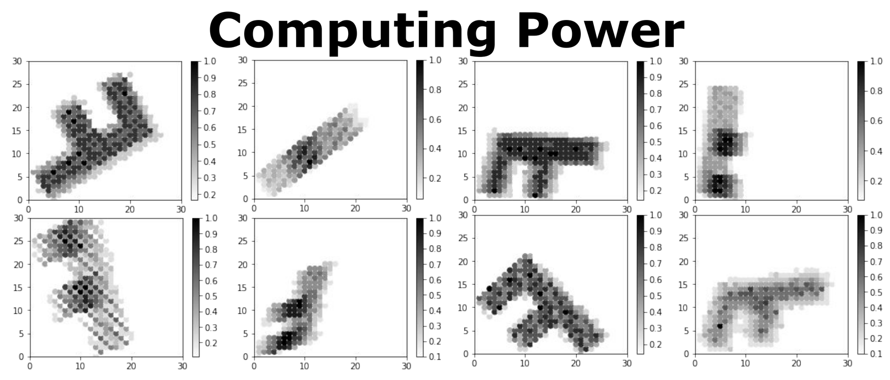
Denoising Images



Recognizing the Same Object



Computing Power



Keywords: Conditional variational autoencoders, Cryo EM, LSTM, tensor decomposition

Variational AutoEncoders (VAE)

The MNIST dataset is a set of written numbers

Latent Space Clustering

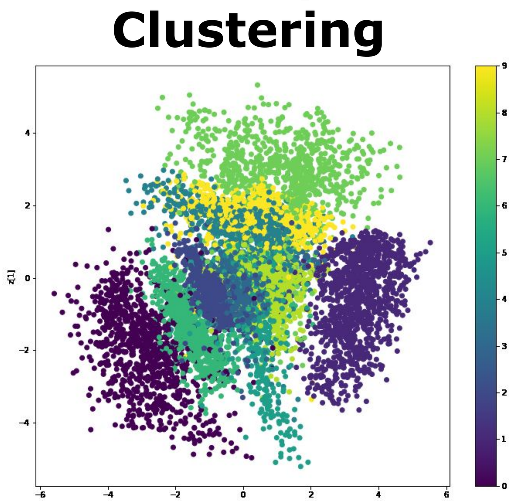


Fig. 2 We want the label of a number given the image. Latent clustering shows that labels aggregate in latent space.

Probabilistic Inference

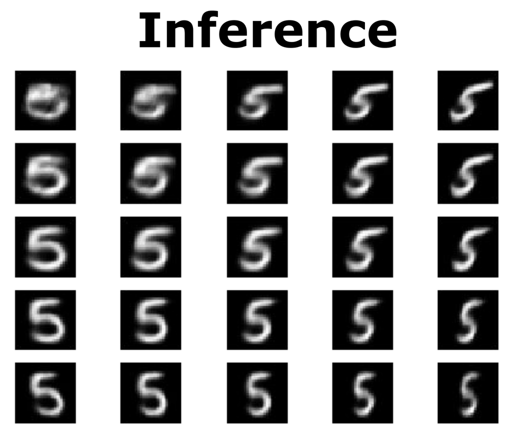


Fig. 3 Variations in a digit uncovered by conditional VAE as a function of latent dimensions

Can VAE's learn rotations?

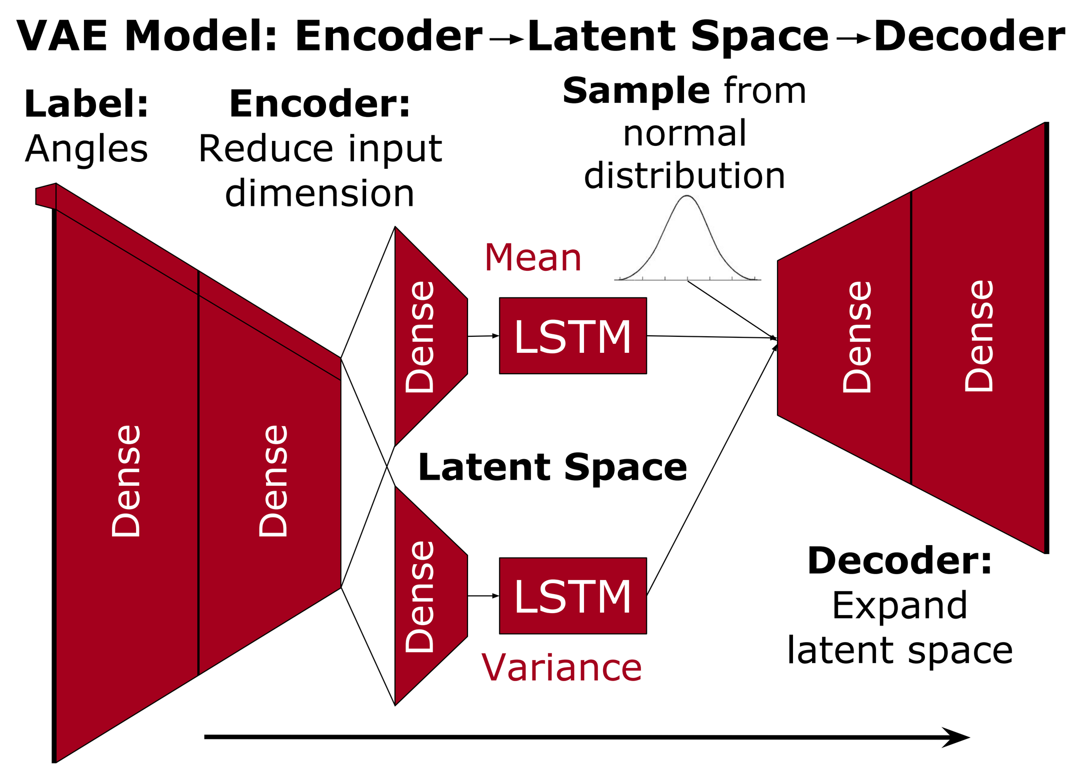


Fig. 4 My VAE model, conditioned on Euler angles, with latent space of size 15 and a LSTM before sampling from the normal distribution (to create variance in decoding).

LSTM Layer

LSTM takes a **sequence** of shadows as input and updates its internal state after each element in the sequence.

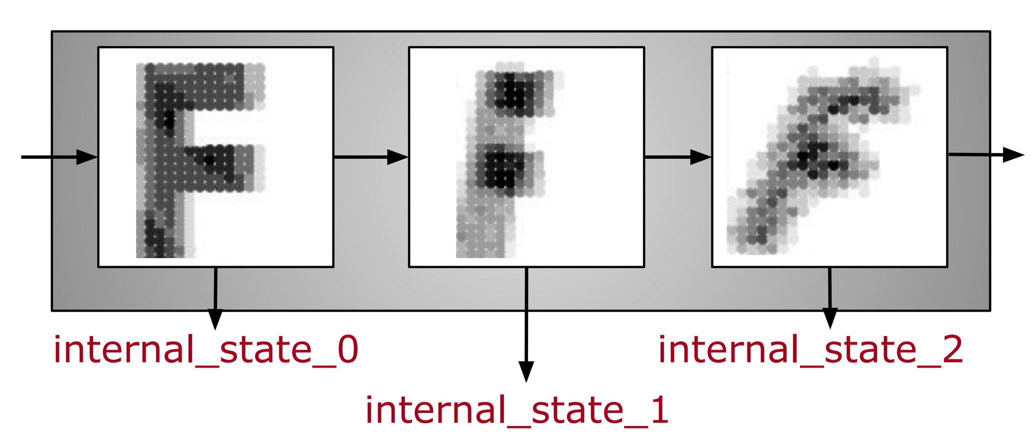
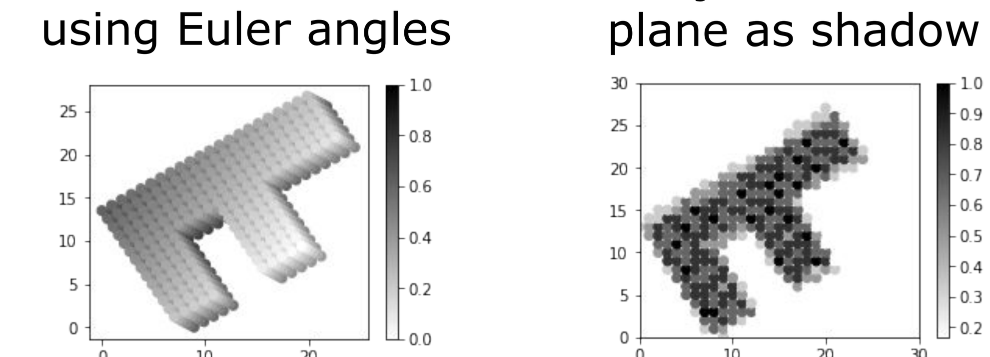


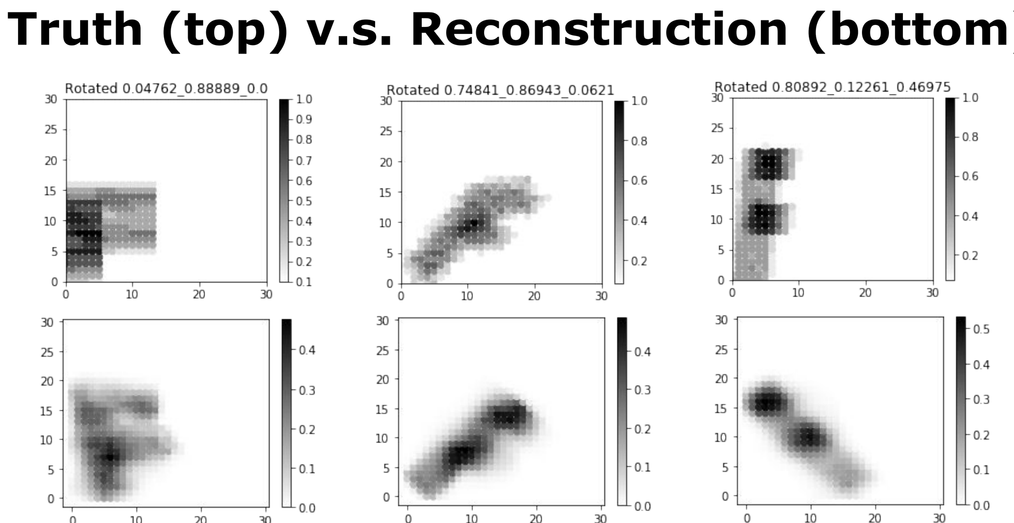
Fig. 5 An unfurled LSTM is like consecutive dense layers. LSTM allows for a stronger connection between orientations.
Choy et al., 3D-R2N2, Stanford University, 2016

Reconstructing Shadows

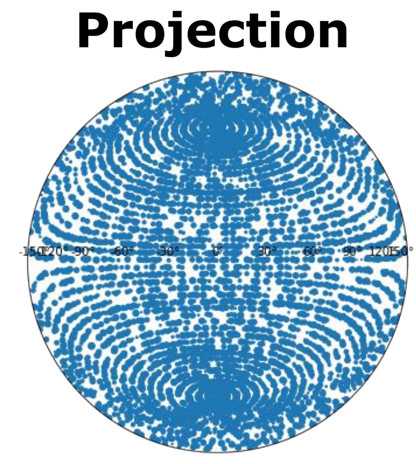
Rotated 3D 'F' using Euler angles | Projection onto plane as shadow



Truth (top) v.s. Reconstruction (bottom)



Euler Angle Projection



Probabilistic Inference

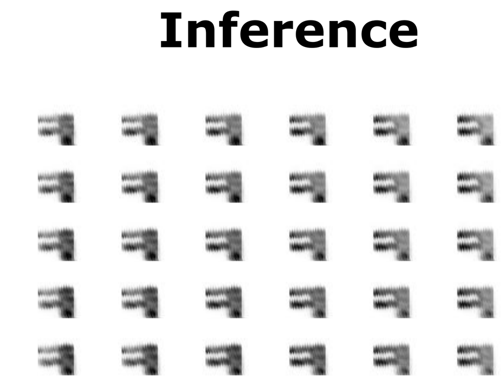


Fig. 6 Lambert projection of Euler angles (left) and variations of the 'F' dataset (right)

Gimbal Lock

Gimbal lock occurs for Euler angles when two axis become aligned and a degree of freedom is lost, resulting in "flips."

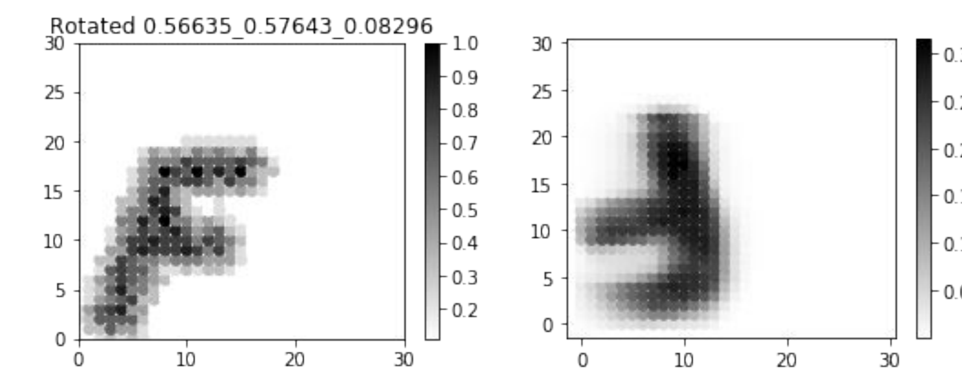


Fig. 7 Flipped reconstructed image (right)

Quaternions are unique (to a negative sign) and are better than Euler angles, so they would be a future implementation.

Tensor Decomposition

A common problem for neural networks is their large number of parameters. A way to combat this issue is to represent them by their tensor decomposition, e.g. finding the CPD of their layers.

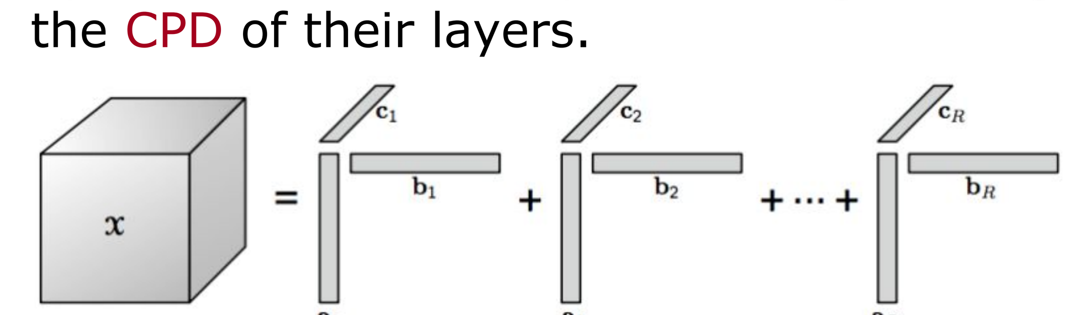


Fig. 8 CPD is a sum of outer products.
Picture Credits: Turgutlu, Medium, 2018

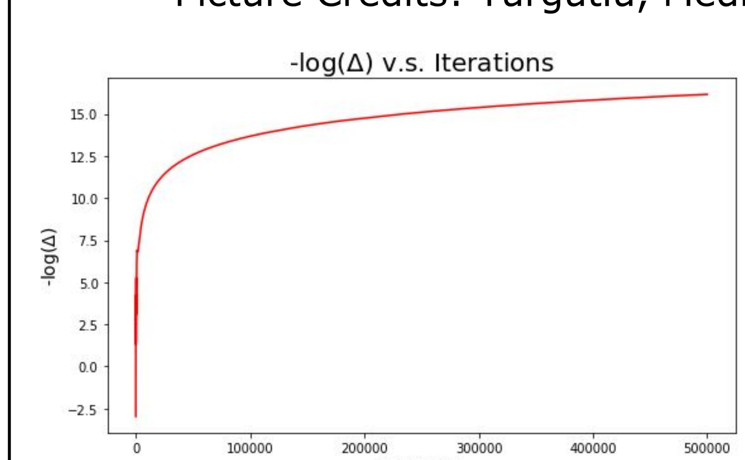
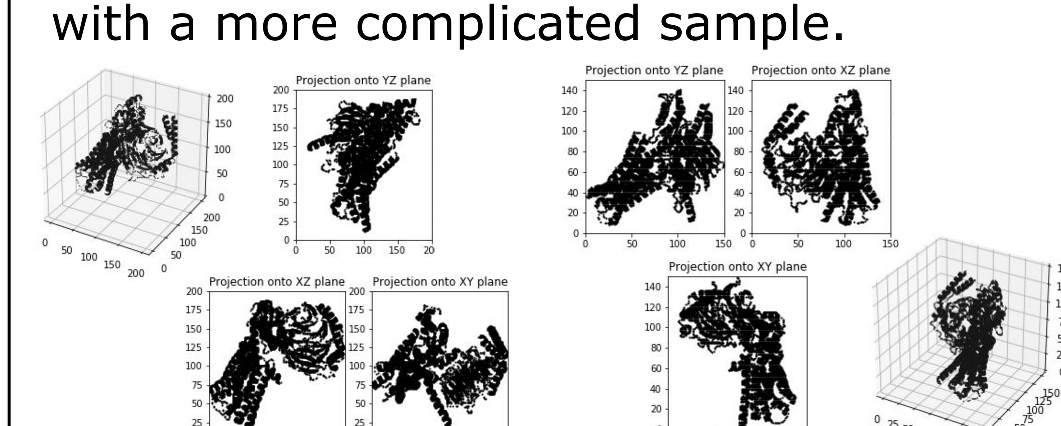


Fig. 9 Convergence of CPD implementing ALS

Future Improvements

The next step would be for the VAE to output orientation given the shadow, and with a more complicated sample.



Acknowledgments

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