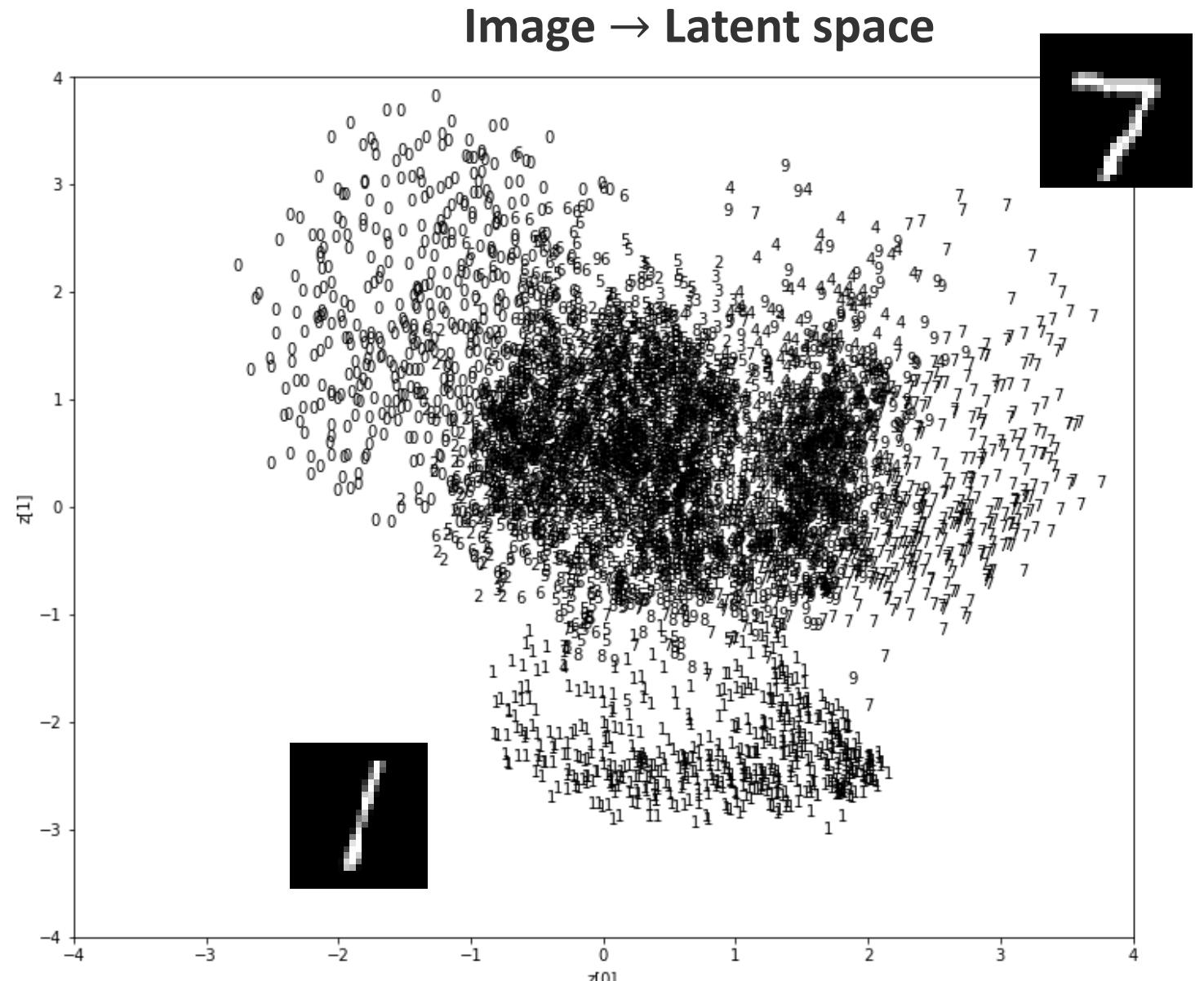
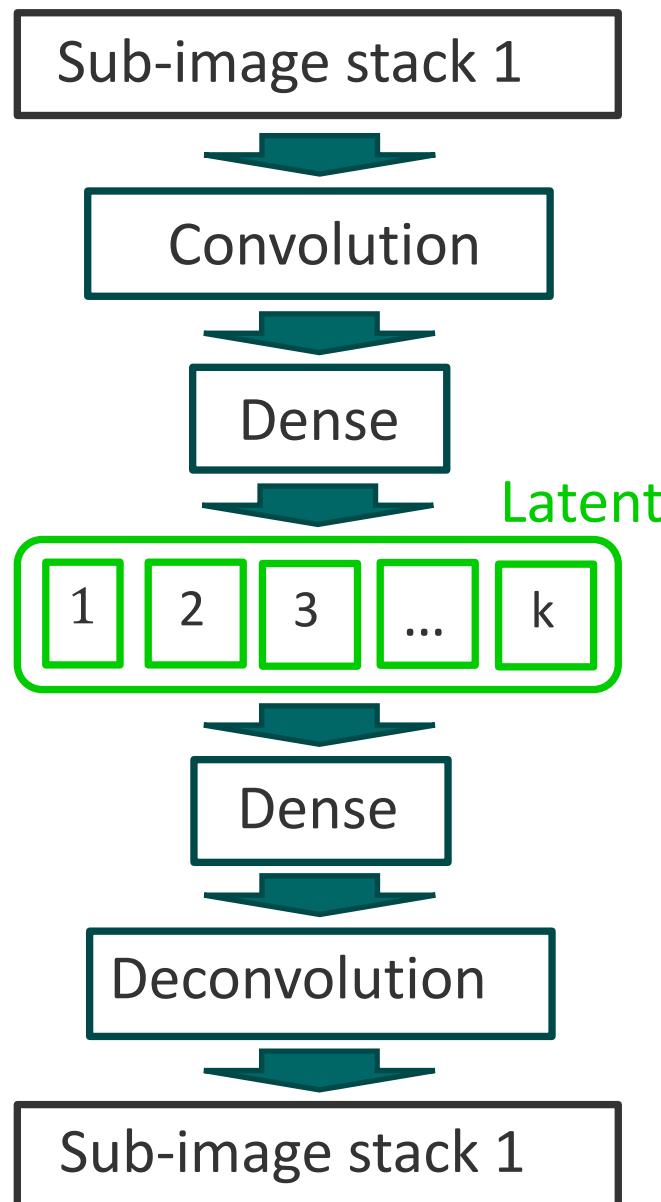


Lecture 23: VAE-BO and DKL

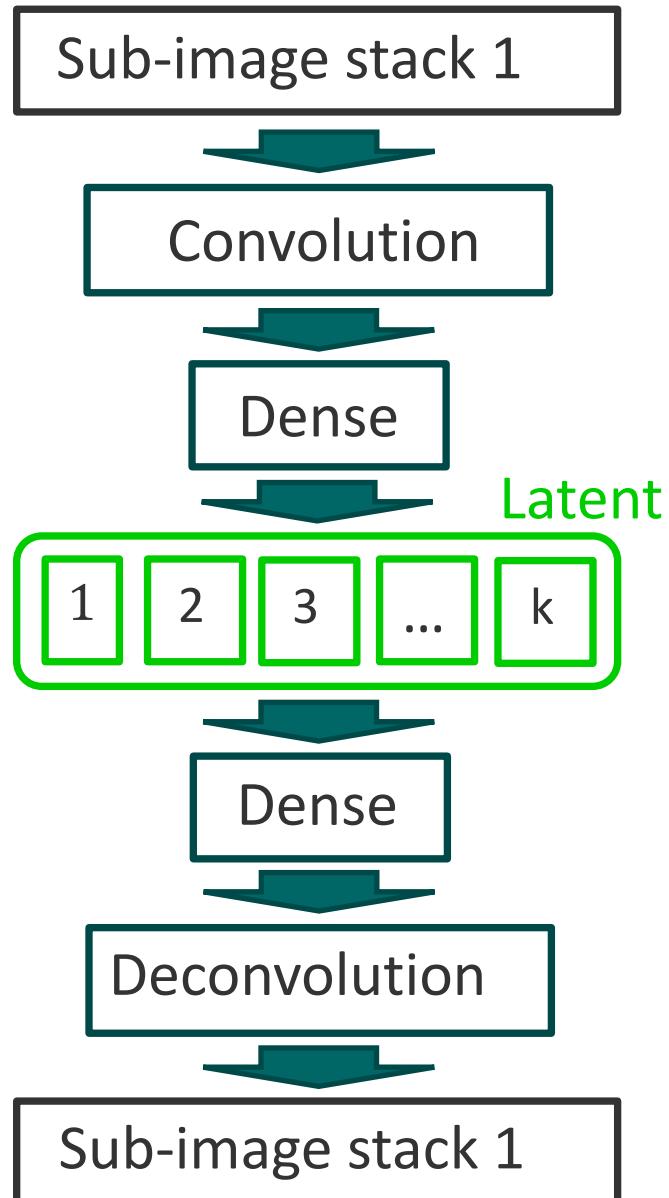
Instructor: Sergei V. Kalinin

Autoencoders: Encoding

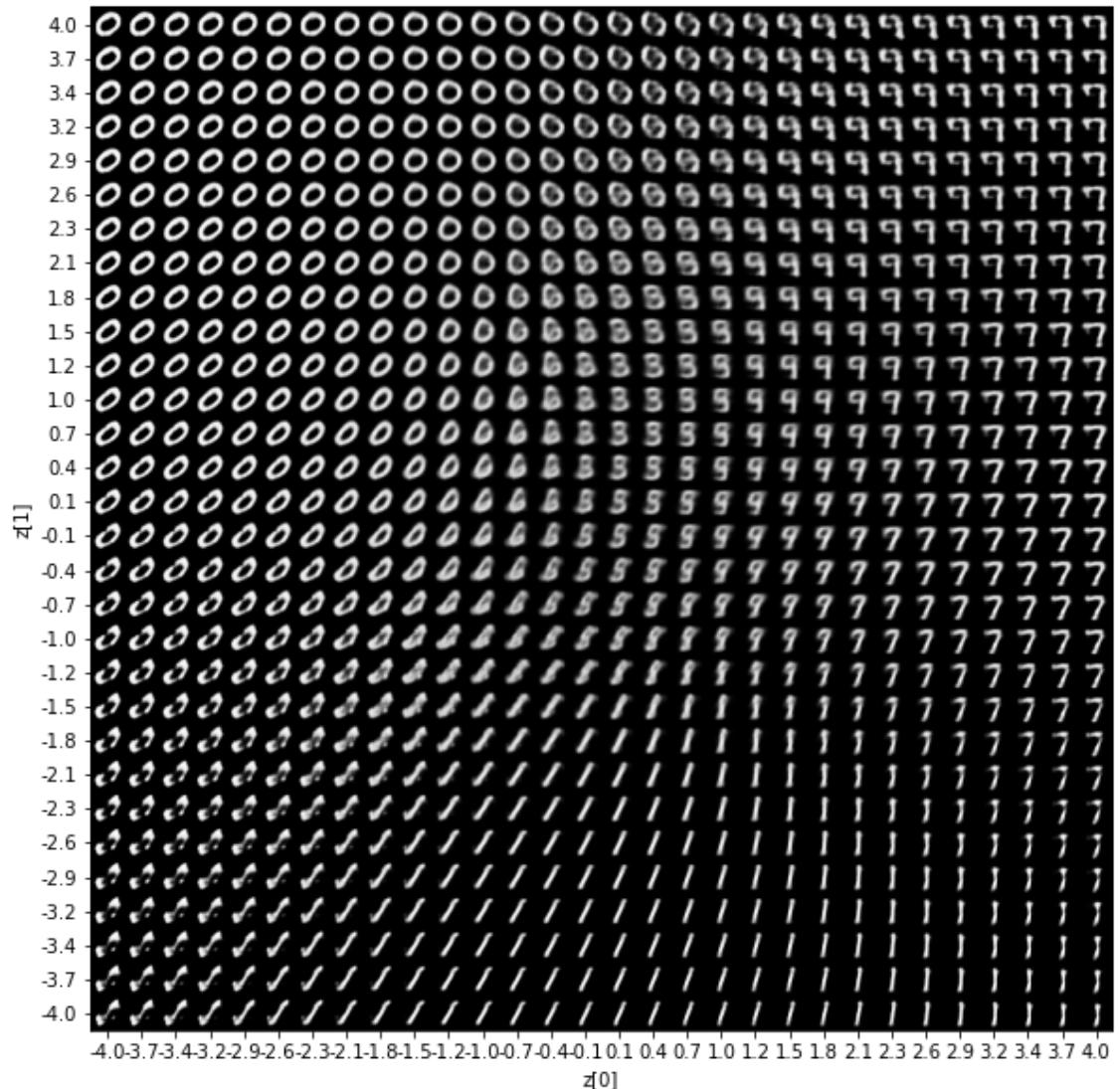


Latent distribution: Encoding the data via low dimensional vector

Autoencoders: Decoding

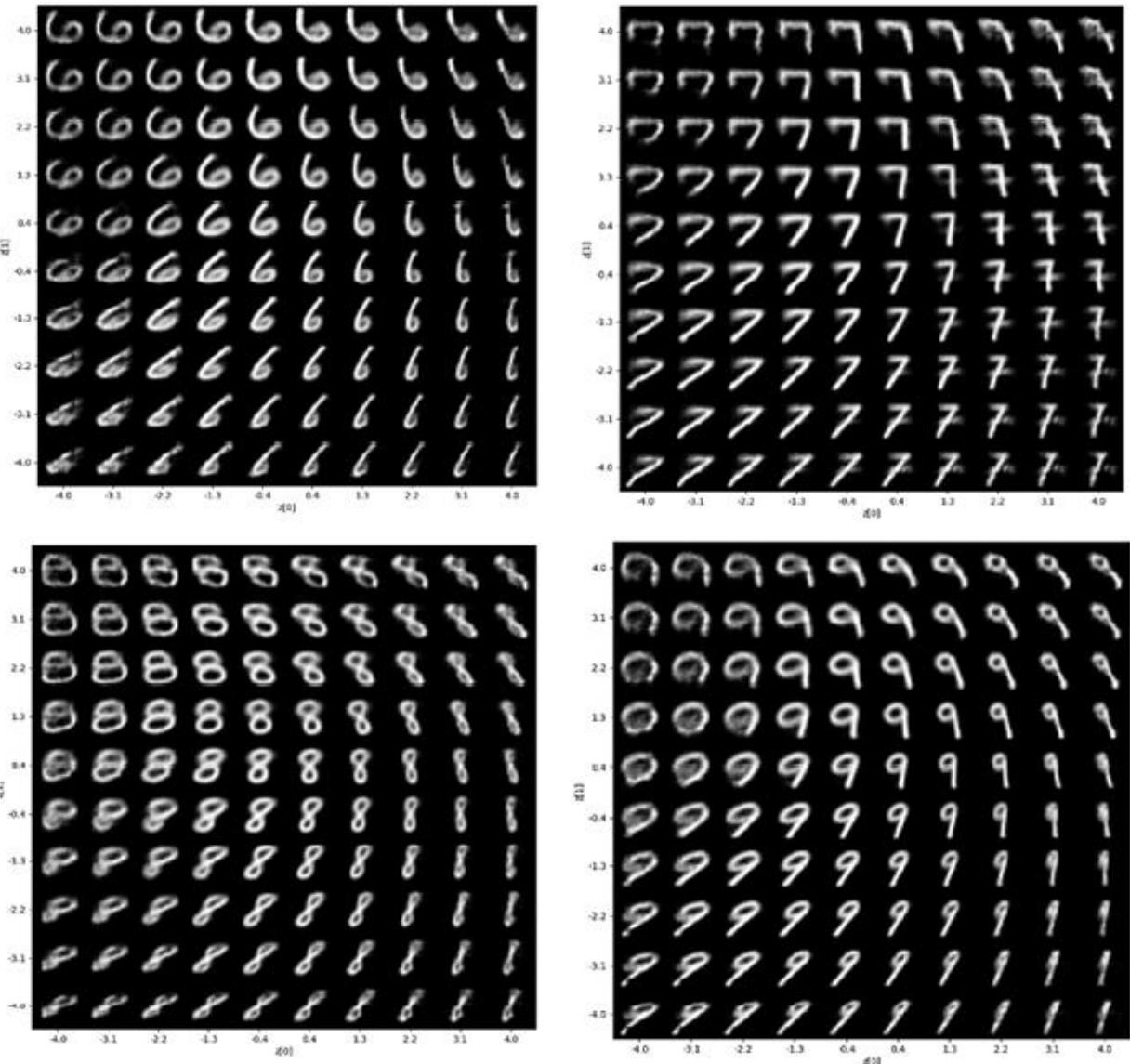
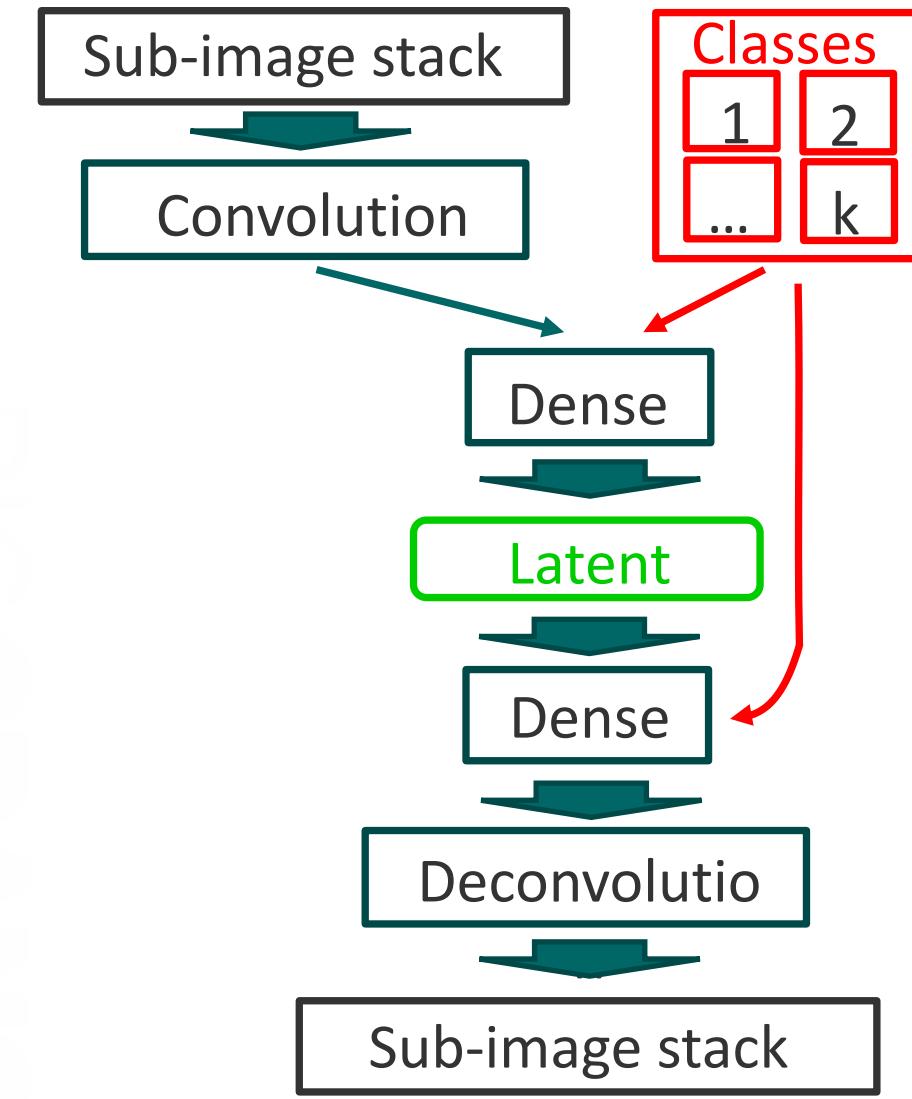


Latent space \rightarrow Image



Latent representation: Decoding images from uniform grid in latent space

Conditional VAE

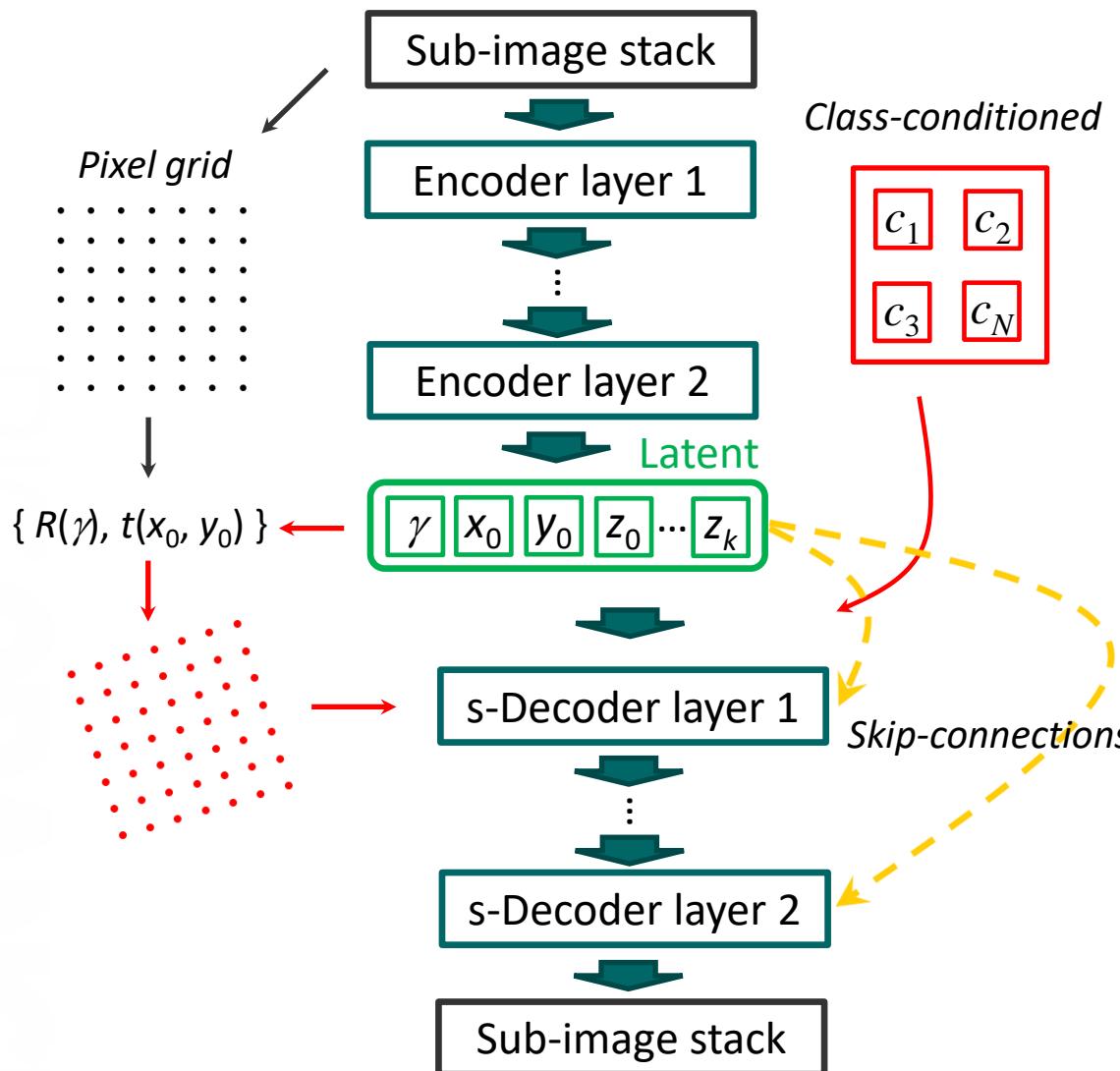


Note the trends in the latent representation for each digit: **disentanglement of the representations**

What if we have multiple classes?

1. Classes are known: conditional (discrete) VAE
2. Factors of variability are known: conditional (continuous) VAE
3. Some classes are known: semi-supervised VAE
4. Number of classes are known: joint VAE

Conditional VAE



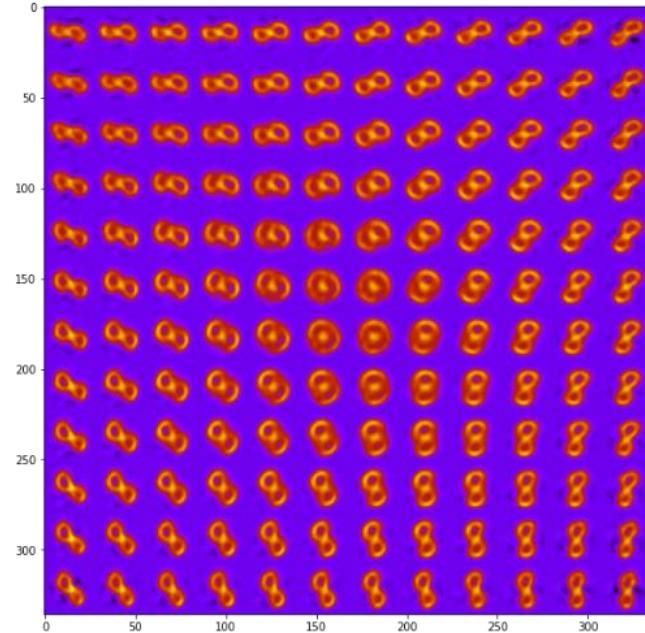
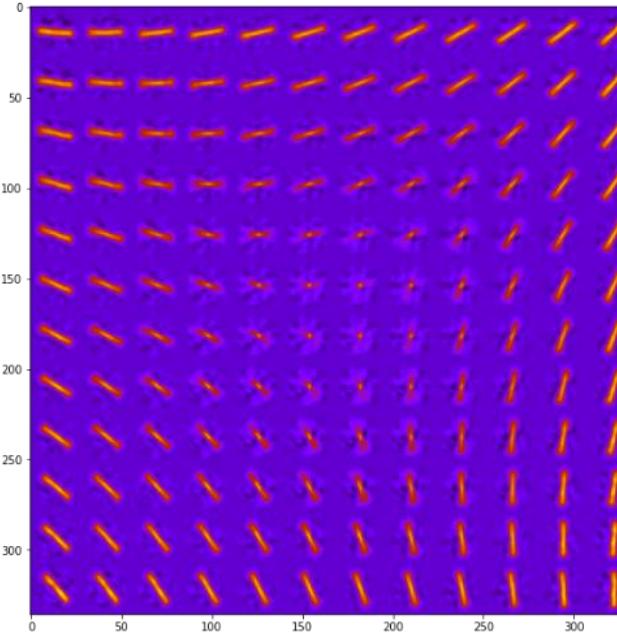
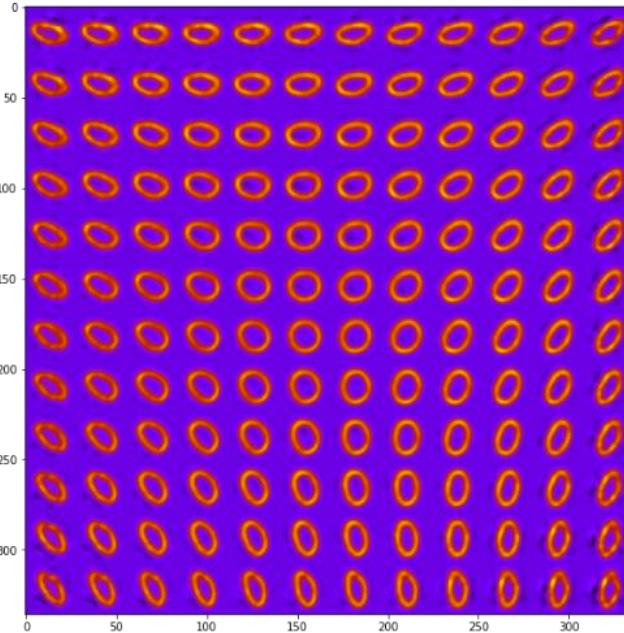
- Generative model is a function of spatial coordinate
- 3 additional latent variables to absorb rotations and shifts
- Disentangles rotations and translations from image content
- Ideal for analyzing microscopy sub-images on atomic level

$$\begin{aligned} ELBO &= \text{Reconstruction Loss} \\ &\quad - D_{KL}(q(z|x)\|\mathcal{N}(0,I)) \\ &\quad - D_{KL}(q(\gamma|x)\|\mathcal{N}(0,s_\gamma^2)) \\ &\quad - D_{KL}(q(\Delta r|x)\|\mathcal{N}(0,s_{\Delta r}^2)) \end{aligned}$$

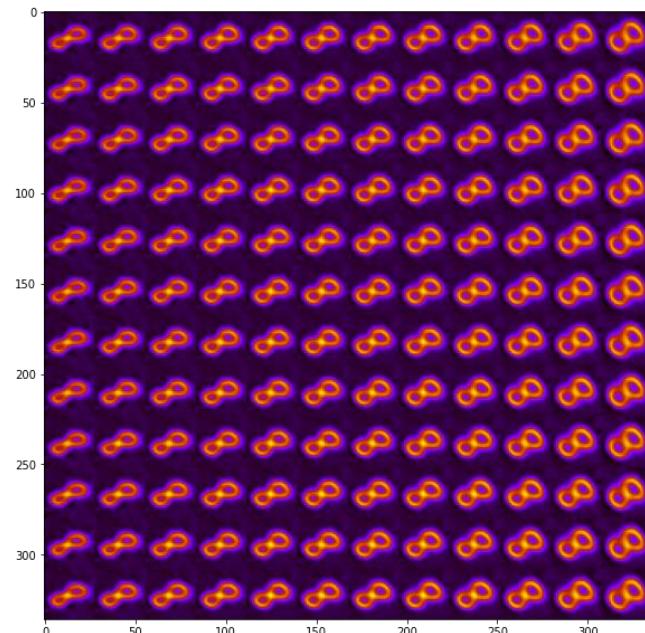
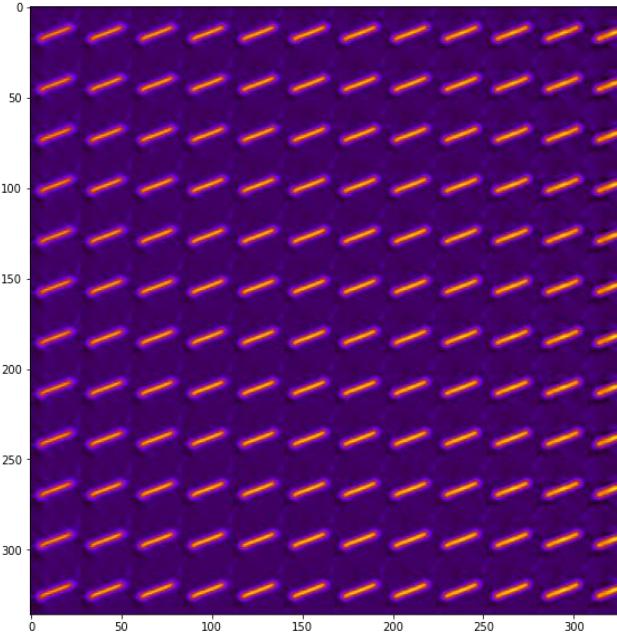
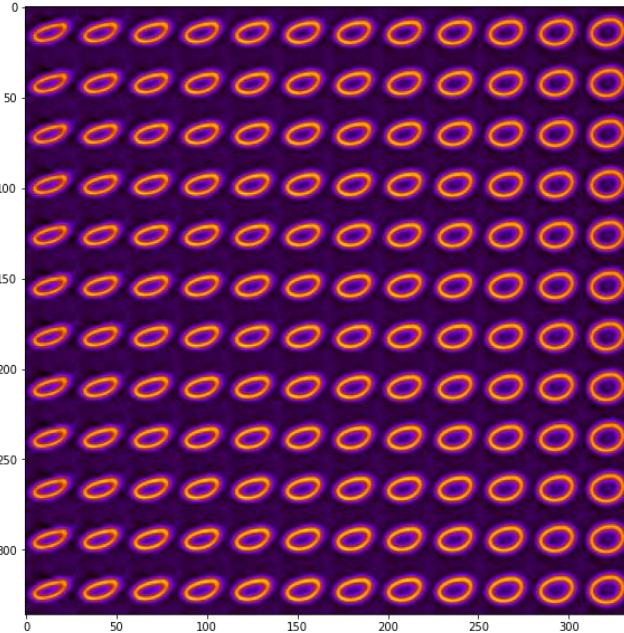
Regular VAE
Rotation
Translation

MNIST cVAE

No rotations

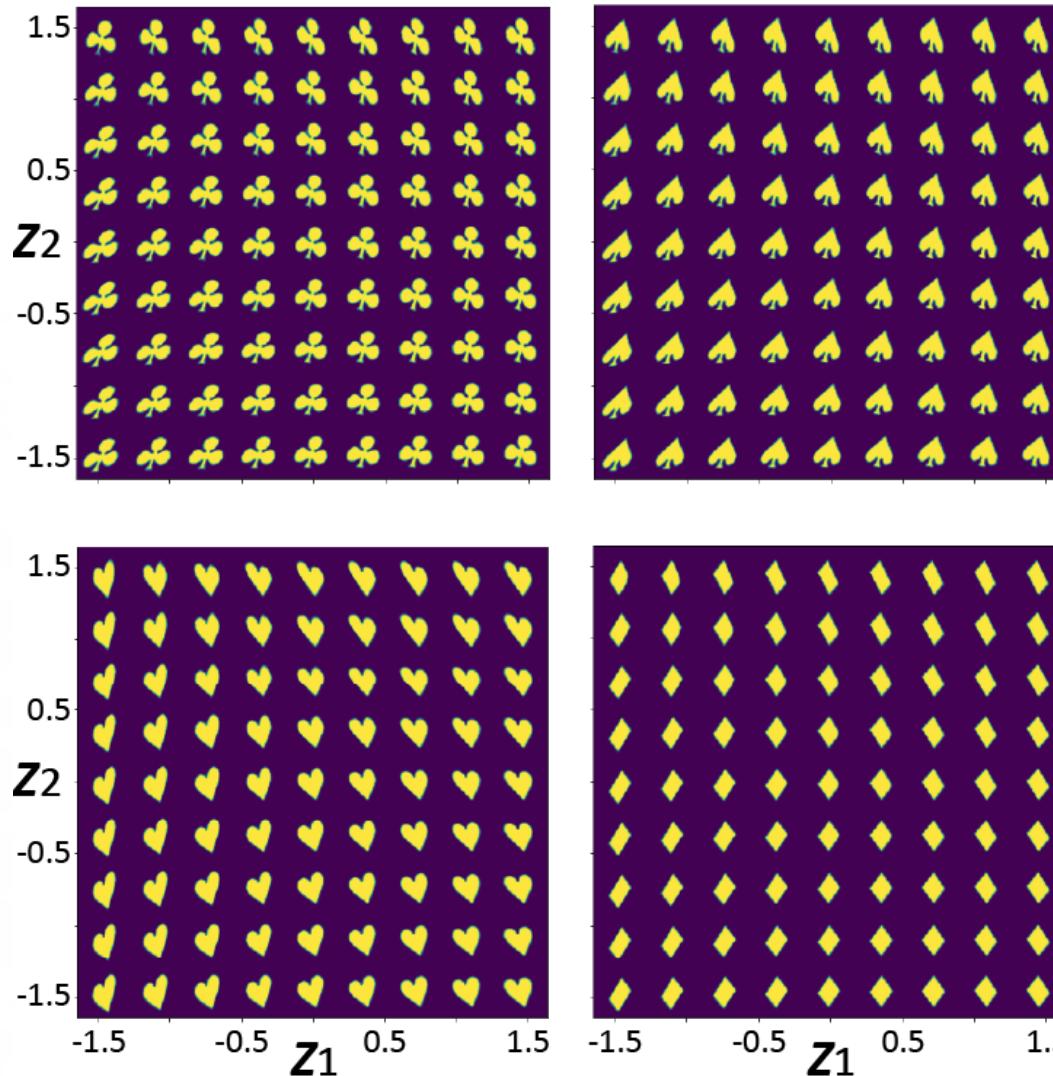


With rotations

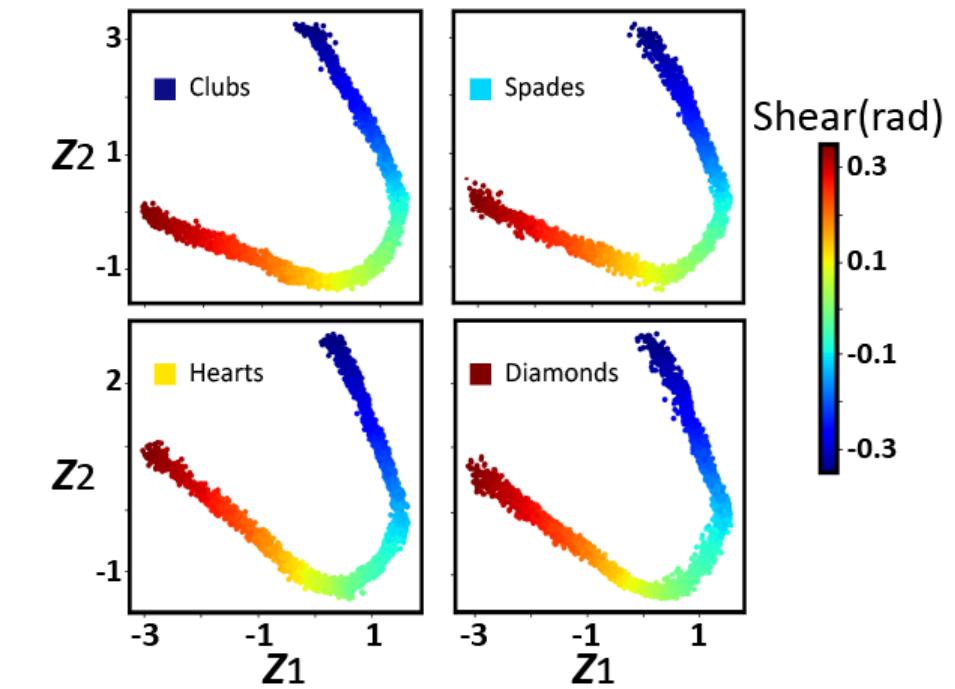


cVAE on cards data set

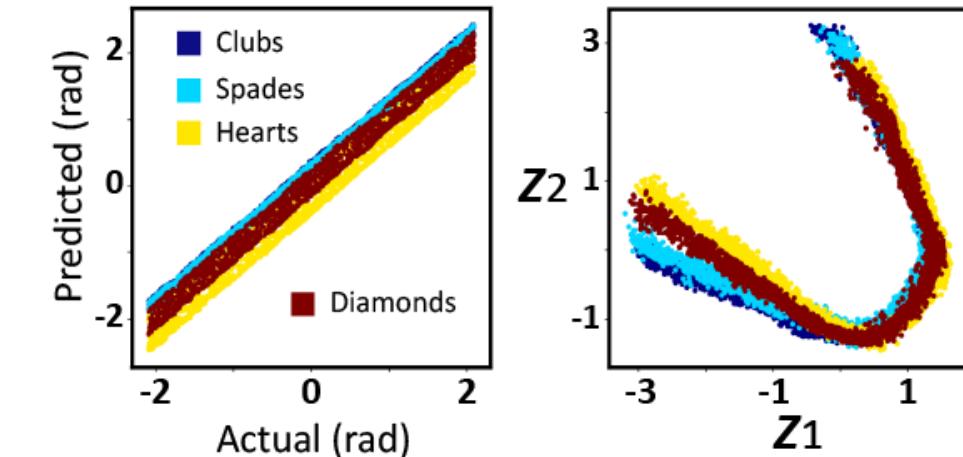
One independent latent space per class



Shear distribution in latent space

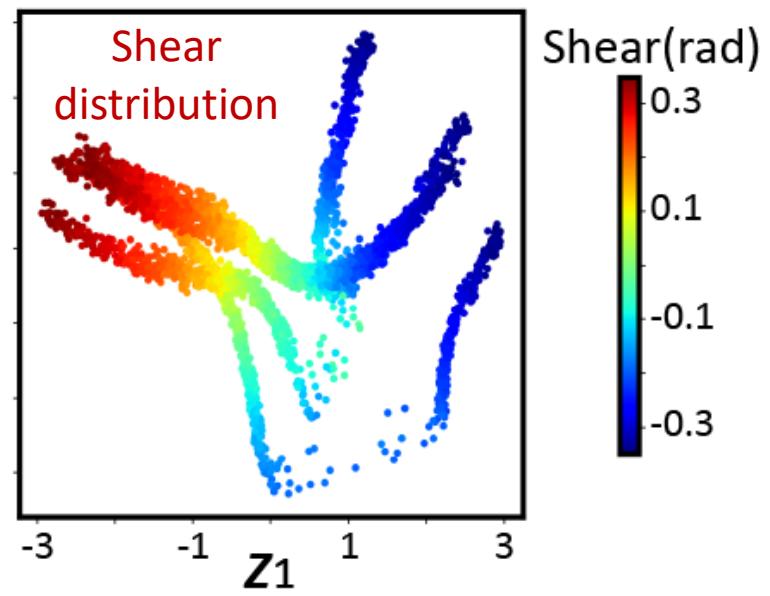
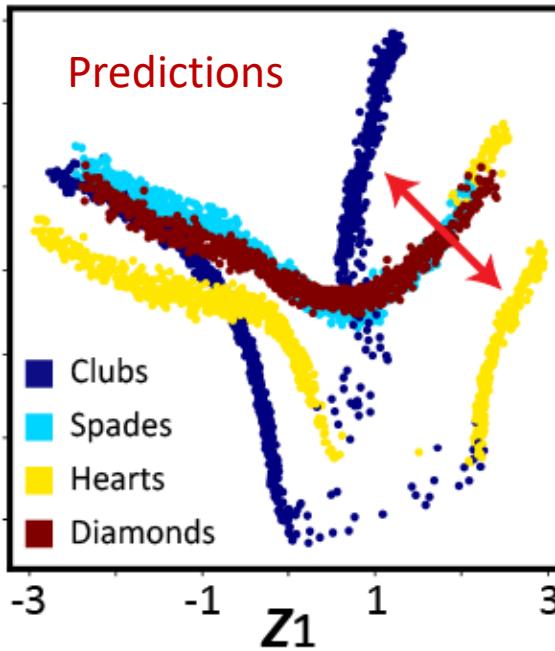
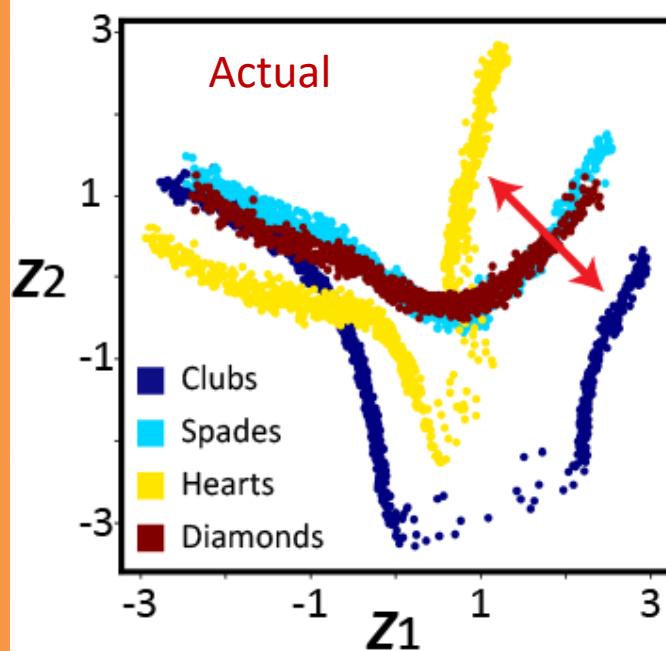
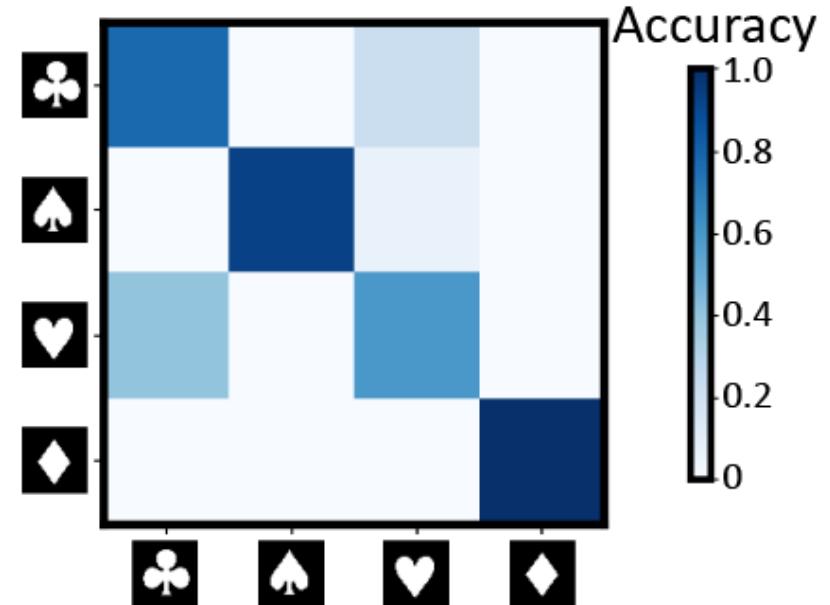
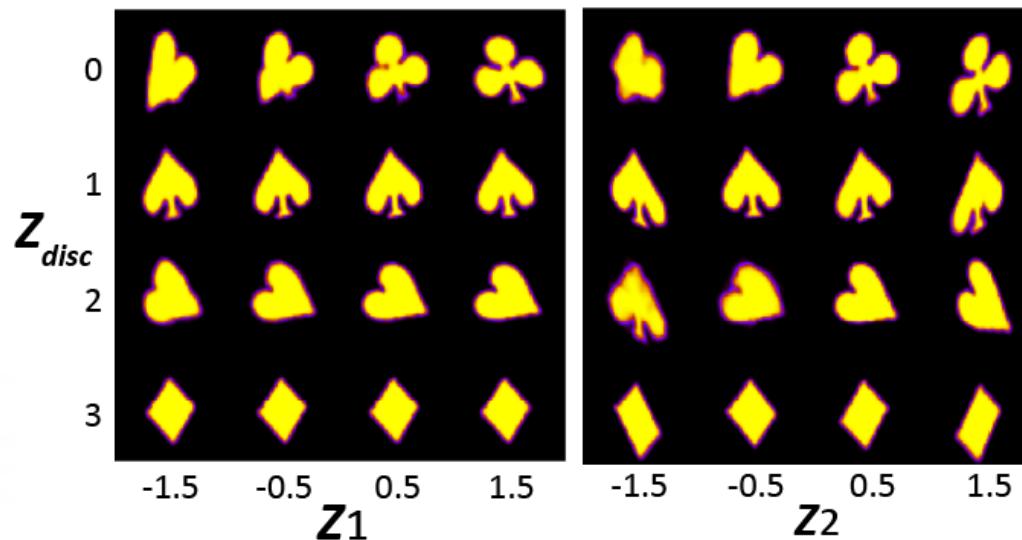


All four plotted jointly

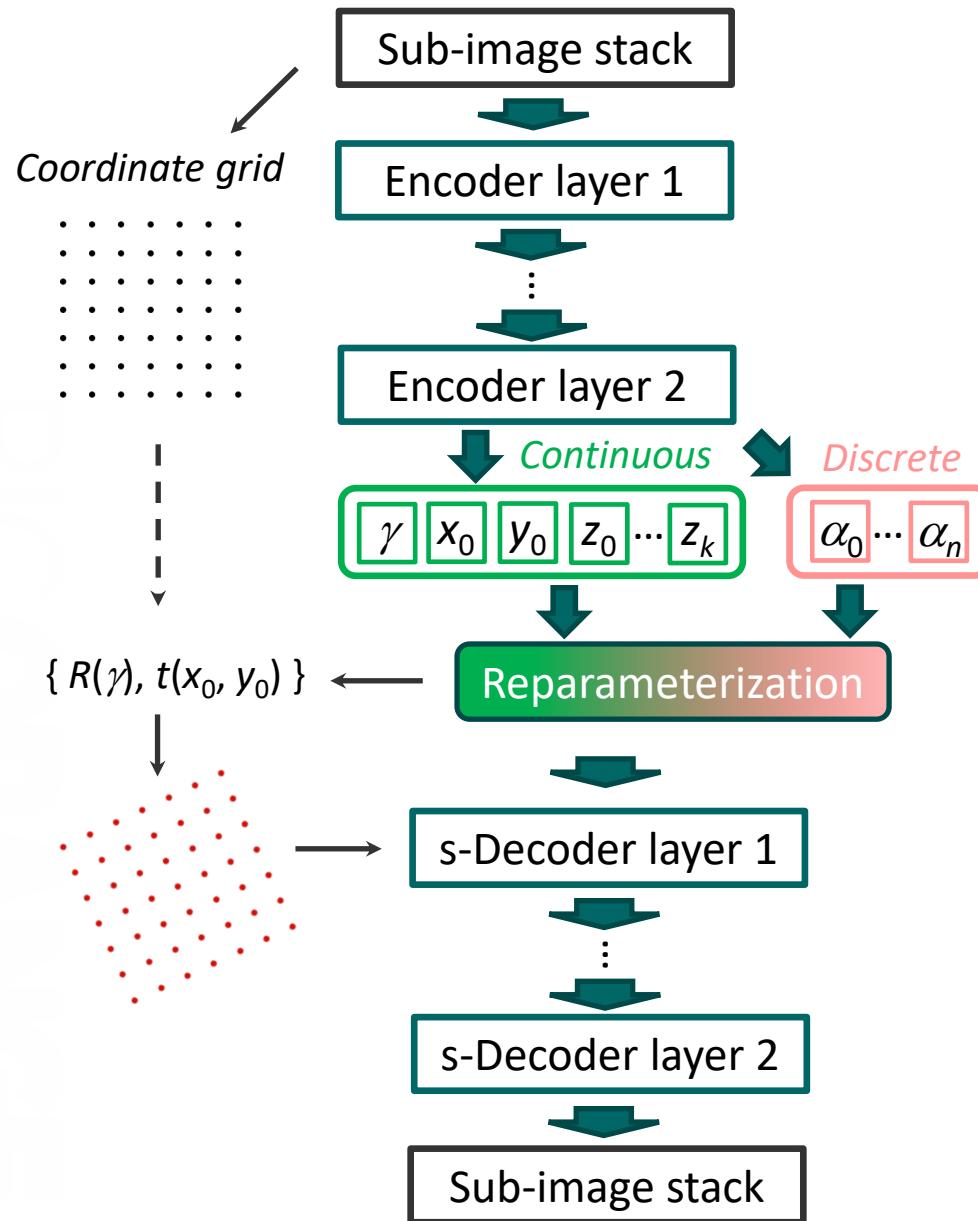


Semi-supervised VAE

Traversal Manifold



Joint VAE

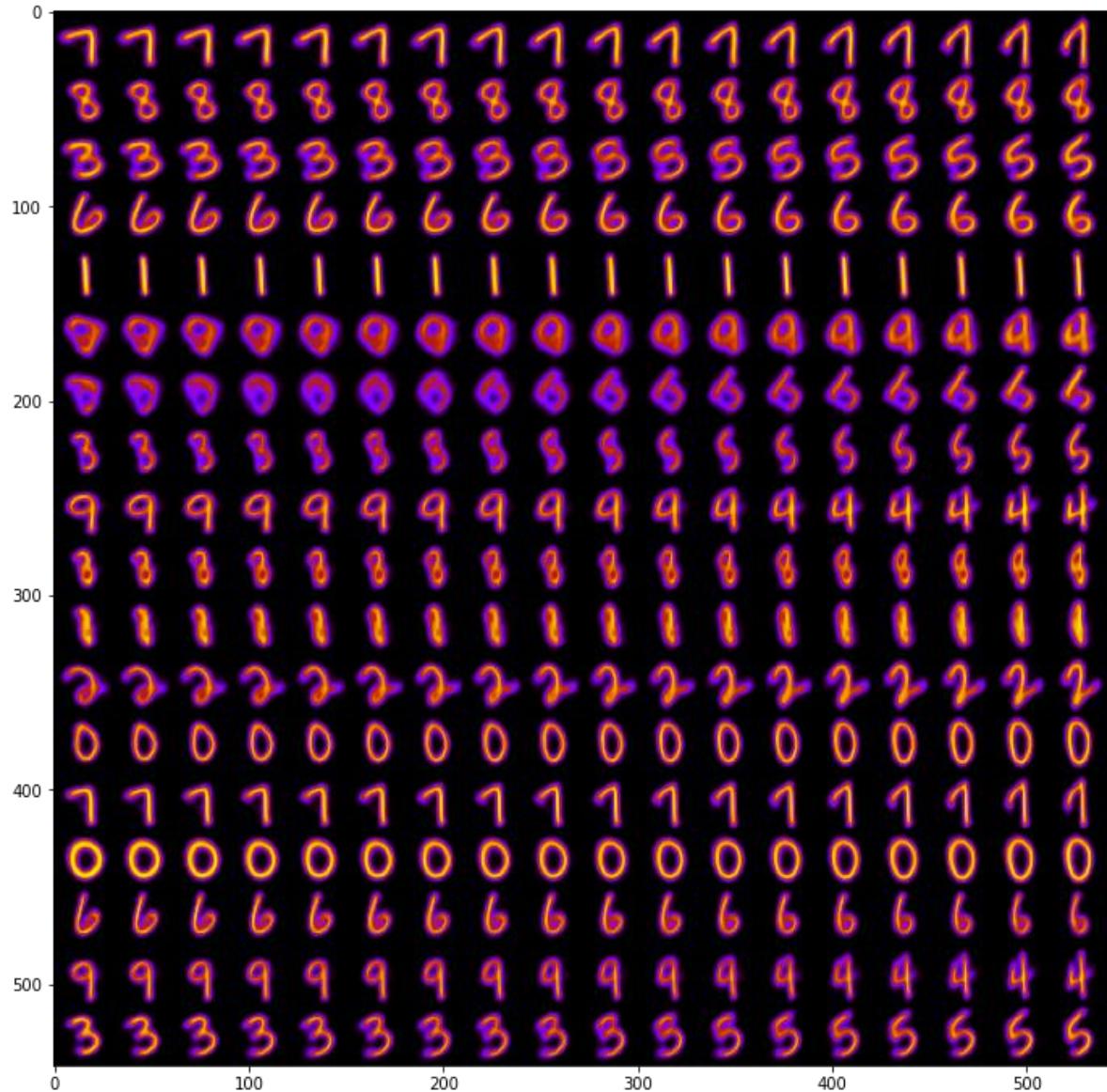
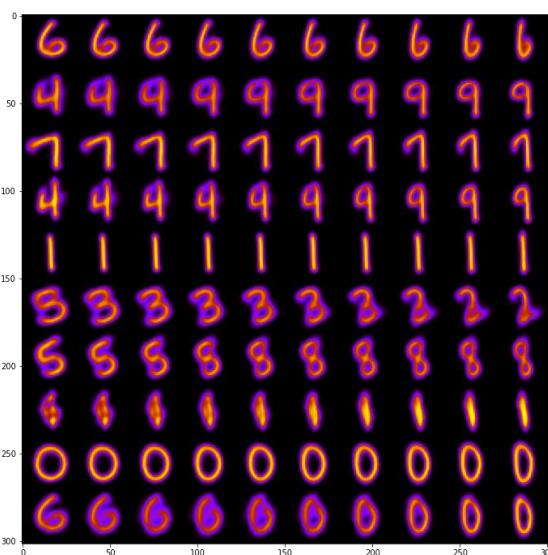
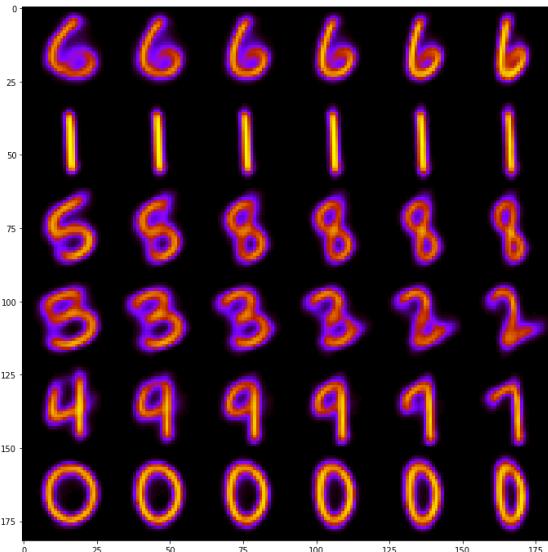


- Generative model is a function of spatial coordinate (e.g., via spatial broadcasting)
- 3 additional latent variables to absorb rotations and shifts
- Disentangles rotations and translations from image content
- Learns discrete classes in unsupervised fashion
- Well-suited for analyzing microscopy (sub-)images on atomic and molecular levels

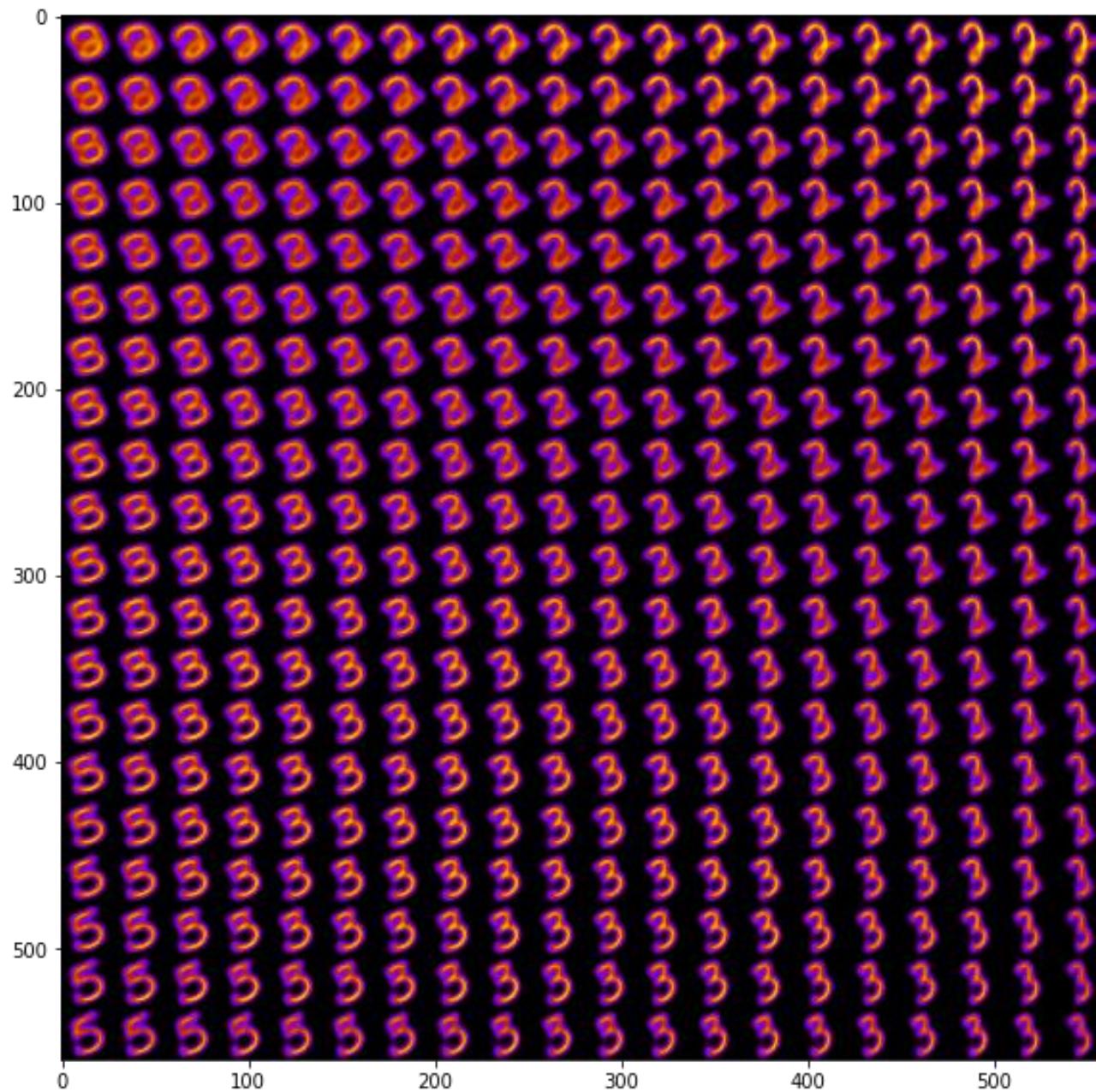
ELBO =

$$\begin{aligned} & - \text{Reconstruction Loss} \\ & - \beta_c(t) |(D_{KL}(q(z|x) \parallel p(z)) + D_{KL}(q(\gamma|x) \parallel p(\gamma)) - C_z| \quad \text{Continuous} \\ & - \beta_d(t) |D_{KL}(q(\alpha|x) \parallel p(\alpha)) - C_\alpha| \quad \text{Discrete} \end{aligned}$$

jVAE on MNIST



Latent representations



Ensemble jVAE

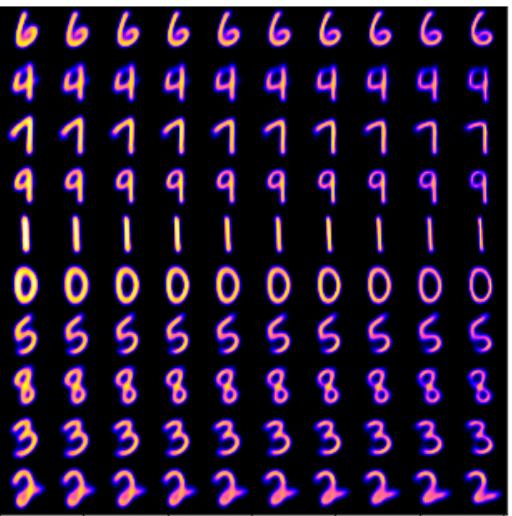
Predictions from different ensemble models



Baseline: 10 epochs
Ensemble models: 8

- The unstable classes show the largest “uncertainty”
- Indication of the quality of separation and/or a guide for selection of the number of classes

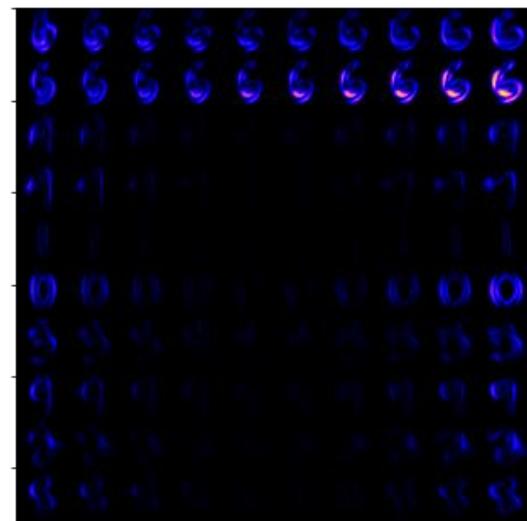
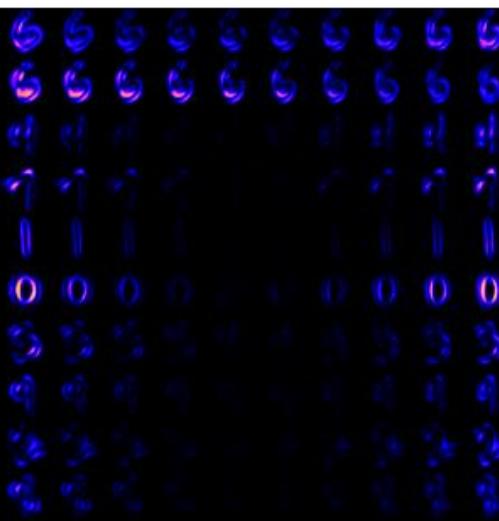
Uncertainty



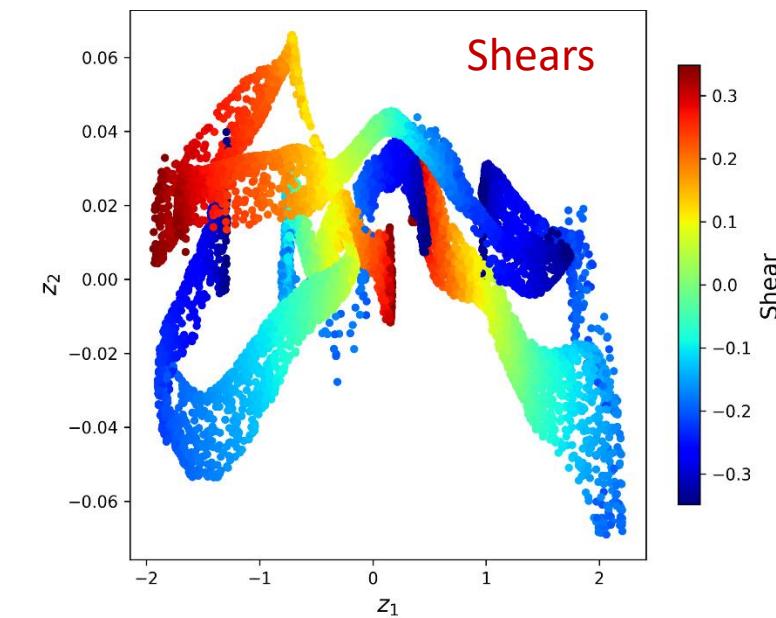
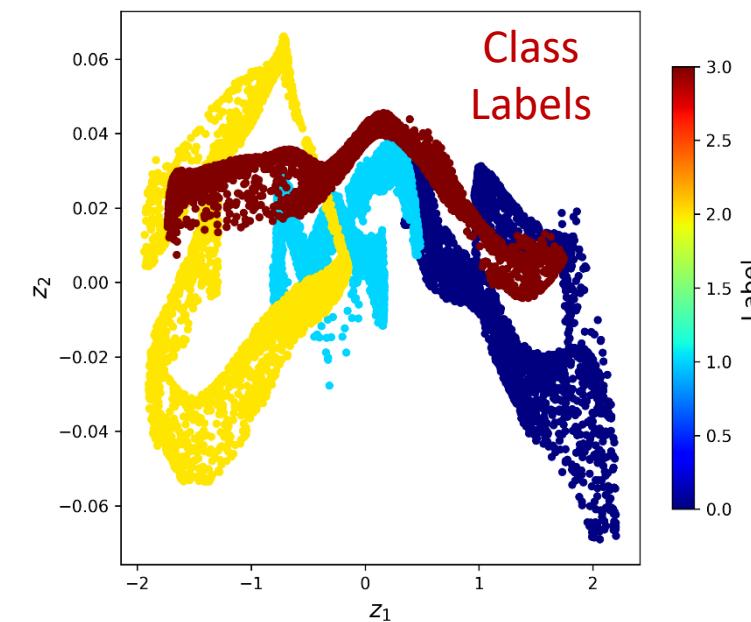
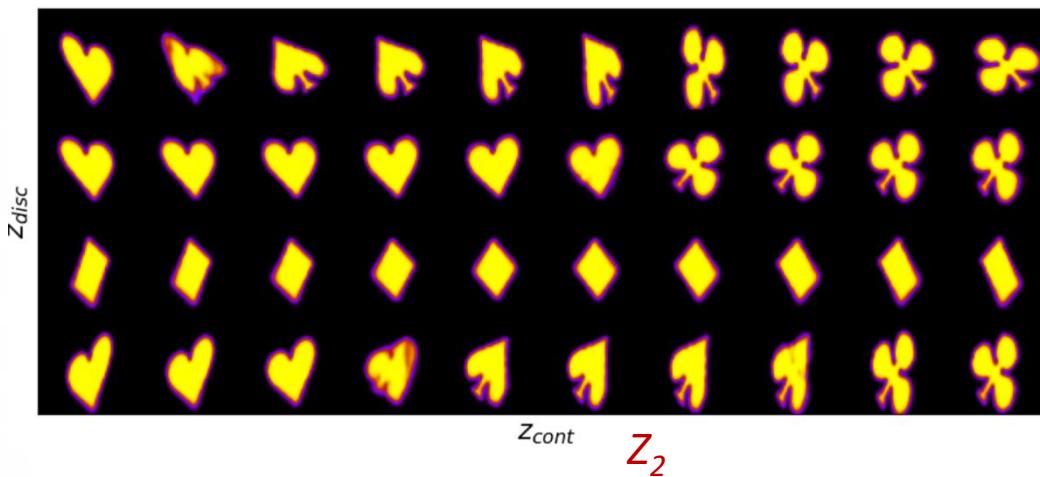
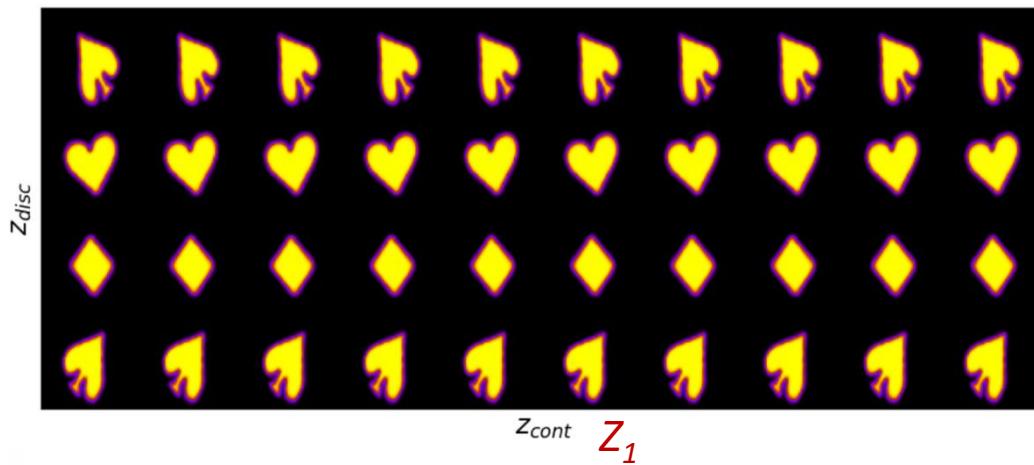
Mean prediction



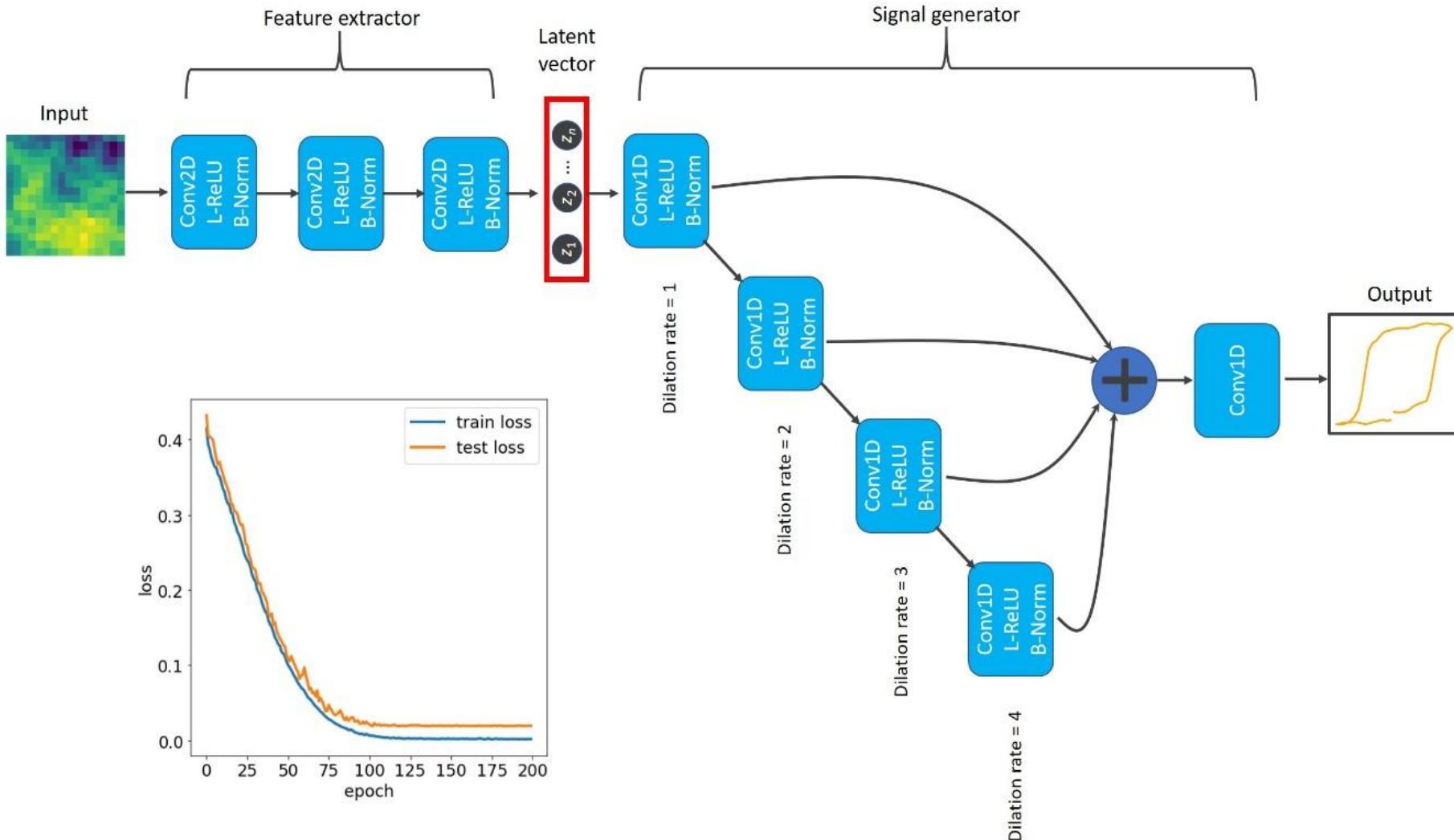
Dispersion in predictions ('uncertainty')



jVAE on cards

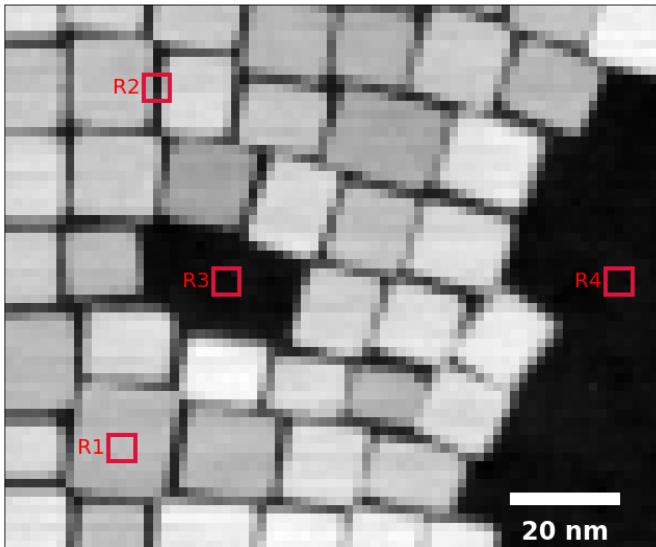


Encoders-Decoders



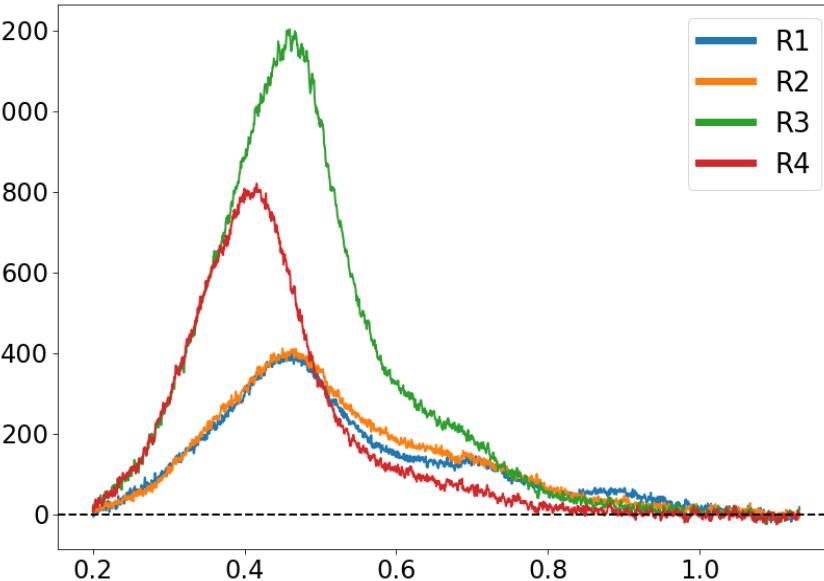
- Use encoder-decoder architecture to transform local structure to local spectra
- And spectra to images
- Predictive within the image

Plasmonic nanoparticles



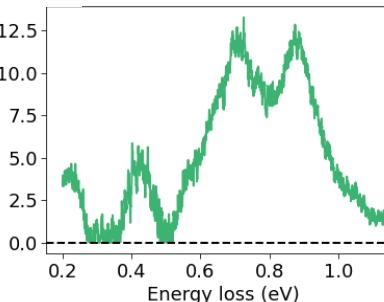
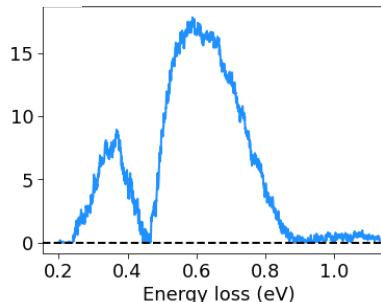
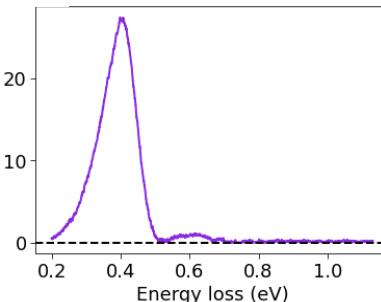
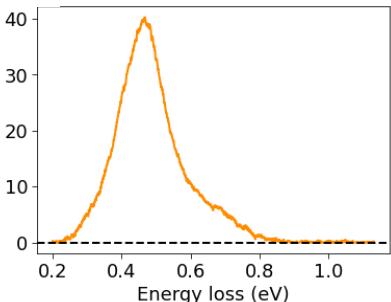
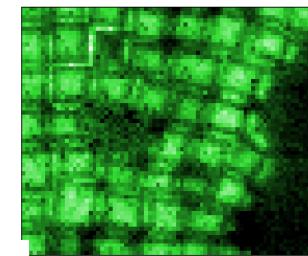
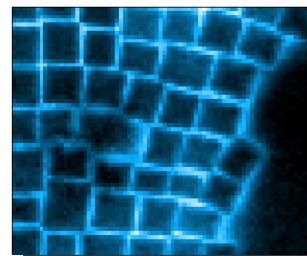
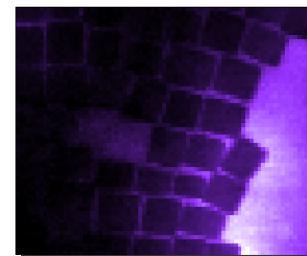
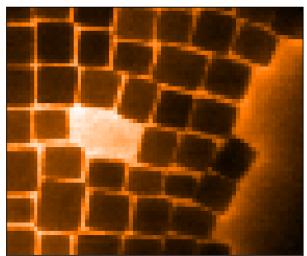
NMF 1

NMF 2

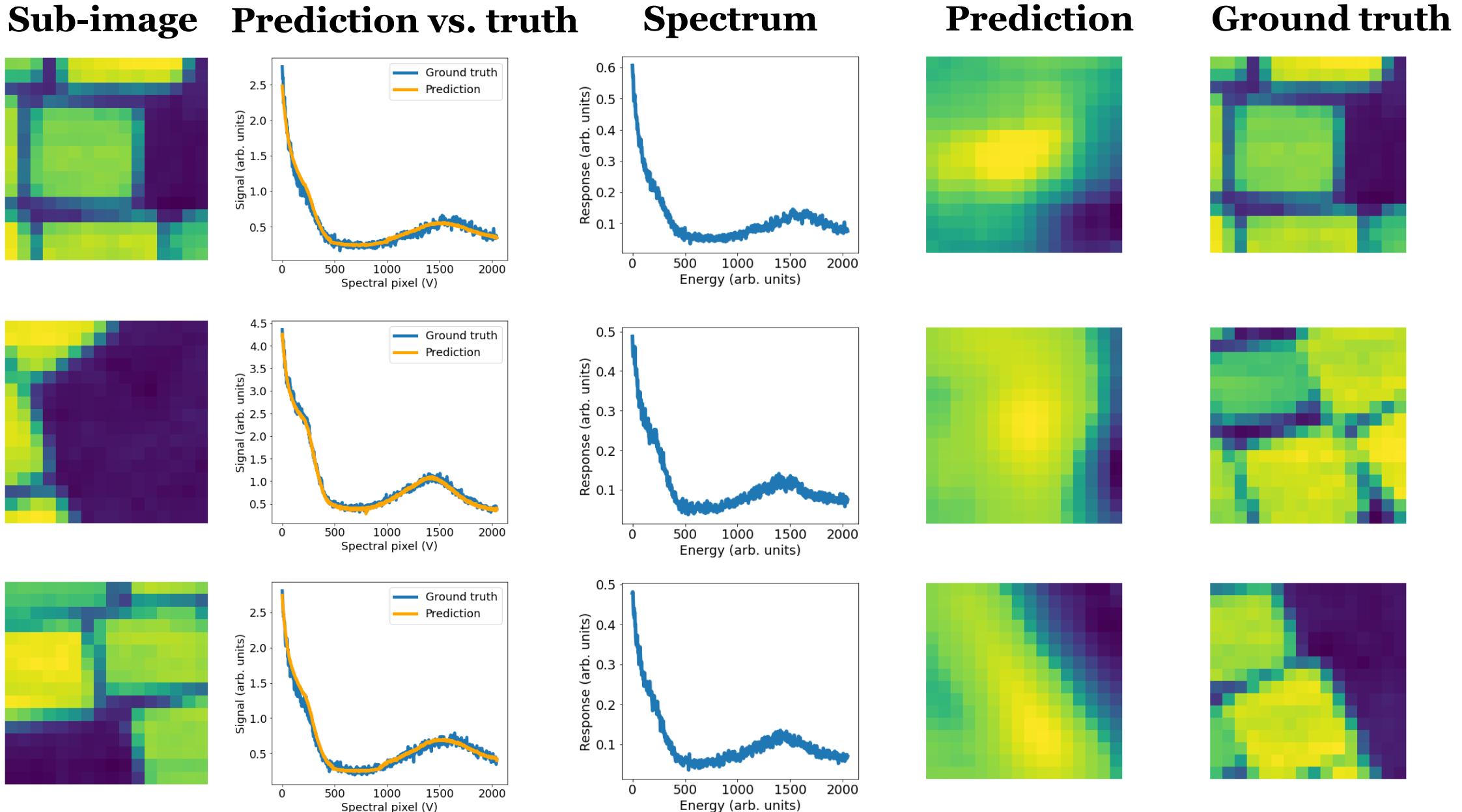


NMF 3

NMF 4

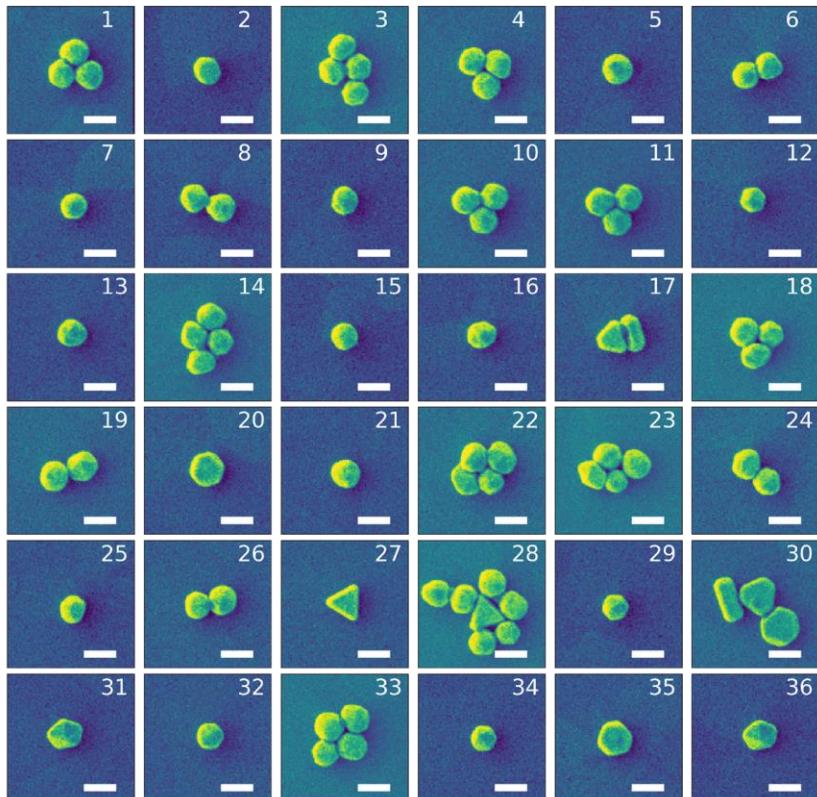


Encoders-Decoders

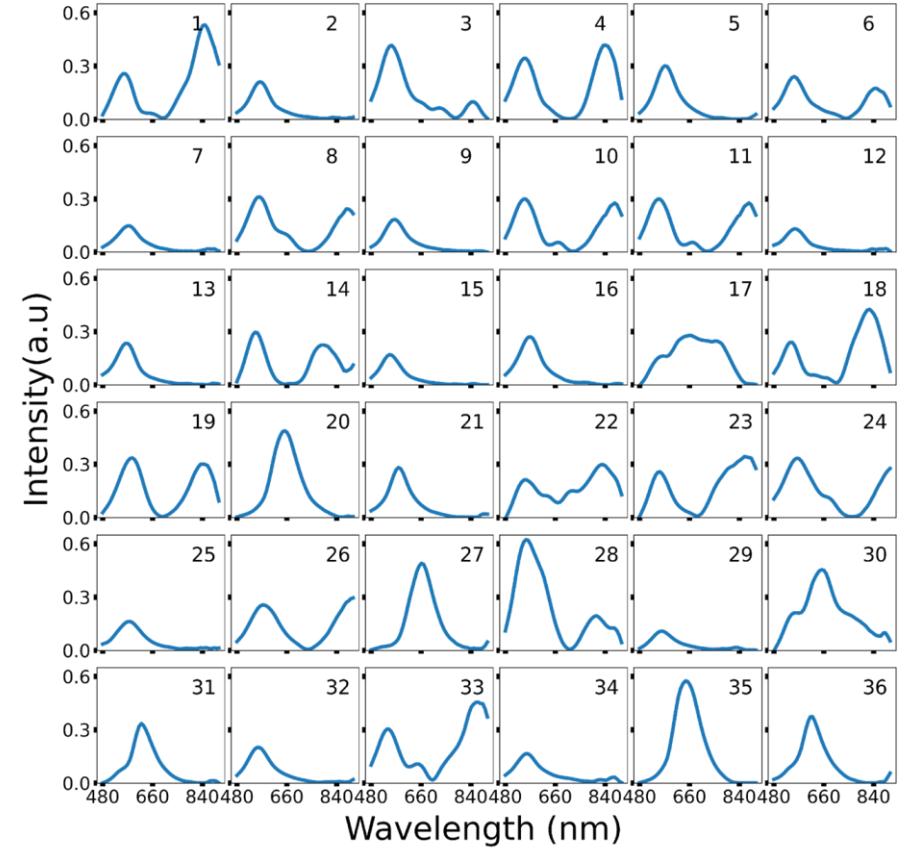


Dual VAE: structure-property relationships

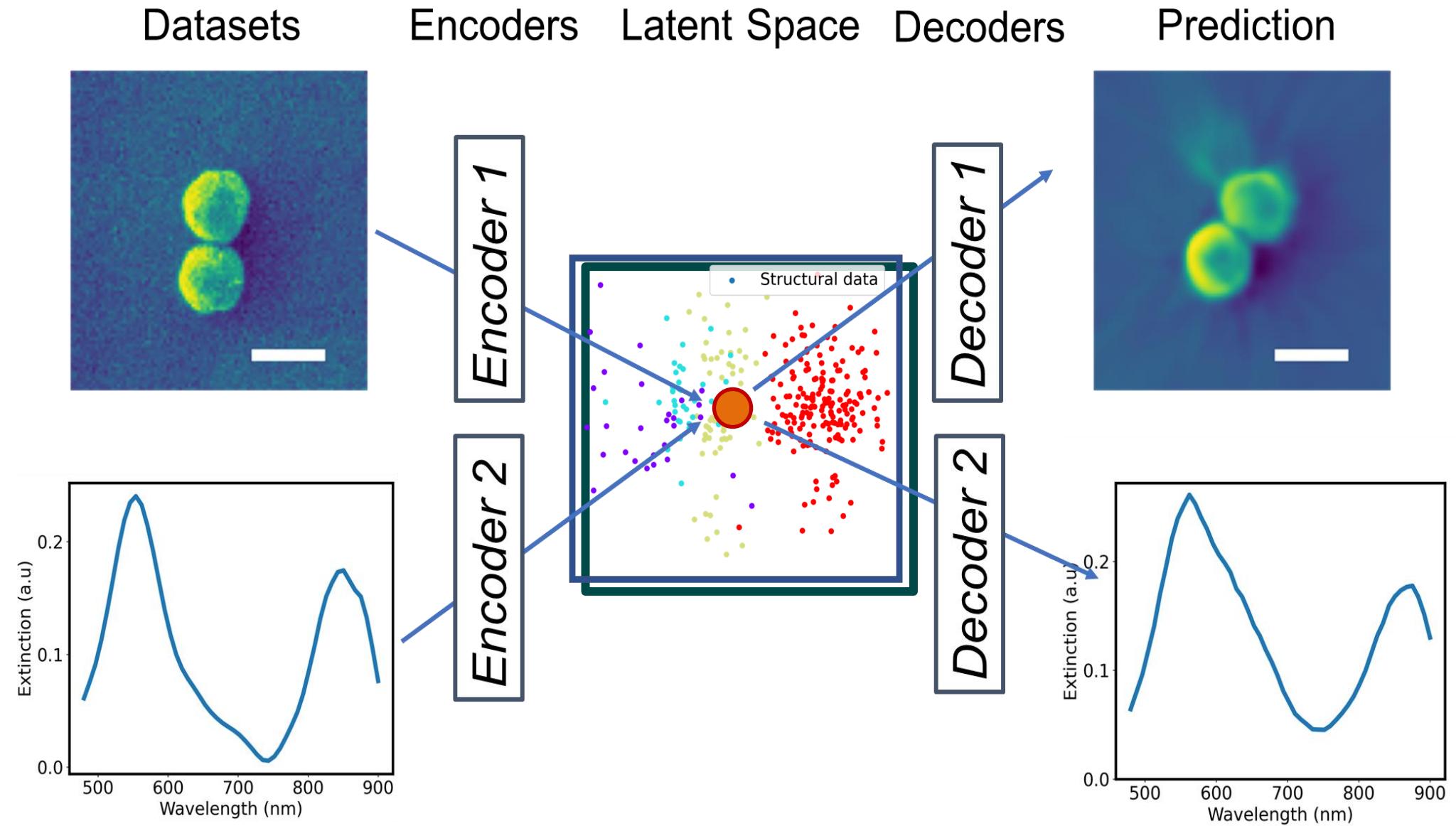
SEM images: "Structure Information"



Hyperspectral microscope: "Property Information"

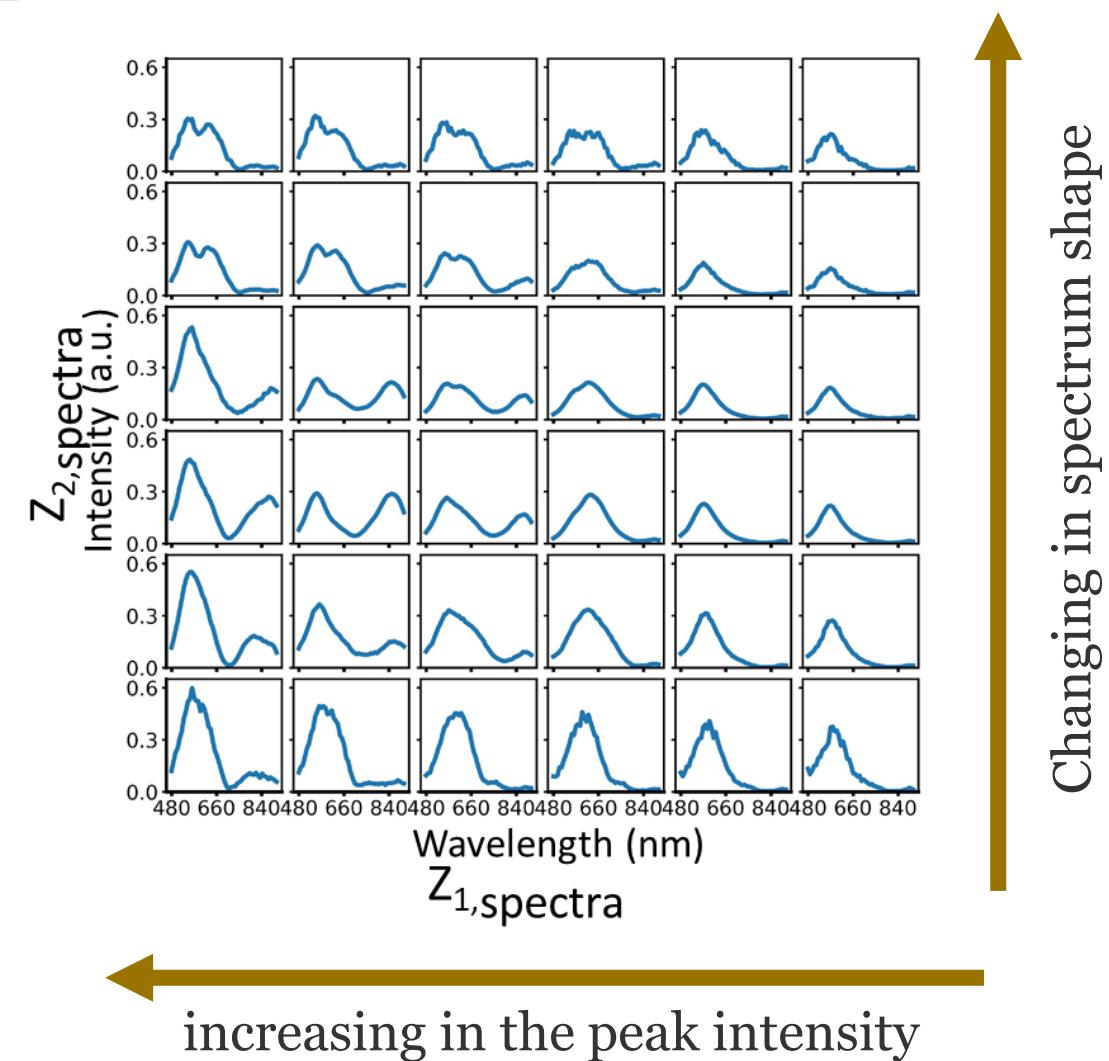
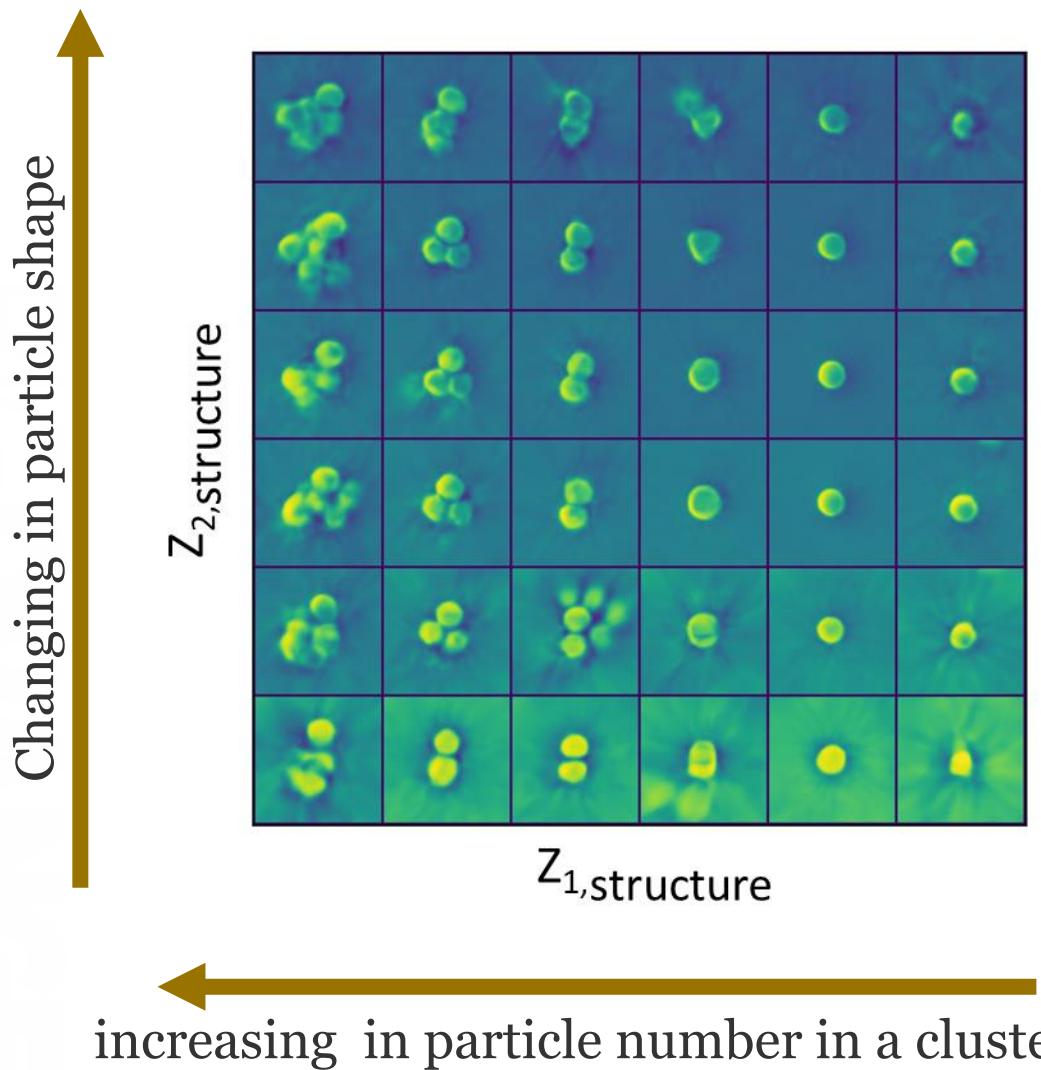


Dual VAE



Dual VAE: Latent Representations

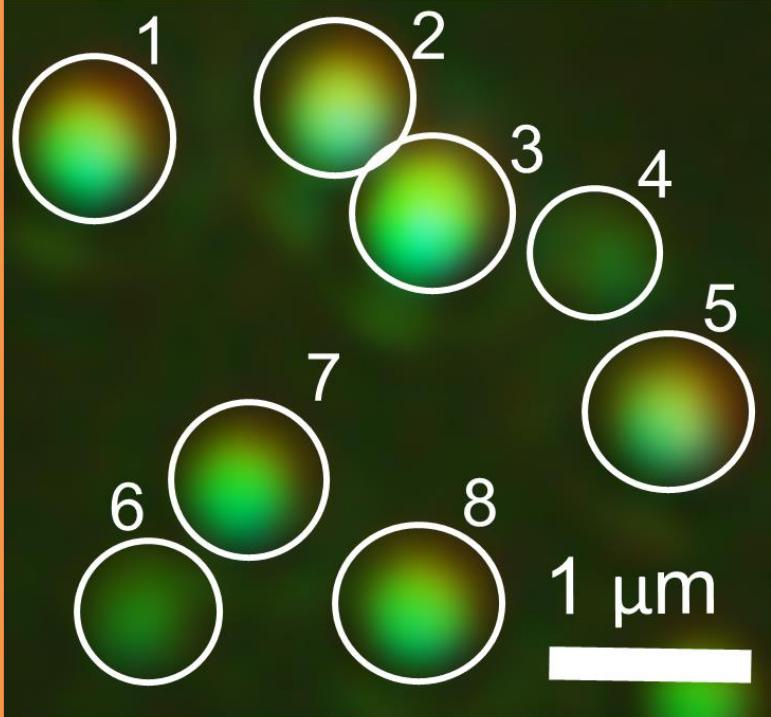
Manifold Representation



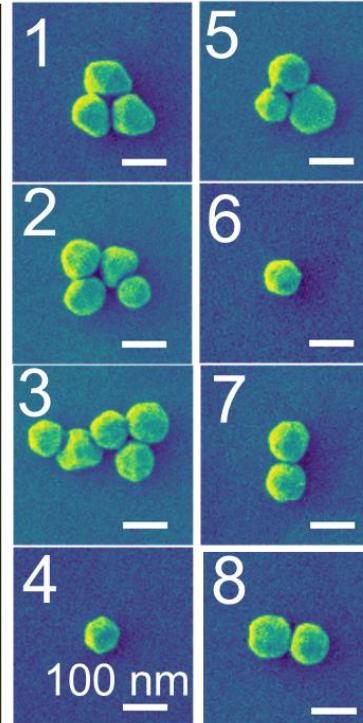
Dual VAE: Predictions

Example

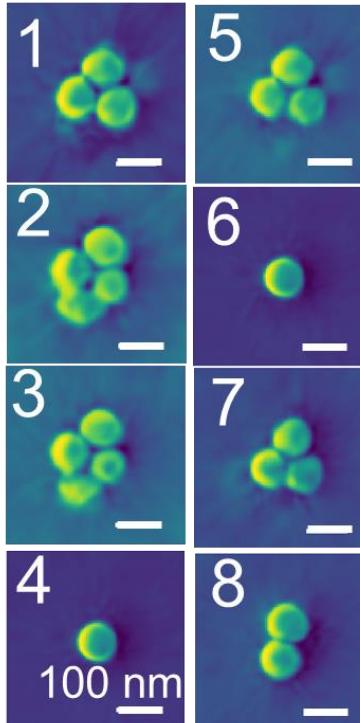
Darkfield Image



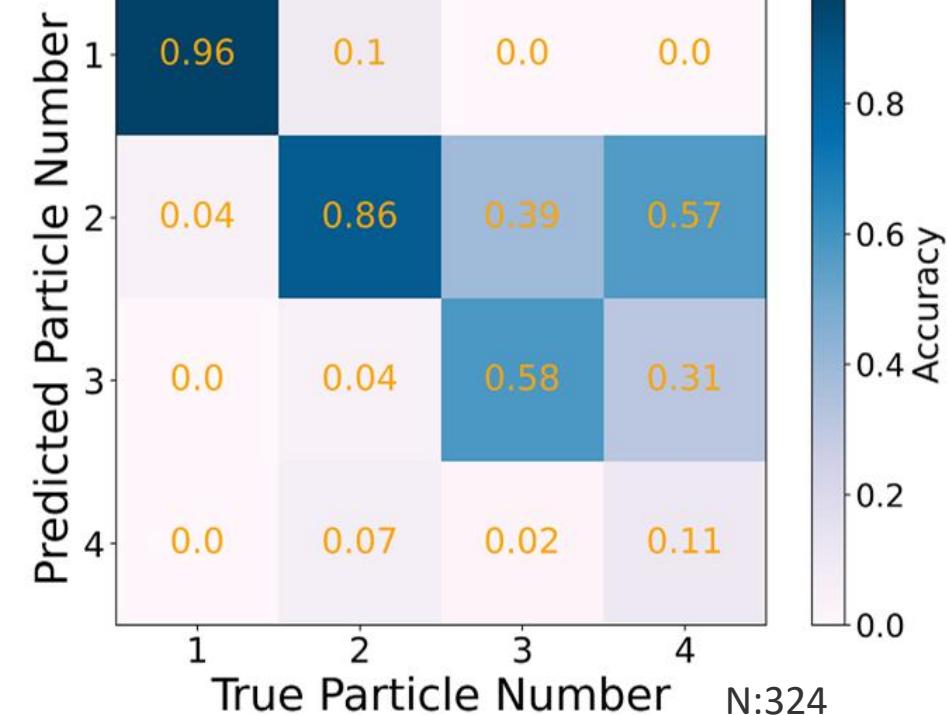
Ground Truth



Prediction



Overall Particles



[2303.18236.pdf \(arxiv.org\)](https://arxiv.org/pdf/2303.18236.pdf)

<https://github.com/saimani5/VAE-tutorials>

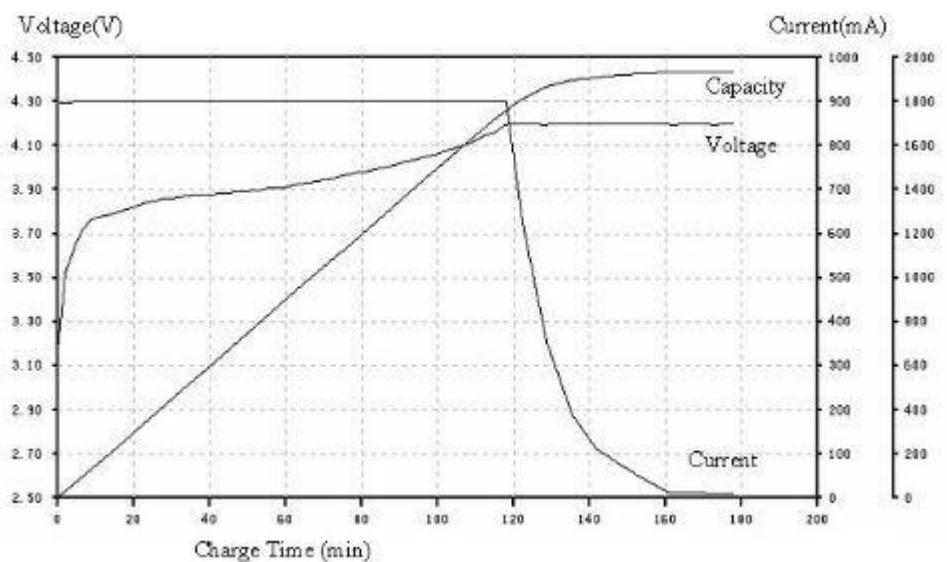
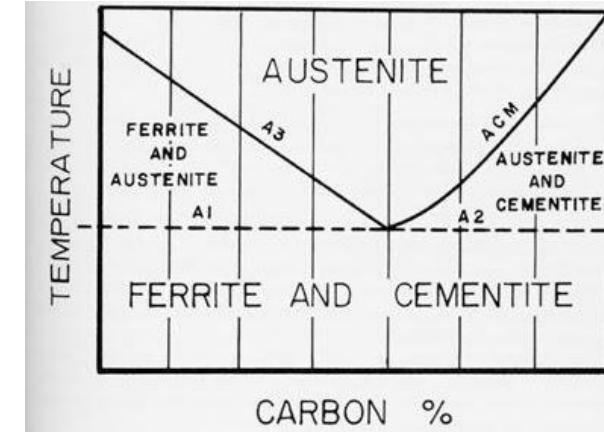
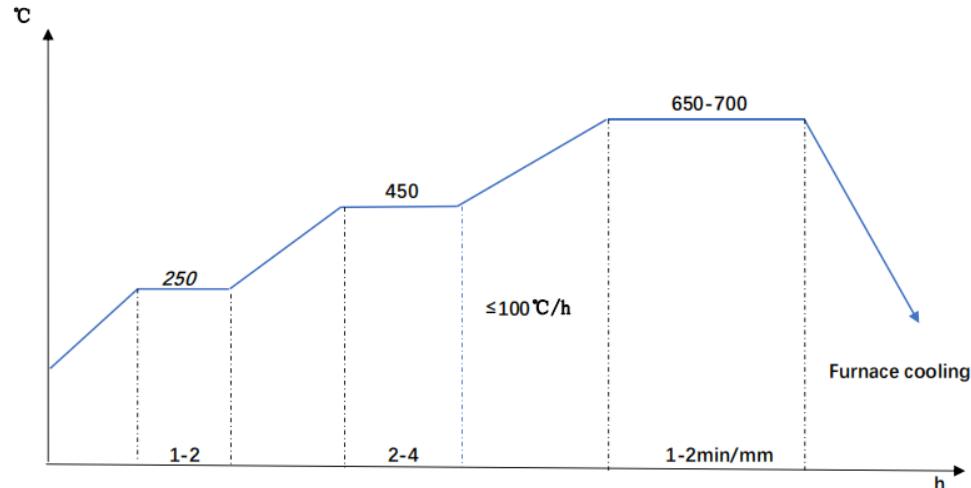
What is the limitation of the GP/BO?

1. Works only in low-dimensional spaces
2. The correlations are defined by the kernel function (very limiting)
3. We do not use any knowledge about physics of the system
4. We do not use cheap information available during the experiment (proxies)

Can we somehow make high dimensional space low-D?

1. Structure-property relationships
2. Molecular discovery and QASR
3. Processing optimization

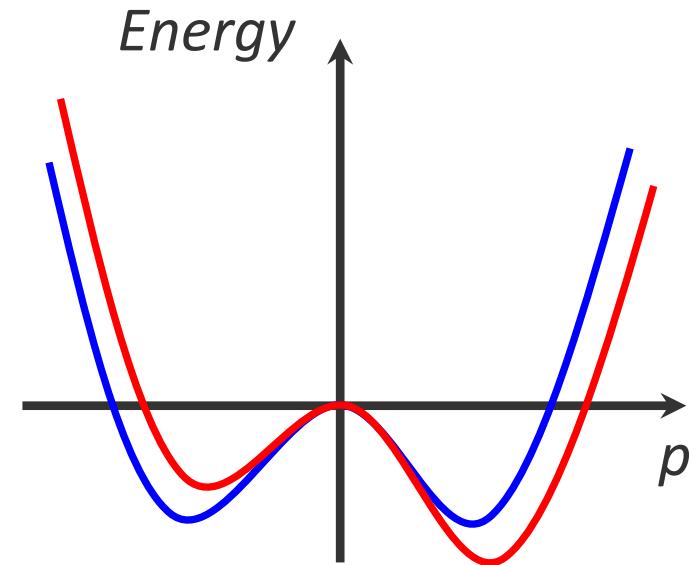
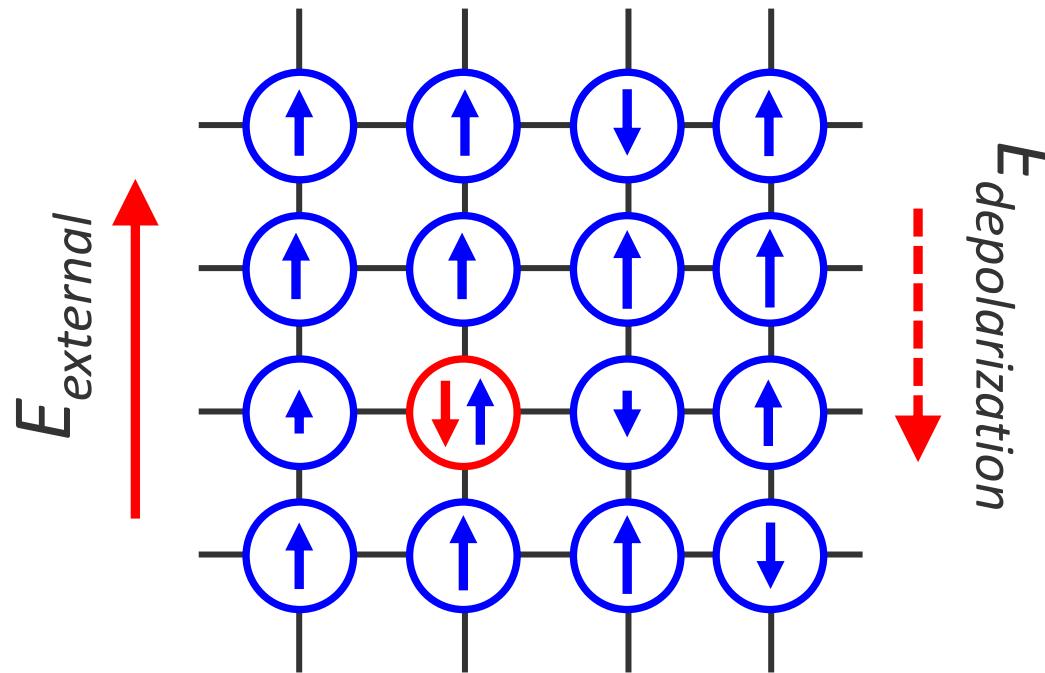
Making materials: process trajectories



- Making steel: complicated and took a lot of time optimize
- Charging battery: obvious economic impact
- Manufacturing: Annealing hybrid perovskite thin films
- Poling ferroelectric

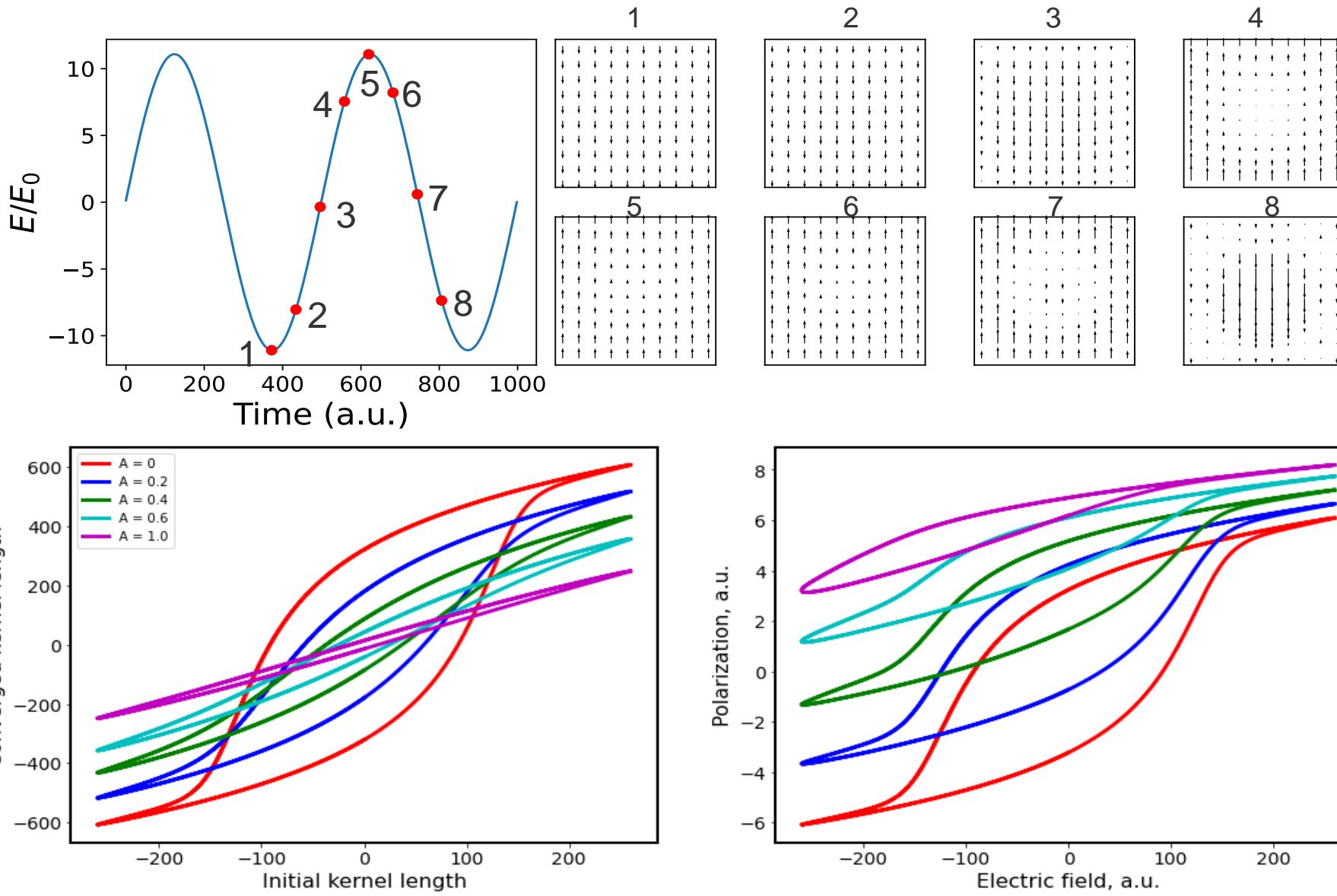
How do we optimize trajectories if we have (a) only limited or no mechanistic information, (b) our experimental budgets are limited, but (c) we have some access to domain expertise?

FerroSIM: the simplest interesting ferroelectric



- A discrete square lattice where a continuous polarization vector resides at each lattice site
- The local free energy at each site takes the GLD form:
 - $F_{ij} = \alpha_1 (p_{x_{ij}}^2 + p_{y_{ij}}^2) + \alpha_2 (p_{x_{ij}}^4 + p_{y_{ij}}^4) + \alpha_3 p_{x_{ij}}^2 p_{y_{ij}}^2 - E_{loc_{x_{ij}}} p_{x_{ij}} - E_{loc_{y_{ij}}} p_{y_{ij}}$
 - Where, $E_{loc} = E_{ext} + E_{dep} + E_d(i,j)$ and $E_d = -\alpha_{dep} < p >$
- The total free energy is the sum of local free energies and coupling terms:
 - $F = \sum_{i,j}^N F_{ij} + K \sum_{k,l} (p_{x_{ij}} - p_{x_{i+k,j+l}})^2 + K \sum_{k,l} (p_{y_{ij}} - p_{y_{i+k,j+l}})^2$
- Polarization at each lattice site is updated to decrease the free energy using $\frac{d}{dt} p_{i,j} = -\frac{\partial F}{\partial p_{i,j}}$

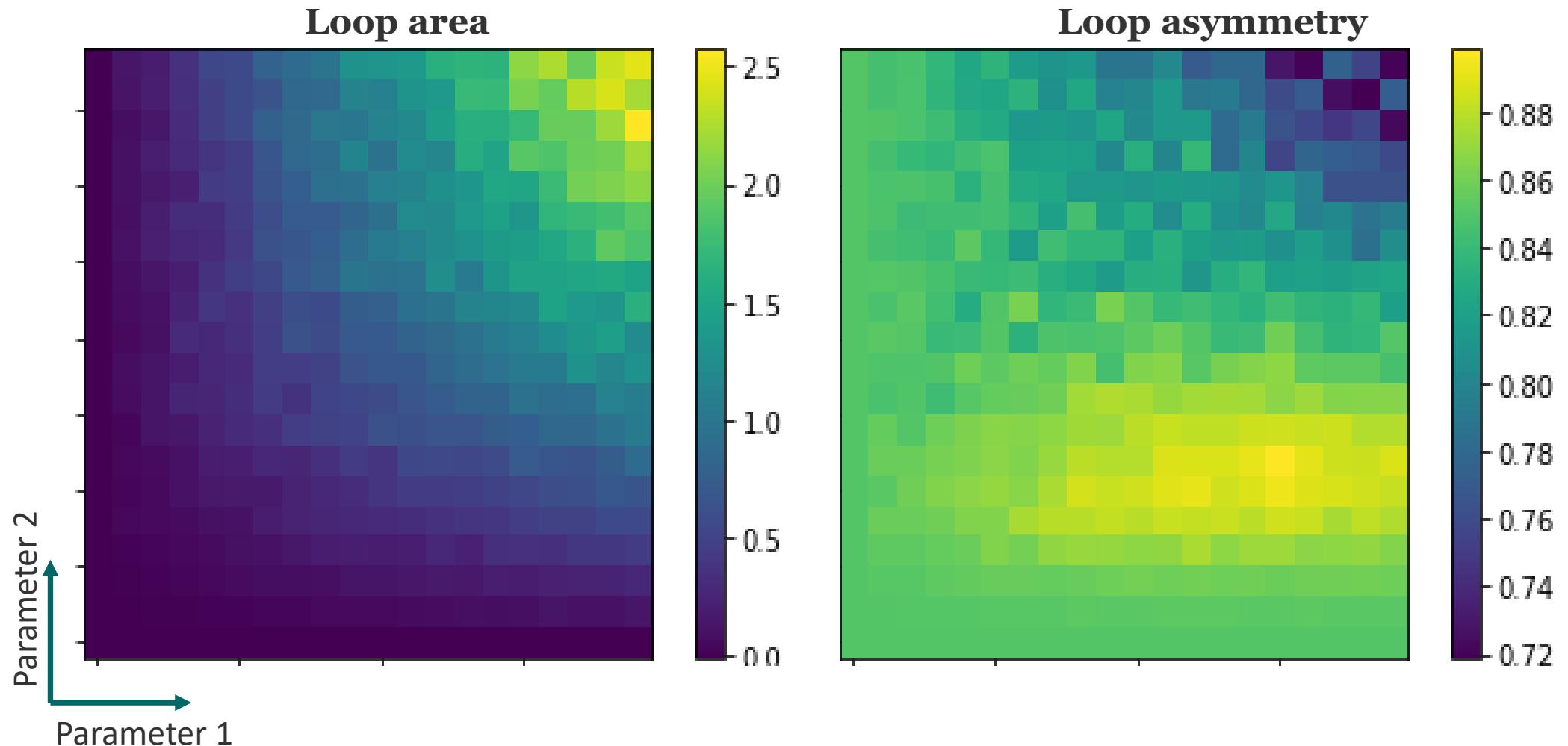
Microstates and Macroscopic Observables



Global response vs. model parameters

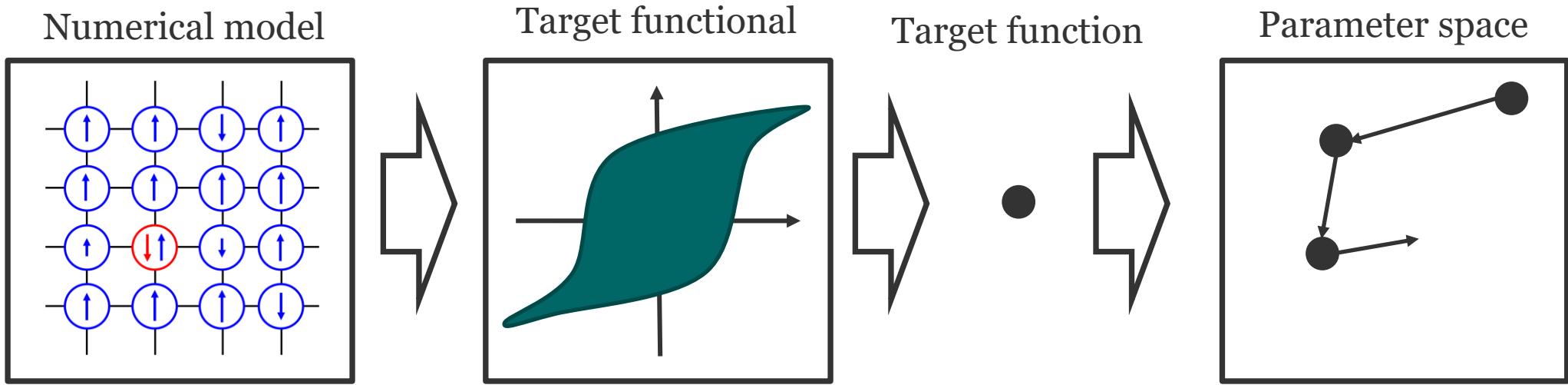
Parameter space 1: Coupling strength

Parameter space 2: Depolarization strength



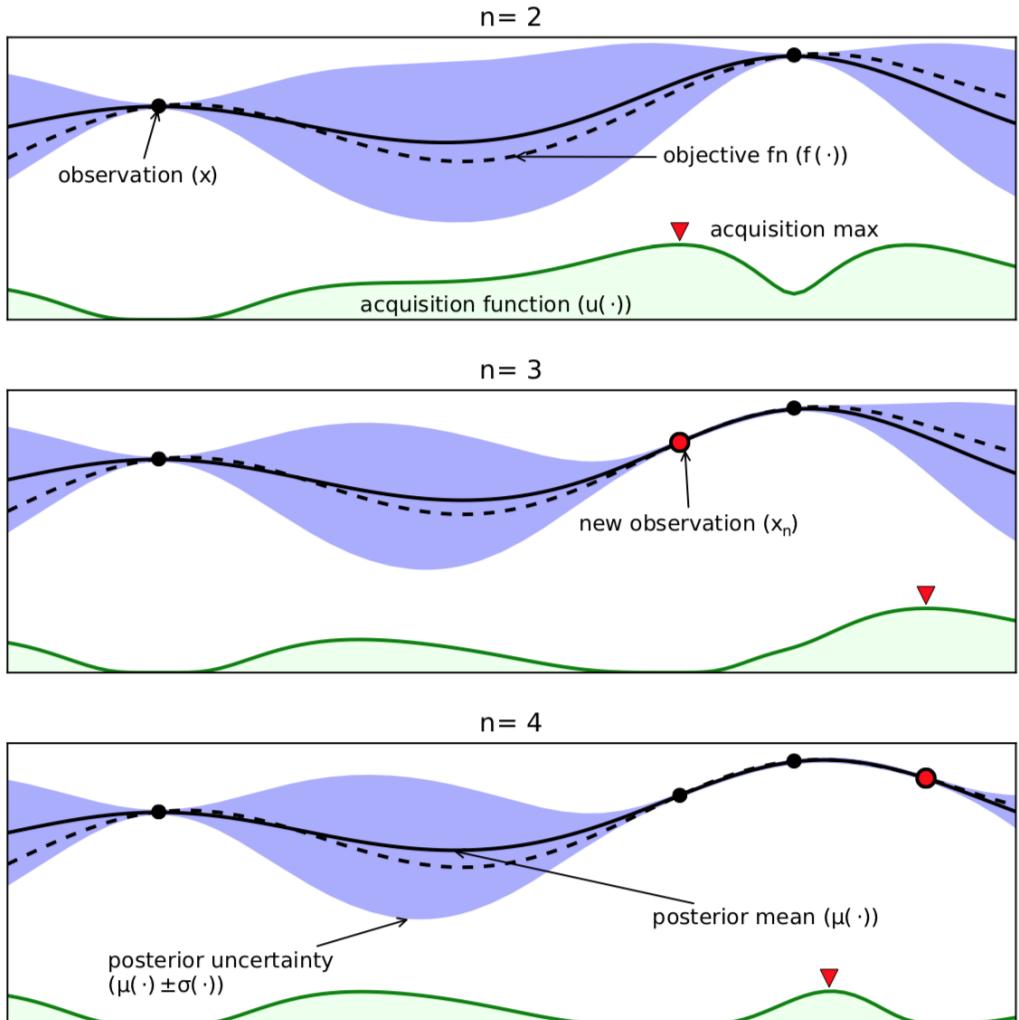
For small dimensional parameter spaces, we can evaluate global responses via the grid search

Can we do better than grid search?



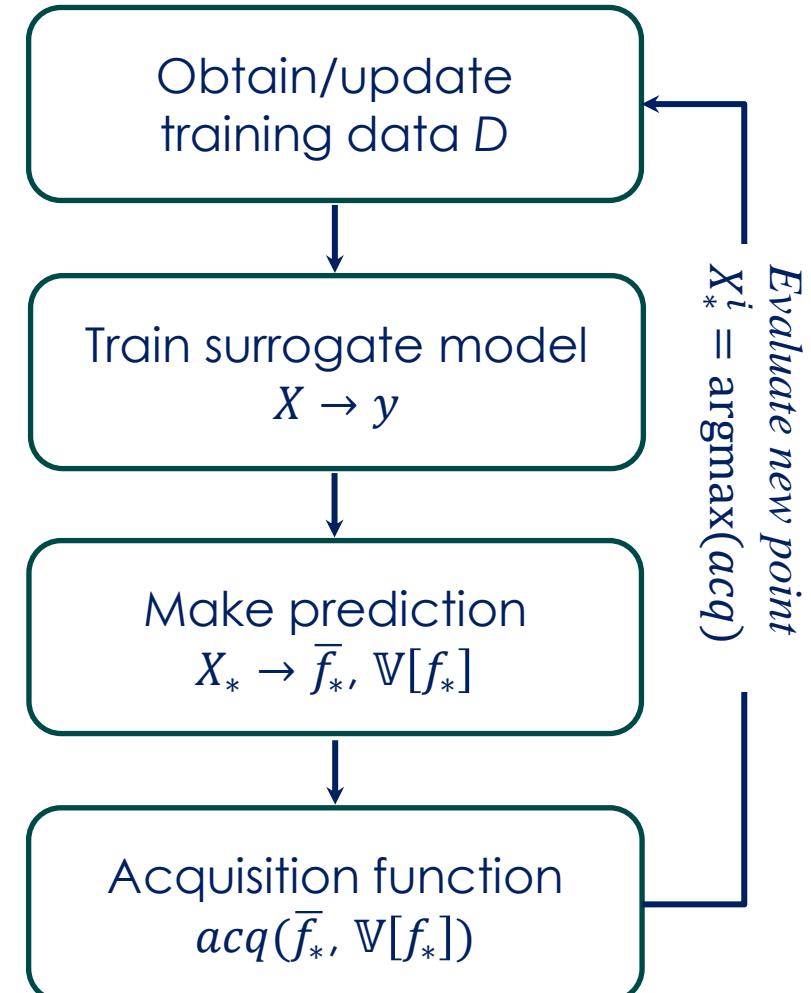
Or we can use simple Gaussian Process-based Bayesian Optimization to do so

Bayesian Optimization!

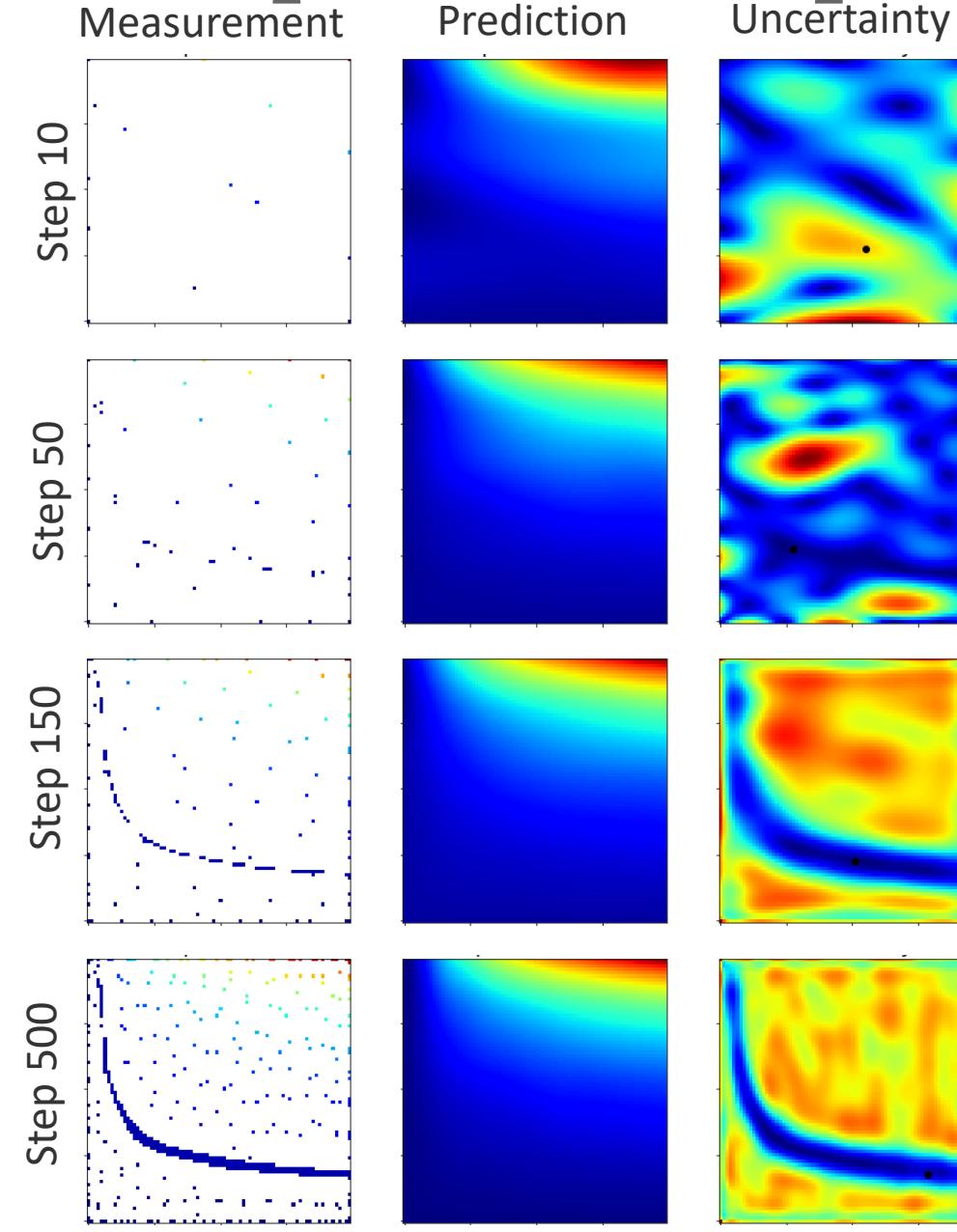


N. de Freitas et al., Taking the Human Out of the Loop: A Review of Bayesian Optimization ,
Proceedings of the IEEE 104, 148 (2015)

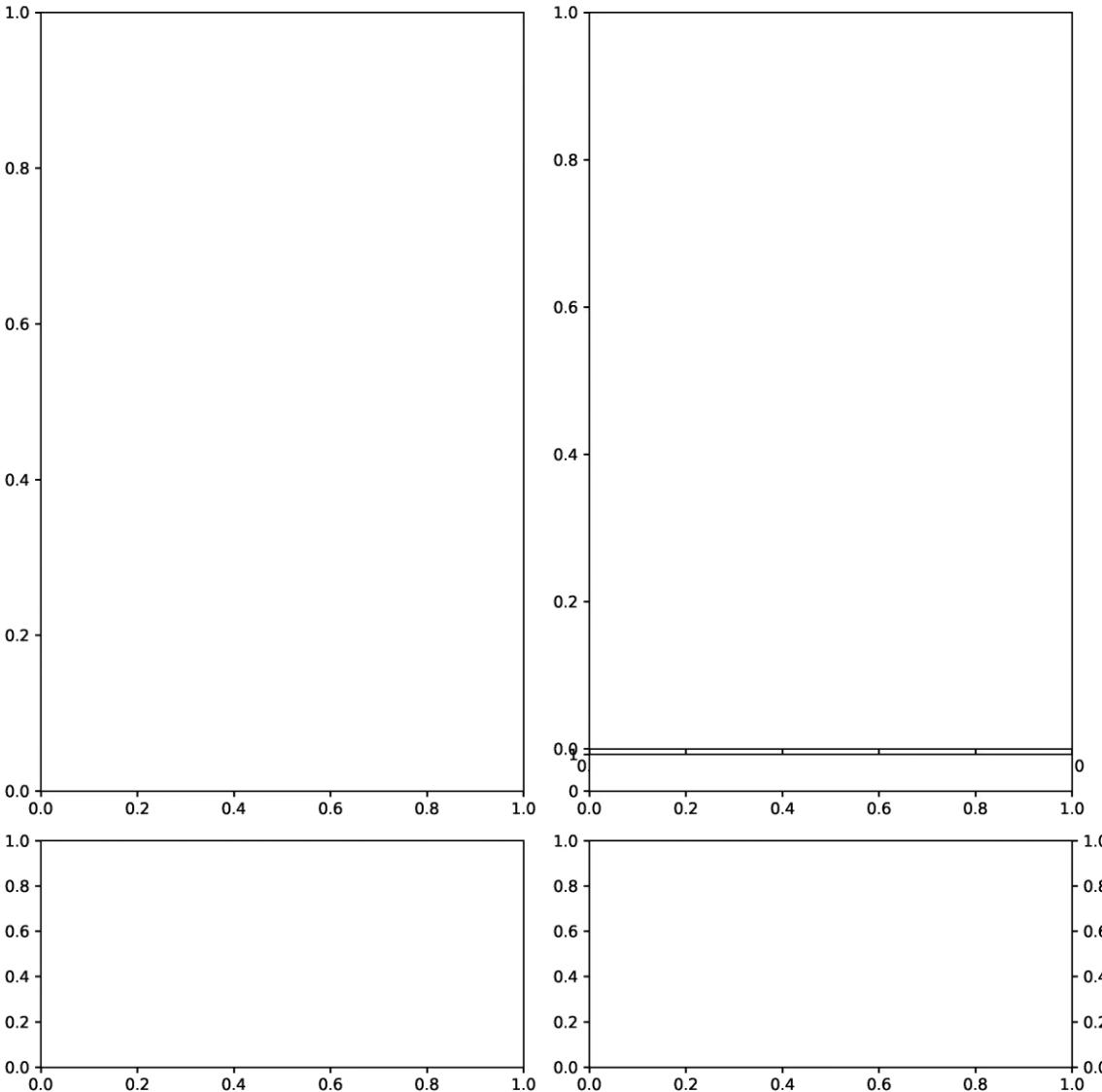
X, y : (sparse) Training data
 X_* : New (not yet evaluated) points



BO exploration of parameter space

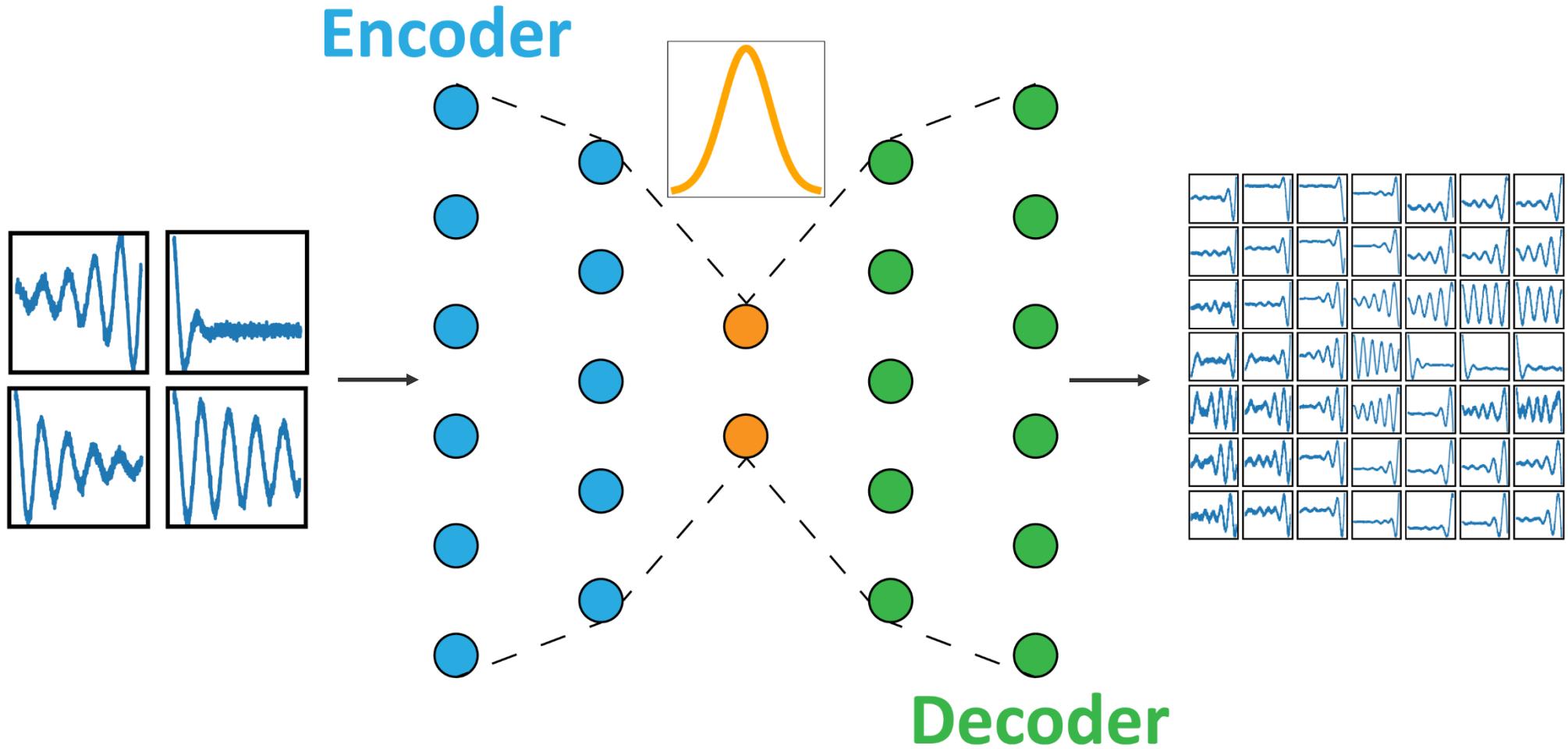


But what about trajectories?



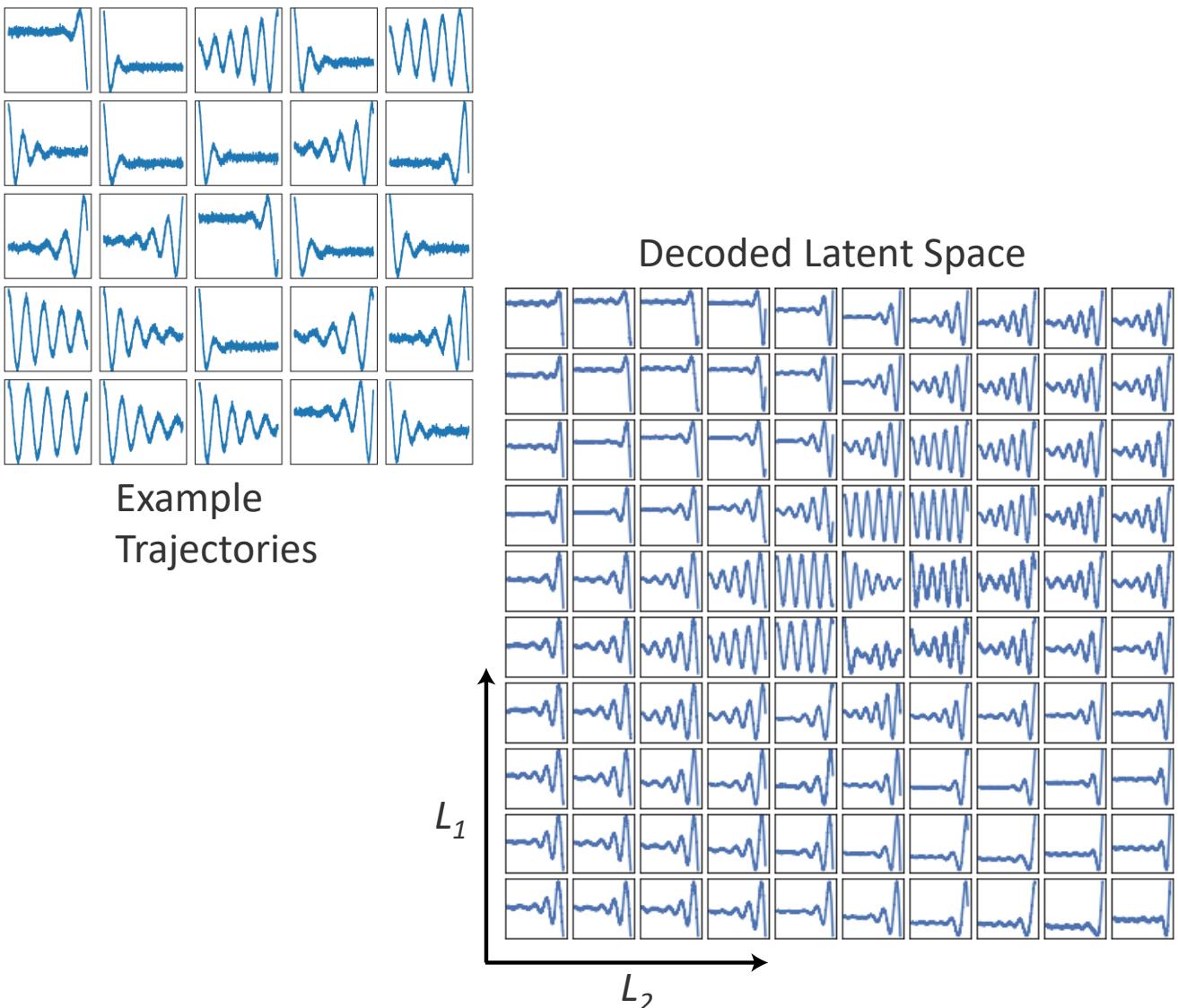
- The model has large number of microstates
- The global state depends on history, i.e. dependence of field vs. time
- Can we somehow optimize the chosen global state in the space of possible histories?
- This space is obviously intractable...
- ... however, we are not interested in ALL possible histories. We are interested in relatively simple histories
- **Thought:** what if we start with the histories that make sense from domain perspective, and look for way to simplify them?

Can VAE help?

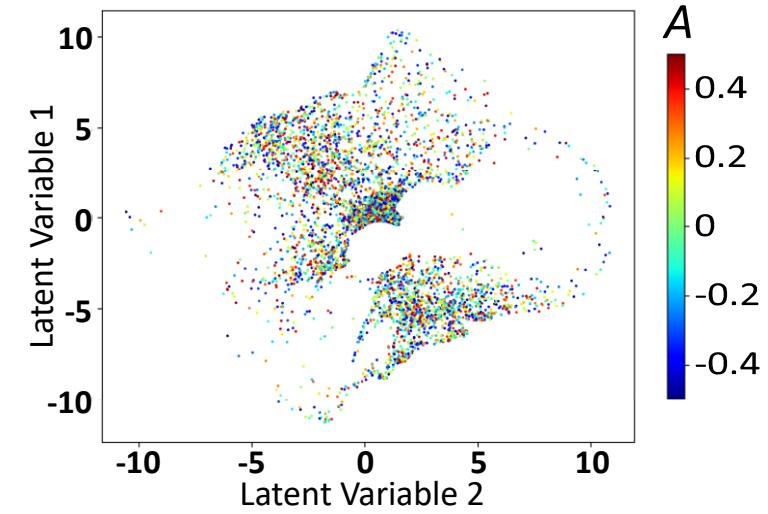
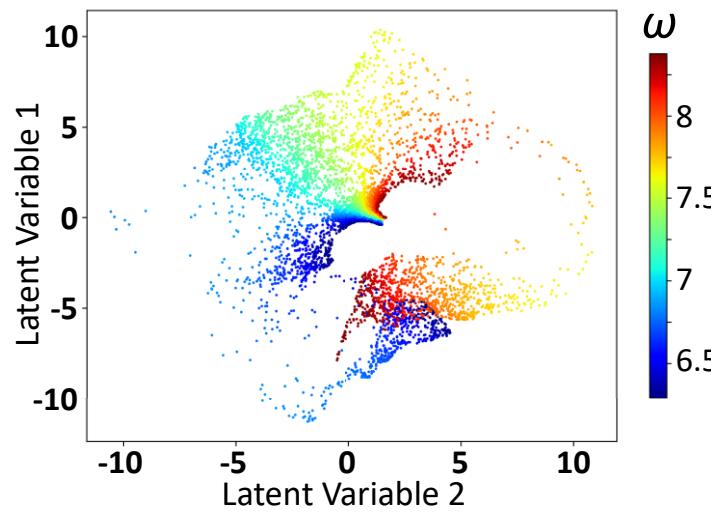
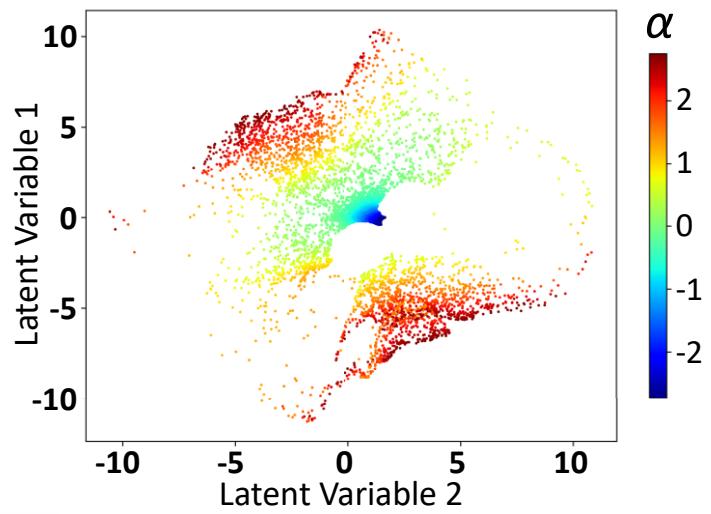


VAE encoding of domain trajectories

- Sinusoidal trajectories with exponential functions as amplitude modulators
 - $A \exp(\alpha t) \sin(\omega t) + B$
- $A: [0, 0.75]$,
- $\alpha: [-2.75, 2.75]$,
- $\omega: [2\pi, \frac{8}{3}\pi]$,
- $B: [-0.5, 0.5]$
- These electric fields are divided into 900 discrete time steps.
- 7500 of these curves are then used to create a smooth latent space using a Variational Autoencoder (VAE)

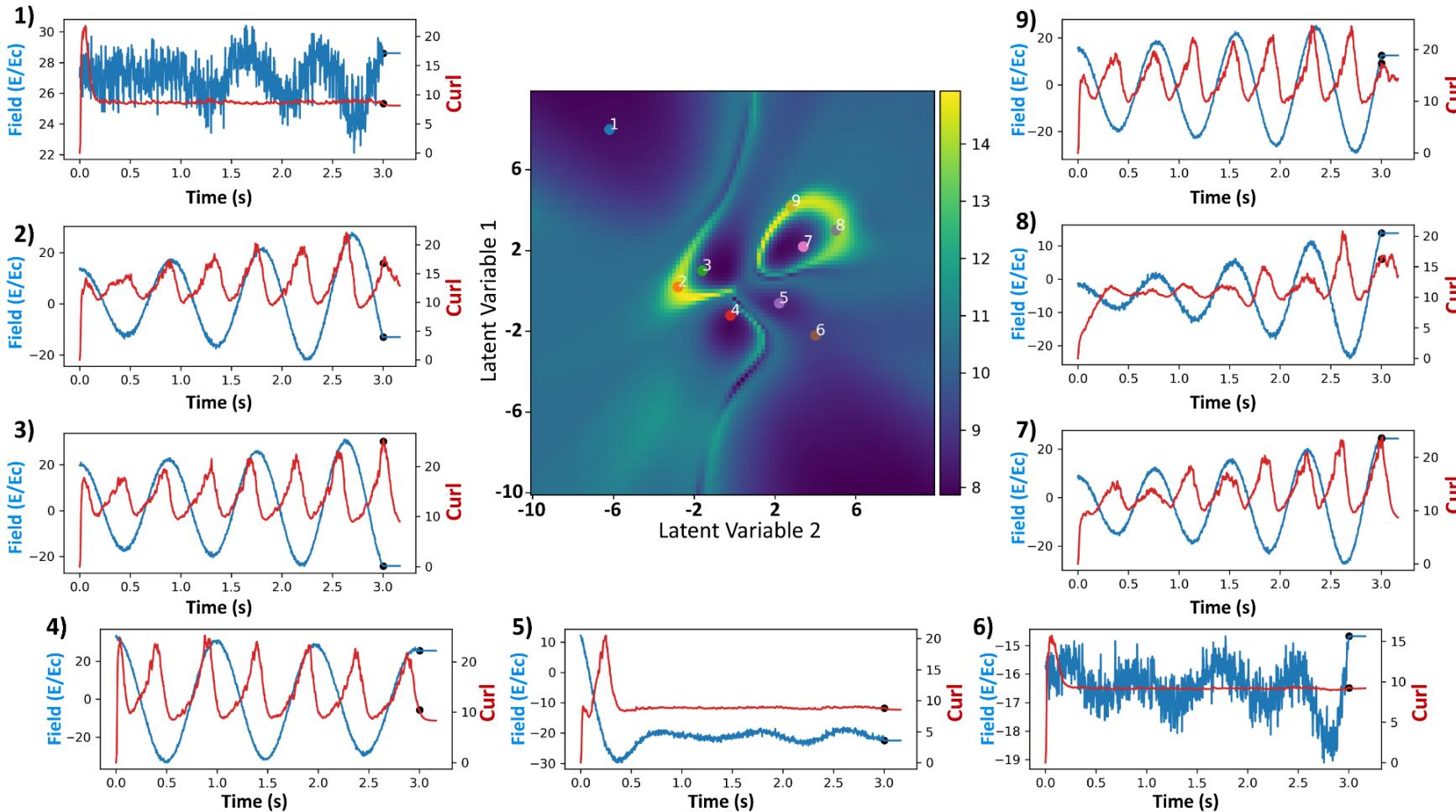


Latent space distributions



Ground truth target function

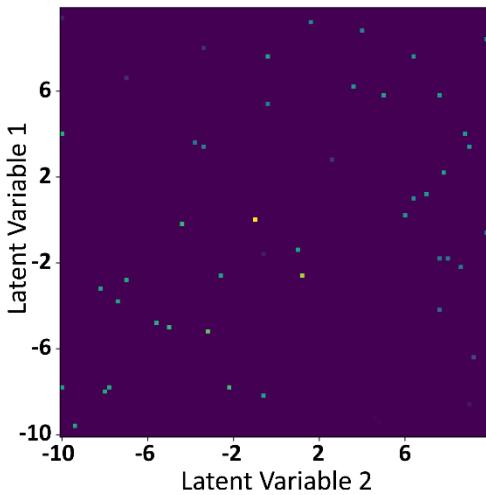
- Latent space is sampled and then decoded back into the space of electric field of 900-dimensions
- An equilibration region of 50-time steps is then added where the electric field is held constant at the final value of the decoded electric field.
- The **sum of absolute value of curl** at each lattice site at the end of the simulation is the target value to be optimized



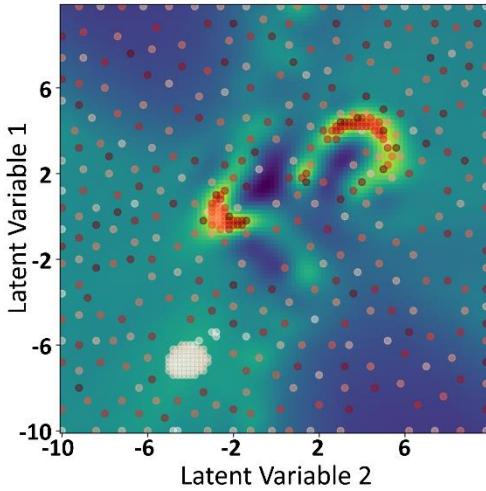
- Curl decays in the equilibration region
- The rate of decay of the curl is proportional to the curl at the onset of the equilibration region
- The local maxima of the curl seemingly coincides with the local optima of the electric field.

Bayesian Optimization in the Latent Space

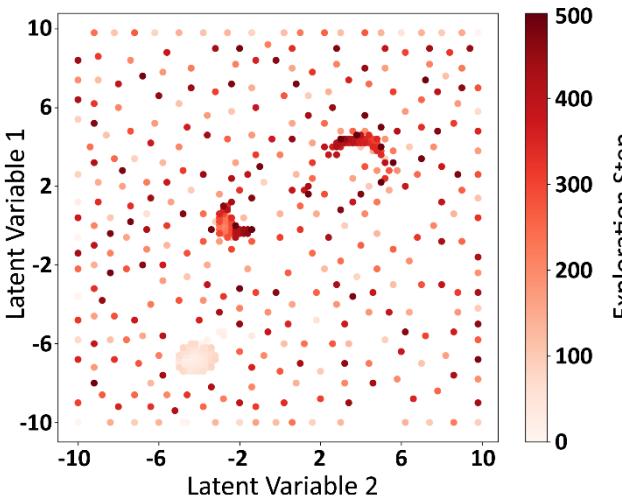
100 initial points



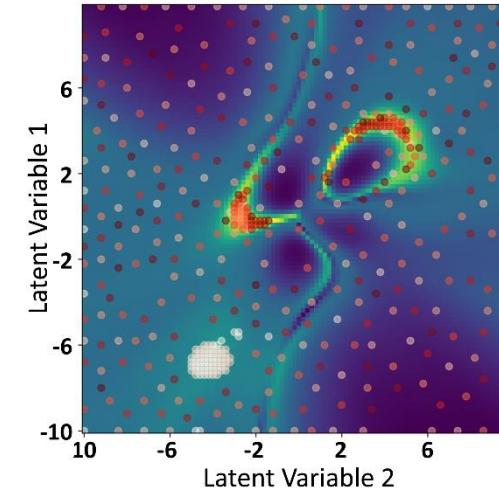
Reconstructed curl surface



Explored points

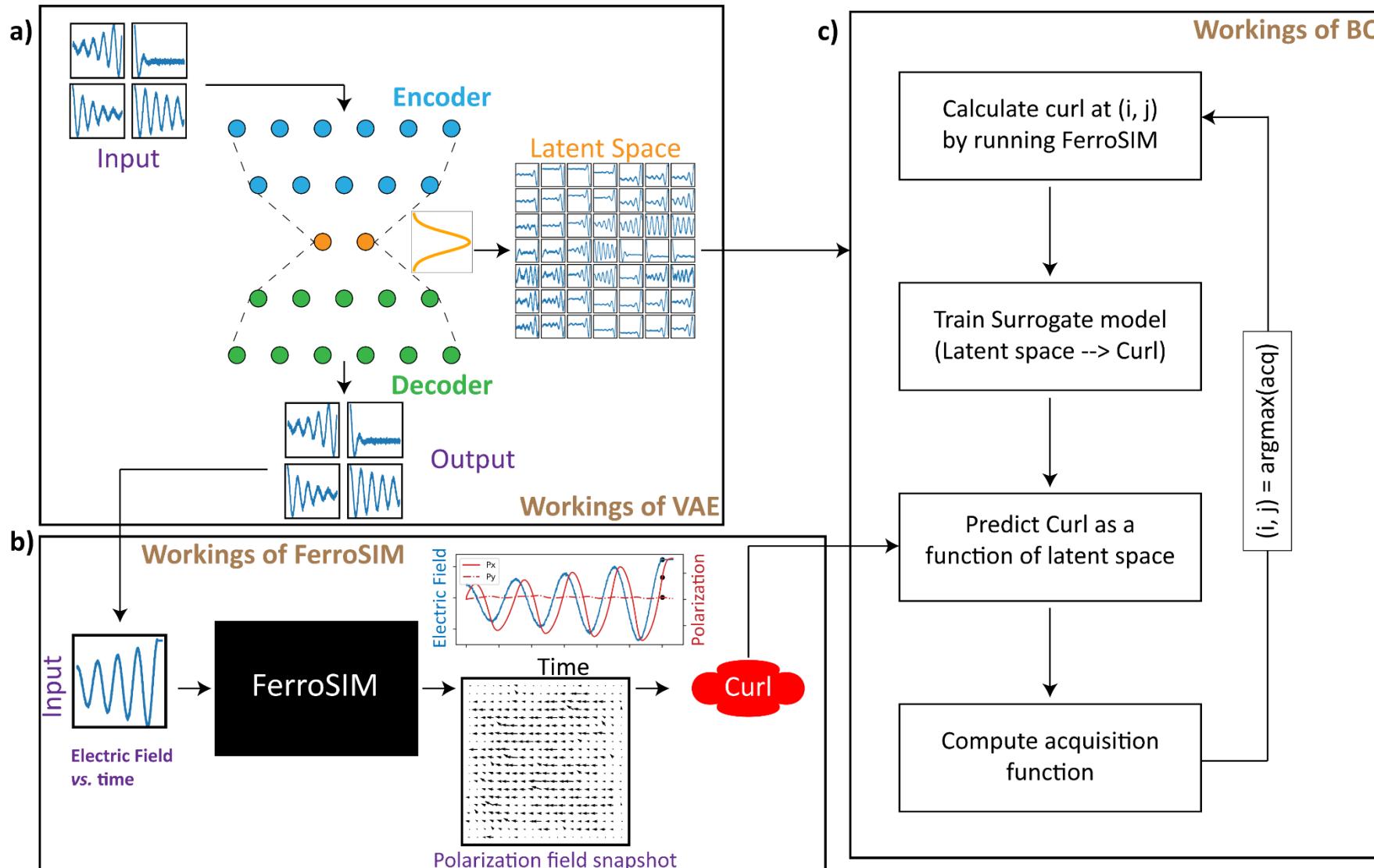


Original curl surface



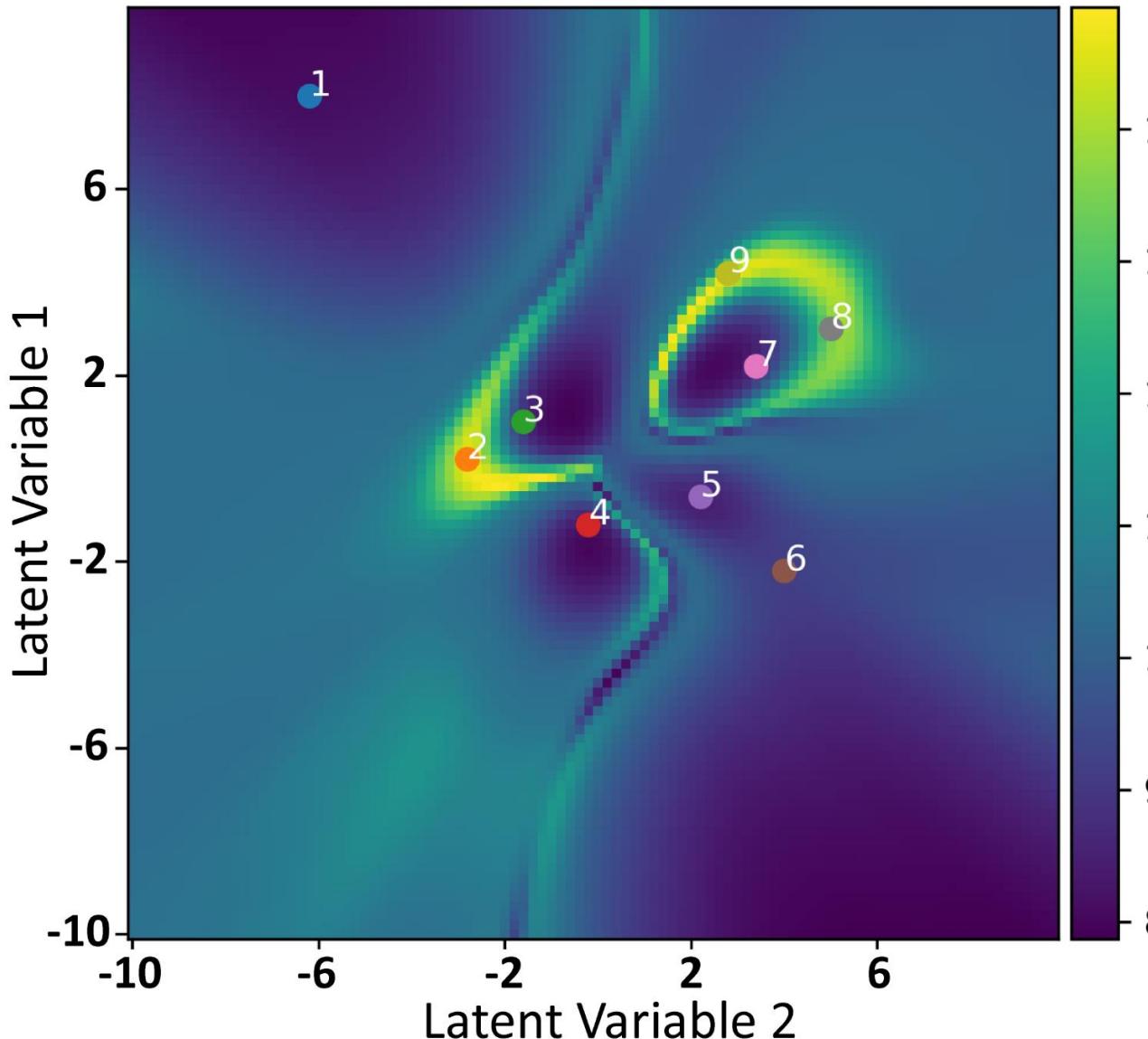
- 100 initialization points and the BO explored the latent space for the next 500 points
- Acq function: $\mu + 10\sigma$
- So, at the end BO only explored a total of 600 points out of 10,000 points the latent space is divided into
- Caveat: we had to tune the Acq with the ground truth data known

Putting everything together



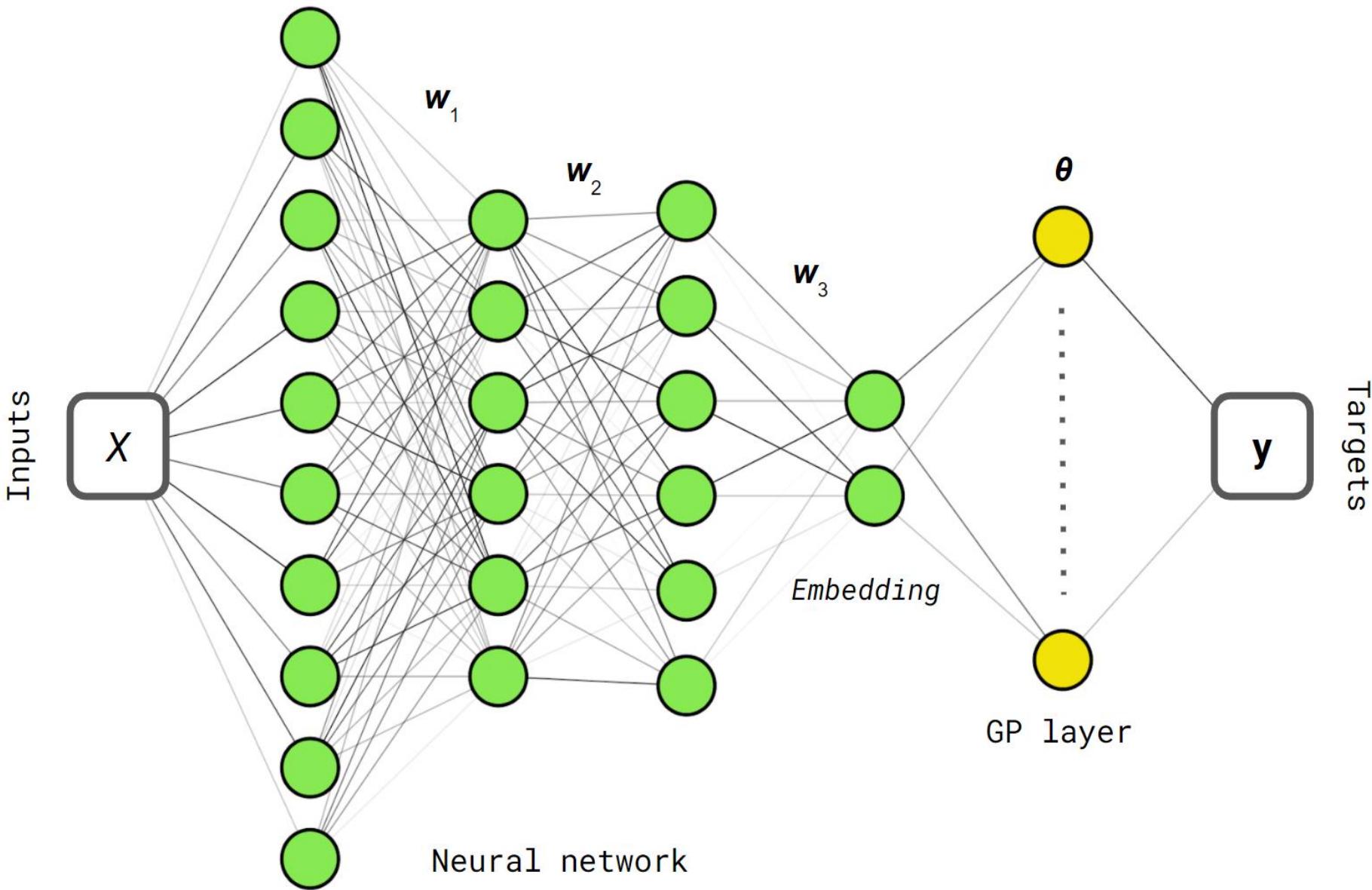
Same approaches are used for molecular discovery, polymers, and biomolecules

What determines success?

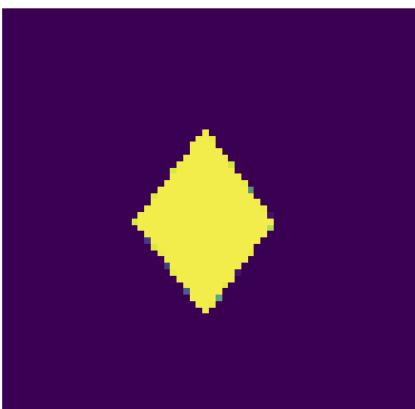
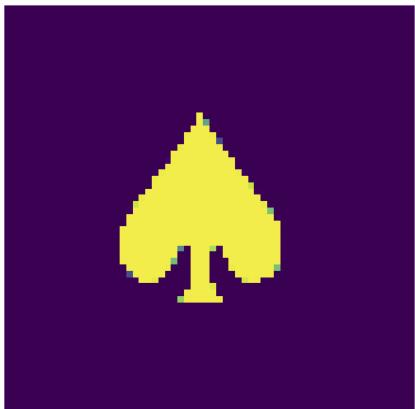
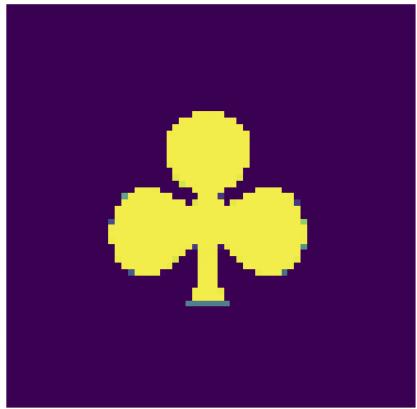


- The success of the BO in the latent space clearly depends on the shape on the manifold that points of interest form.
- For VAE, the shape of the manifold is determined by the properties of the data only, including
 - (a) how strong correlations in data reflect in correlation in properties and
 - (b) weight of the “good” trajectories

Deep Kernel Learning



Card data set



Rotations:
[-120°, 120°]
Shear:
[-20°, 20°]

