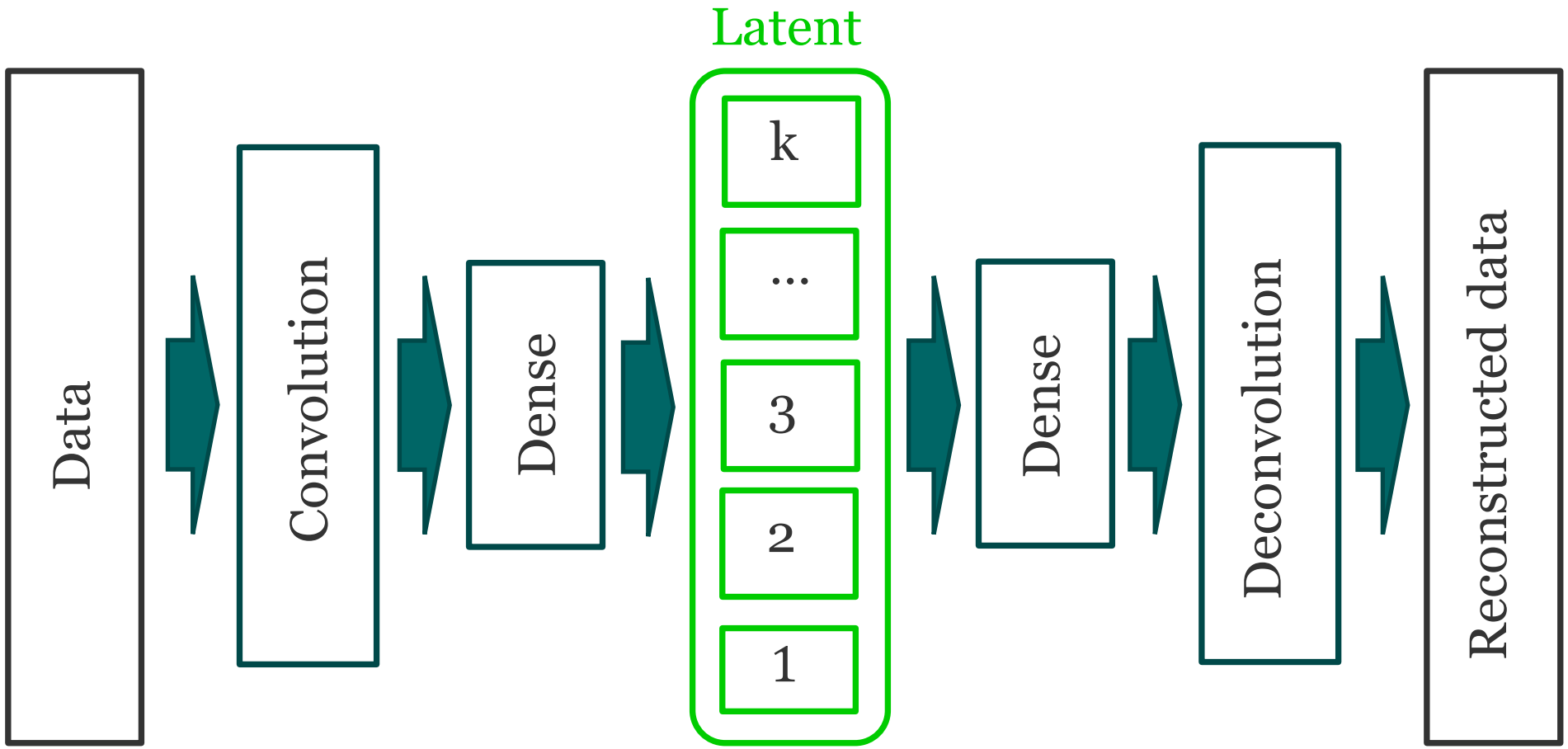
# Lecture 34: VAE Applications

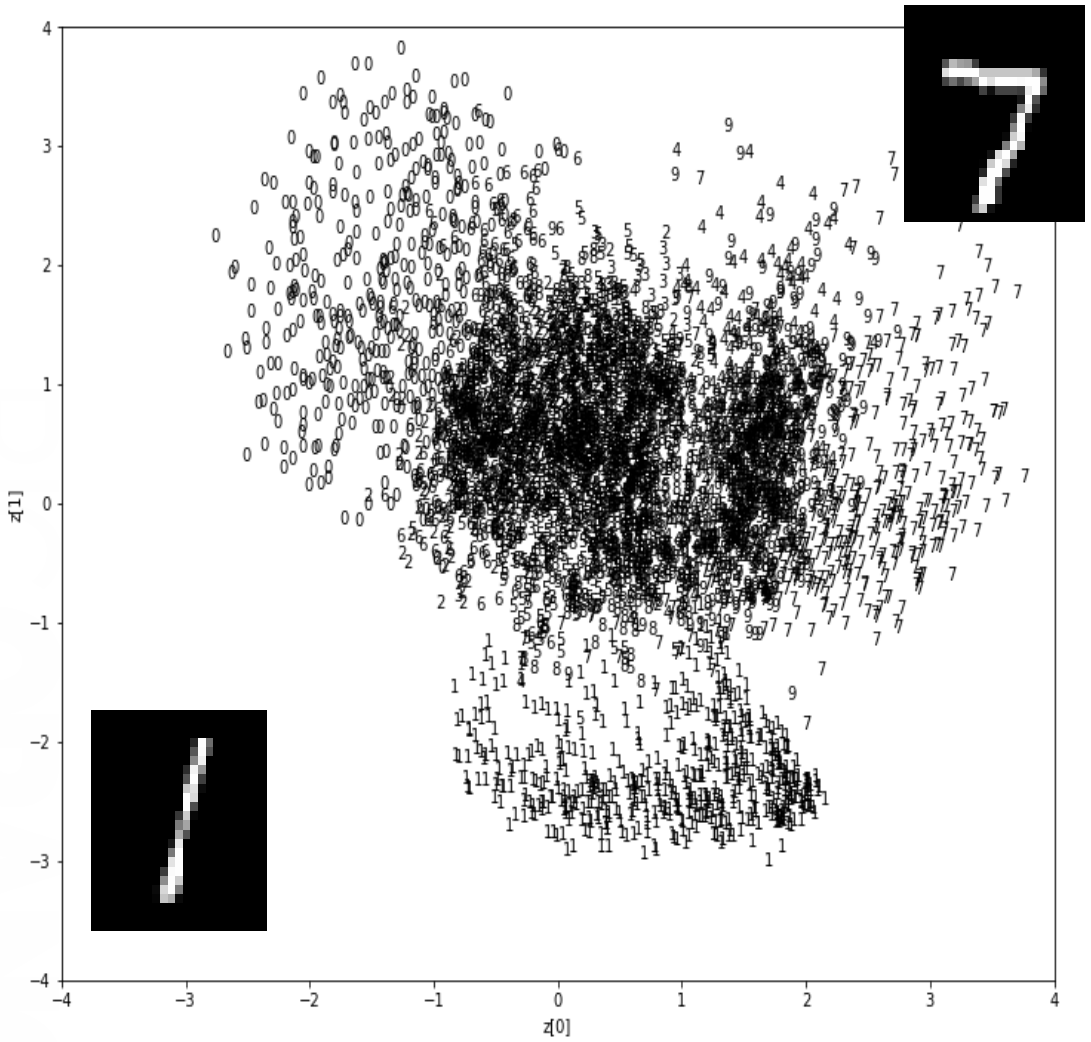
Instructor: Sergei V. Kalinin

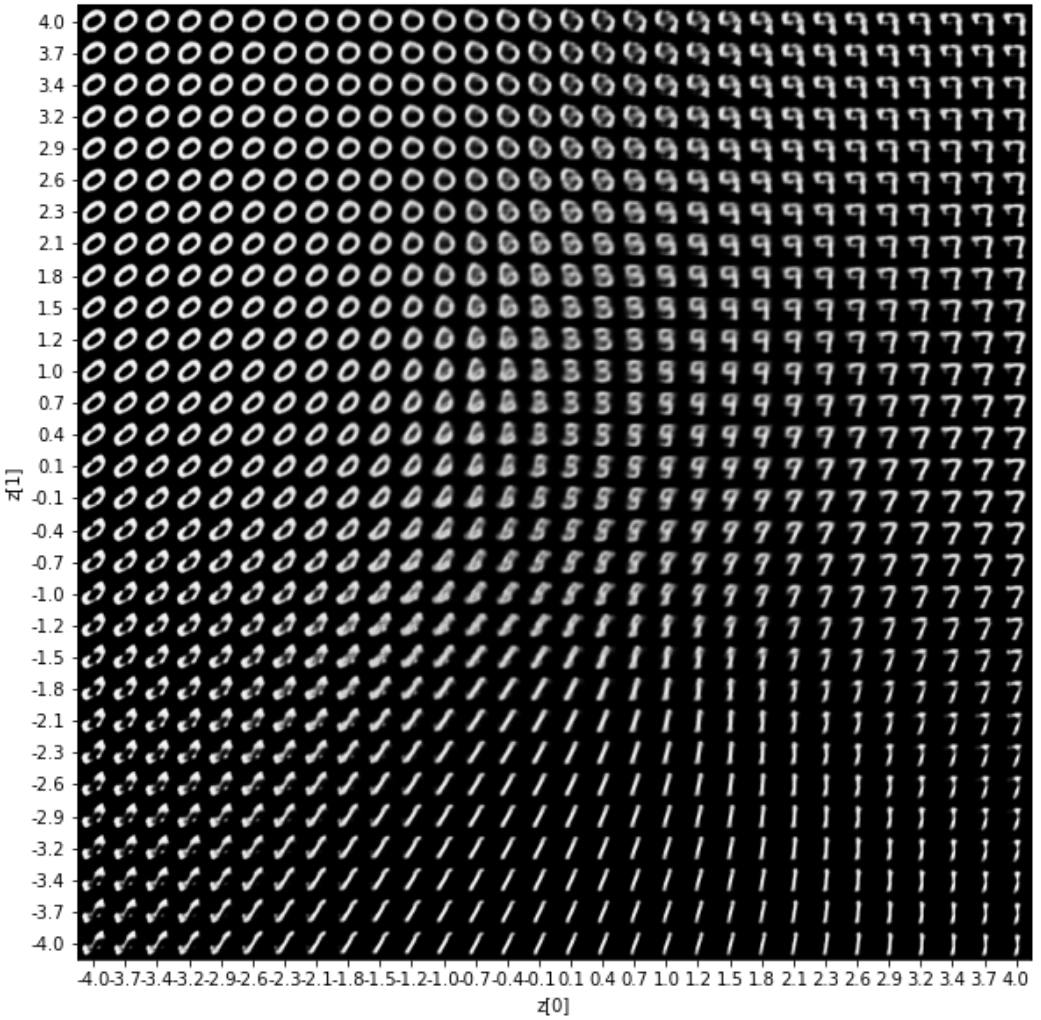
# Autoencoders




**Loss:** reconstruction loss

# Encoding, Decoding, and Latent Space

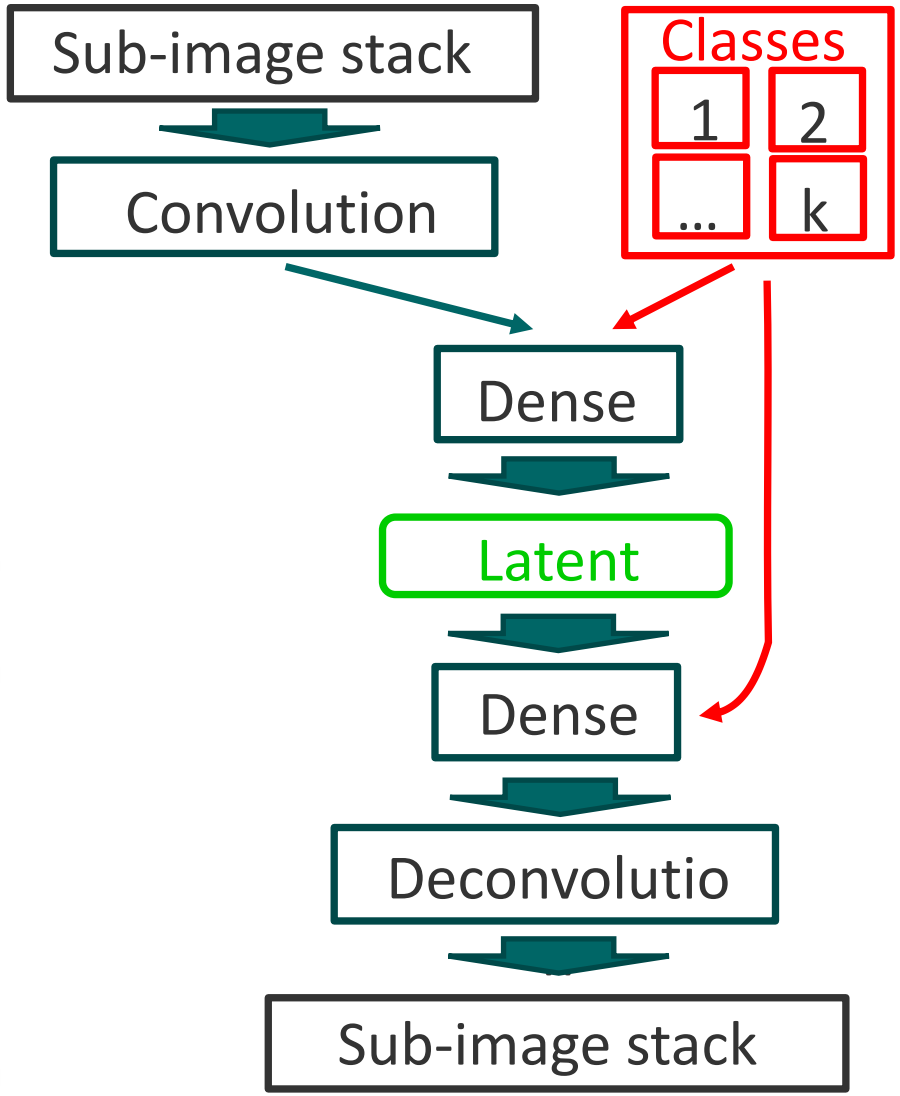


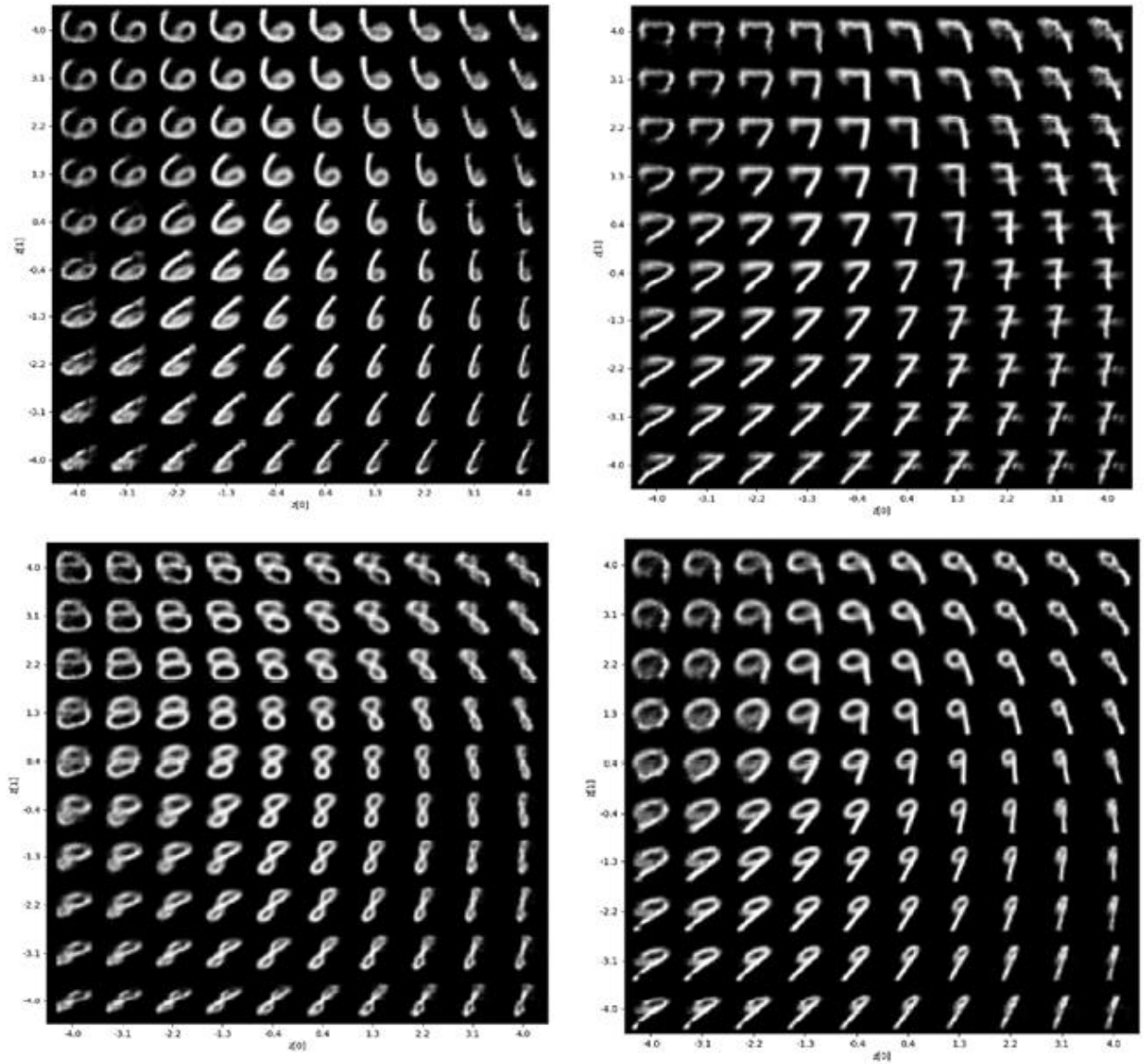




**Latent distribution:** Encoding the data via low dimensional vector

**Latent representation:** Decoding images from uniform grid in latent space

# Conditional VAE



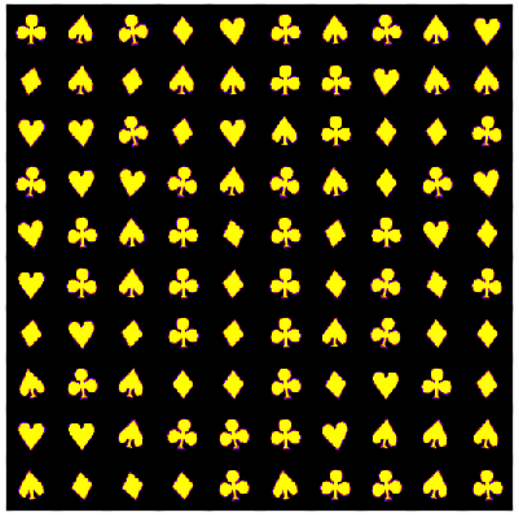
Note the trends in the latent representation for each digit: disentanglement of the representations

# VAE on Cards

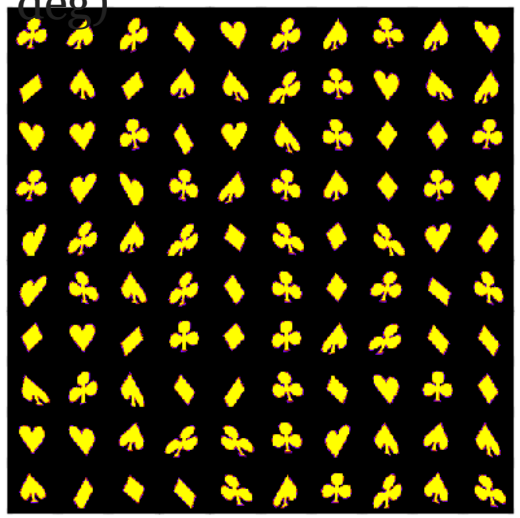
Introduce the **cards** data set:

- Classical 4 hands (diamonds, clubs, pikes, hearts)
- Interesting similarities (pikes and hearts)
- And invariances on affine transforms (e.g. diamonds)

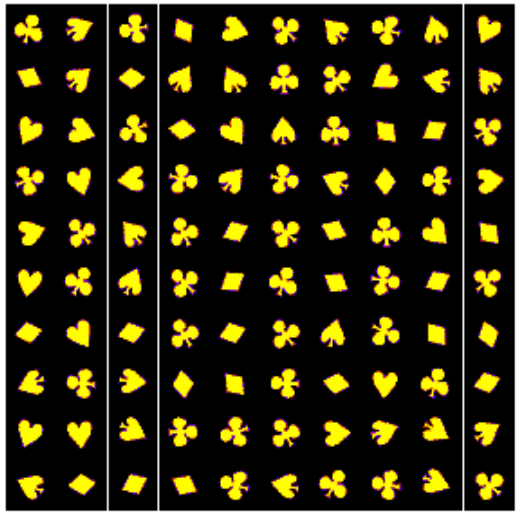
**Cards 1:** Low R (12 deg) and low S (1 deg)



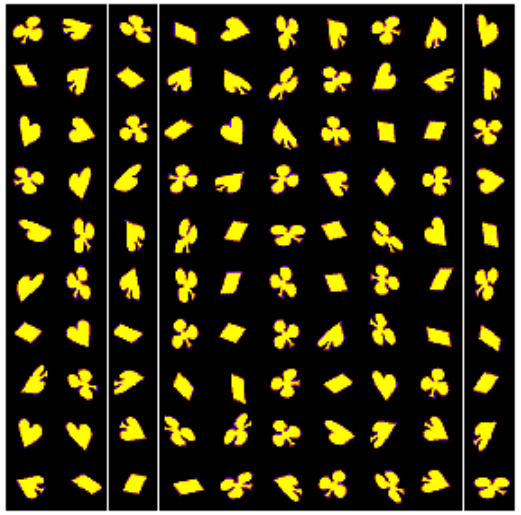
**Cards 2:** Low R (12 deg) and high S (20 deg)



**Cards 3:** High R (120 deg) and Low S (1 deg)



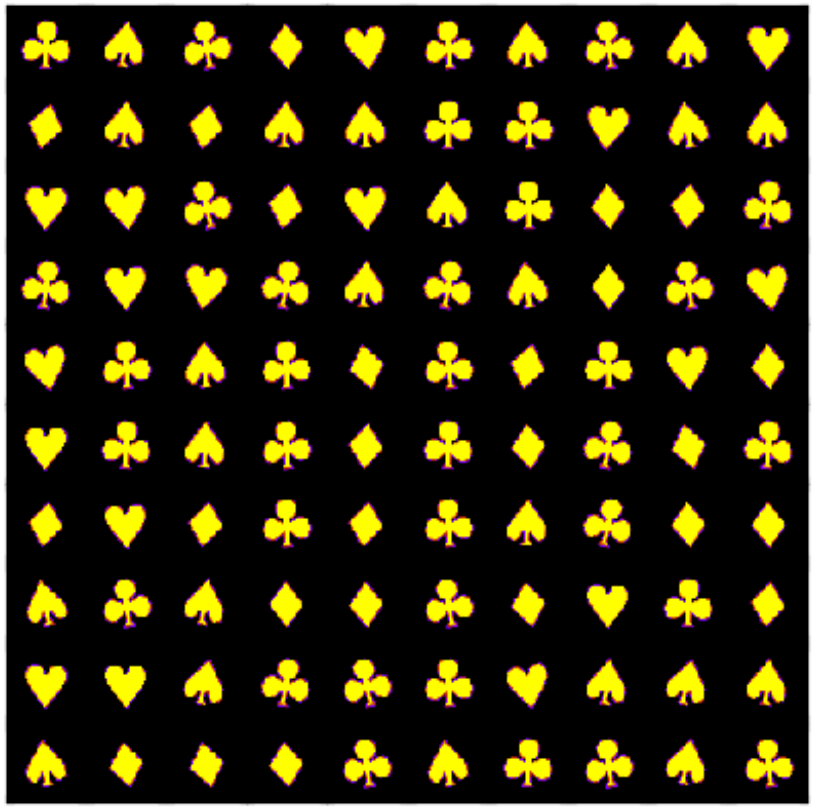
**Cards 4:** High R (120 deg) and high S (20 deg)



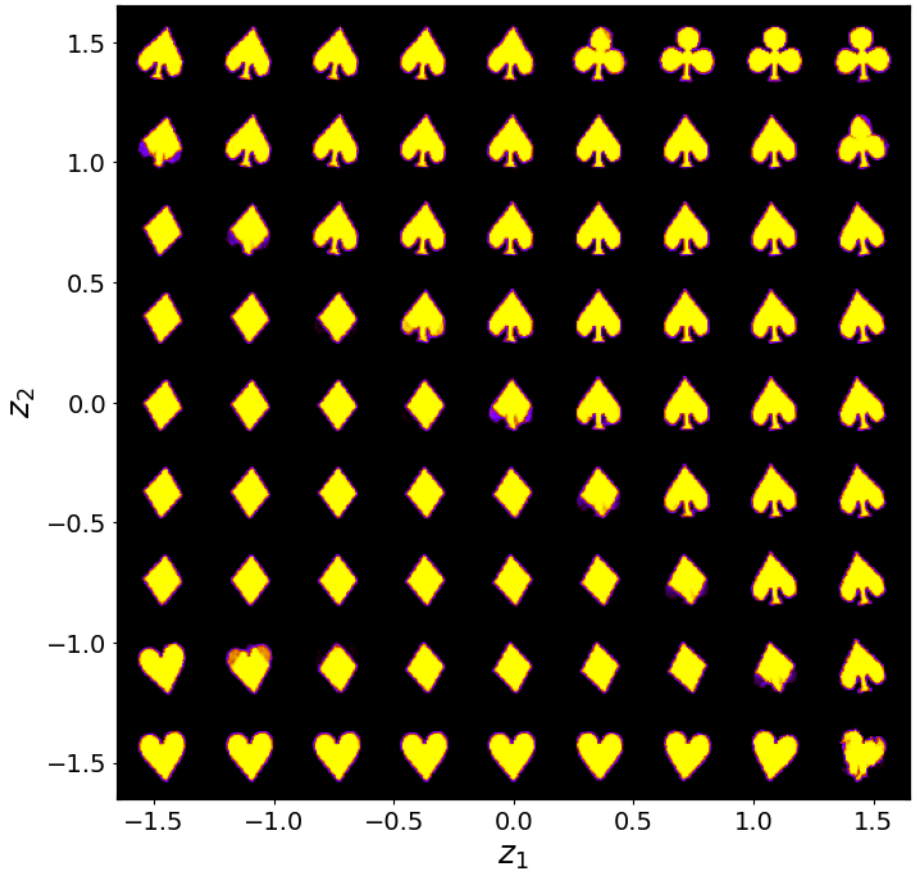
- Shear, rotations, and translations are **known** factors of variability (or traits) in data
- Can VAE disentangle representations and discover these factors of variability

# VAE on Cards

**Example of data**

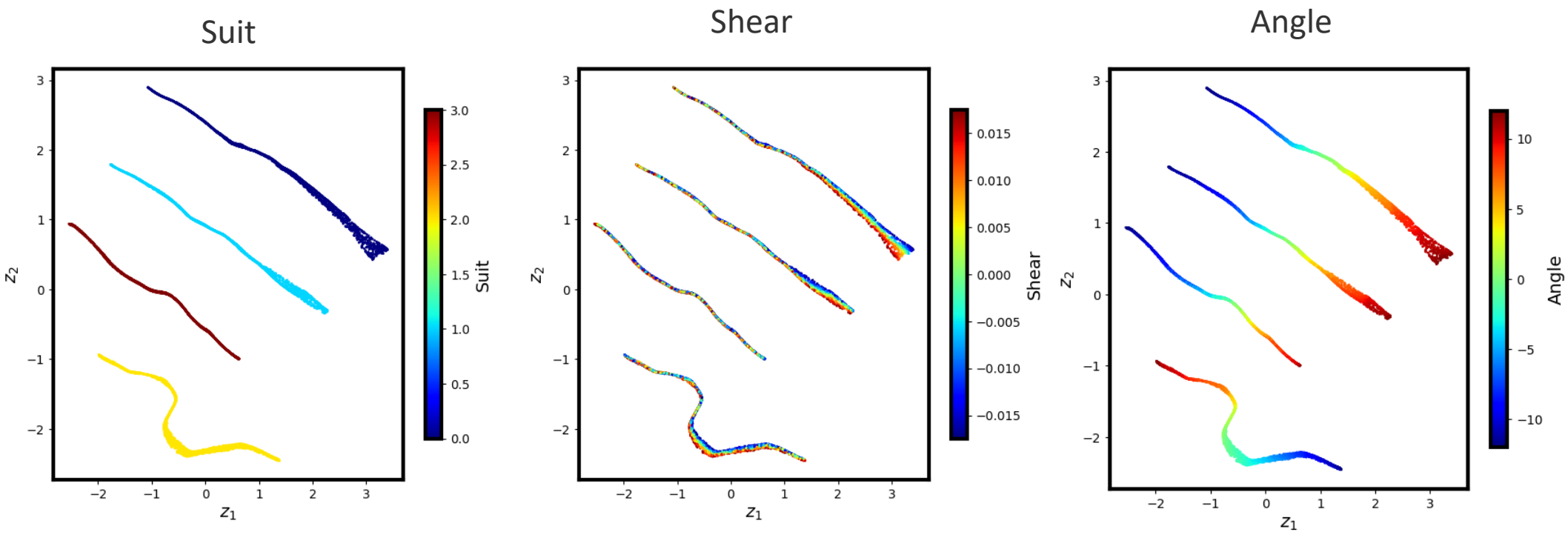


**Latent representation**




**Cards 1:** Low rotation (12 deg) and low shear (1 deg)

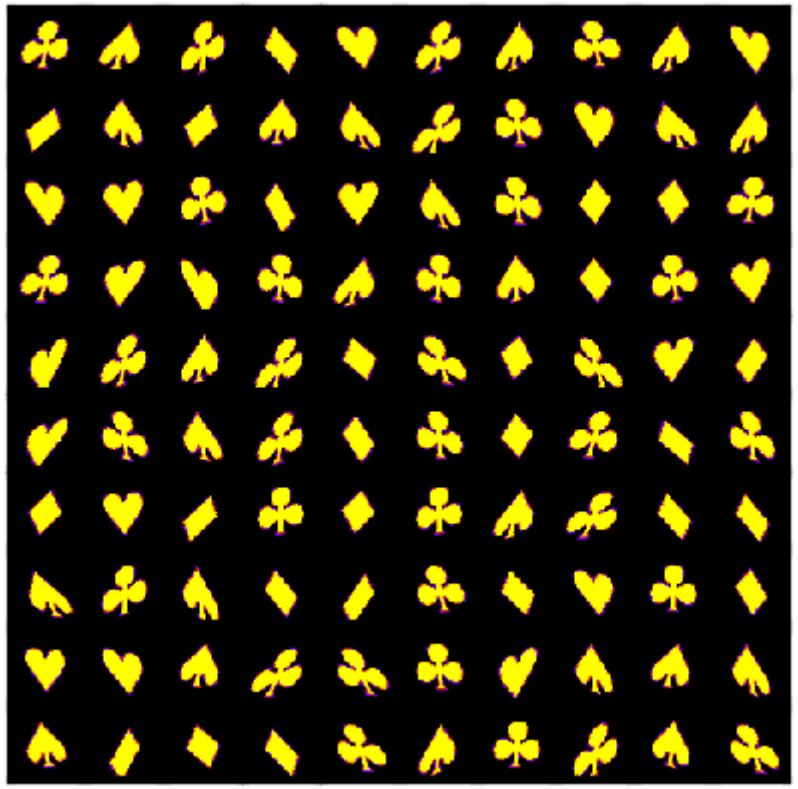
# VAE on Cards



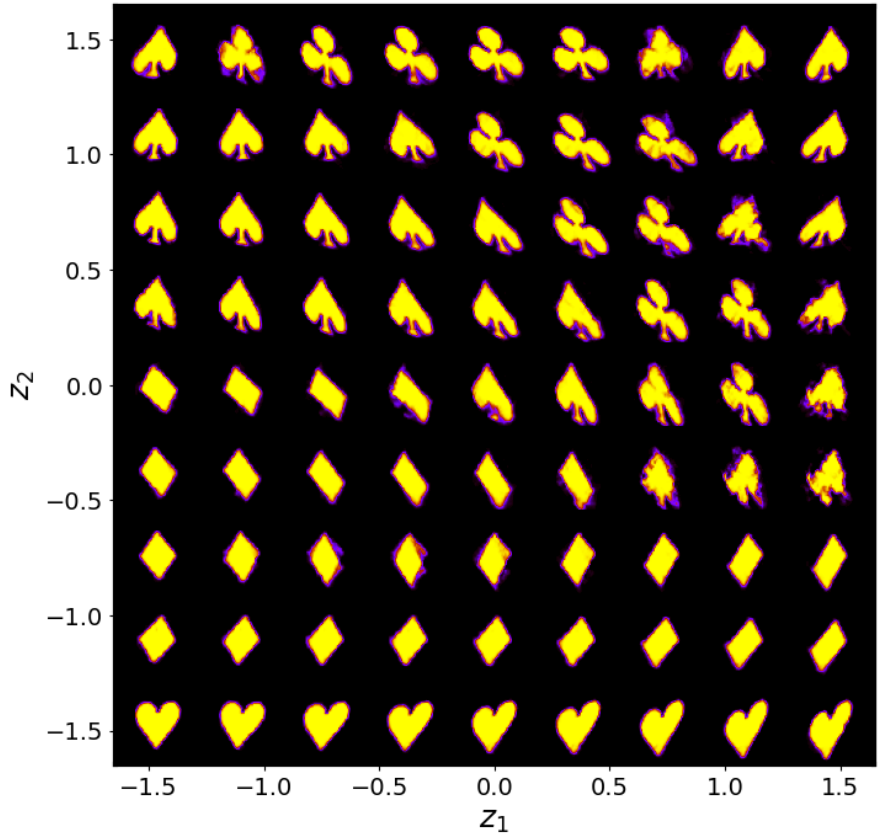

**Cards 1:** Low rotation (12 deg) and low shear (1 deg)

# VAE on Cards

**Example of data**

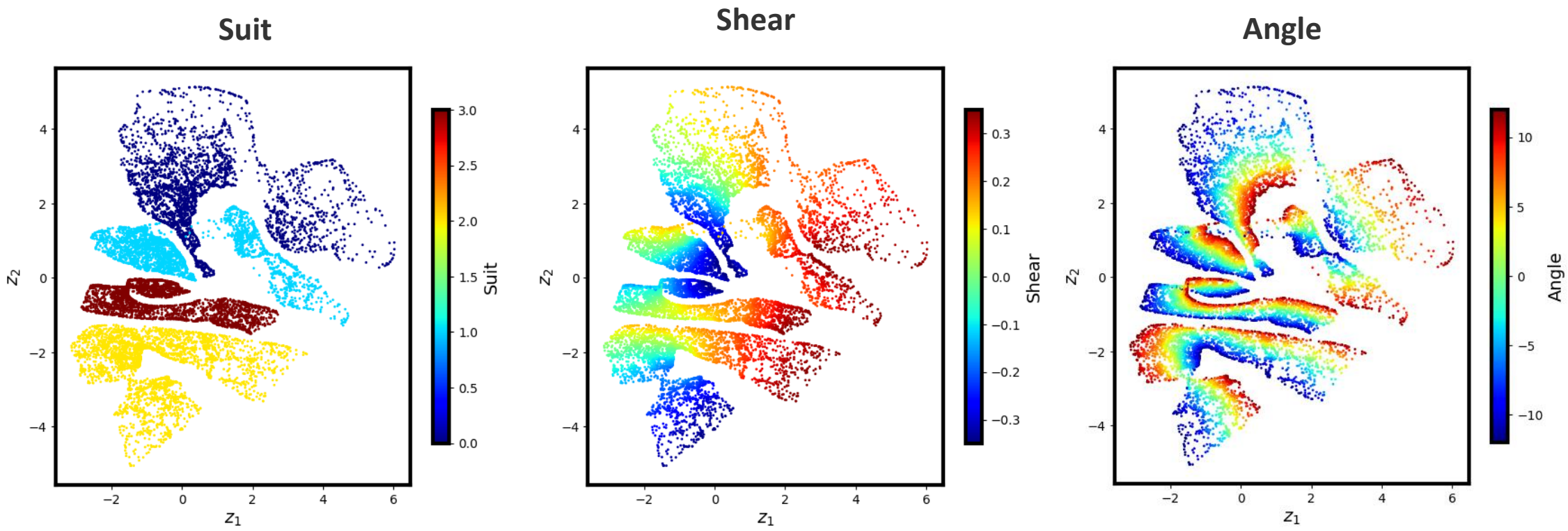


**Latent representation**




**Cards 2:** Low rotation (12 deg) and high shear (20 deg)

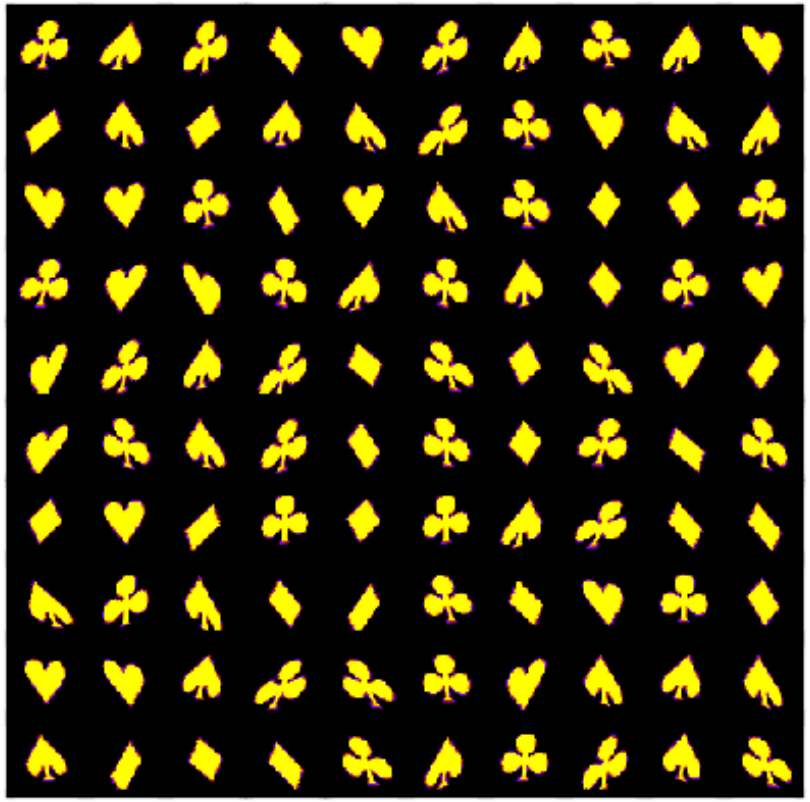
# VAE on Cards



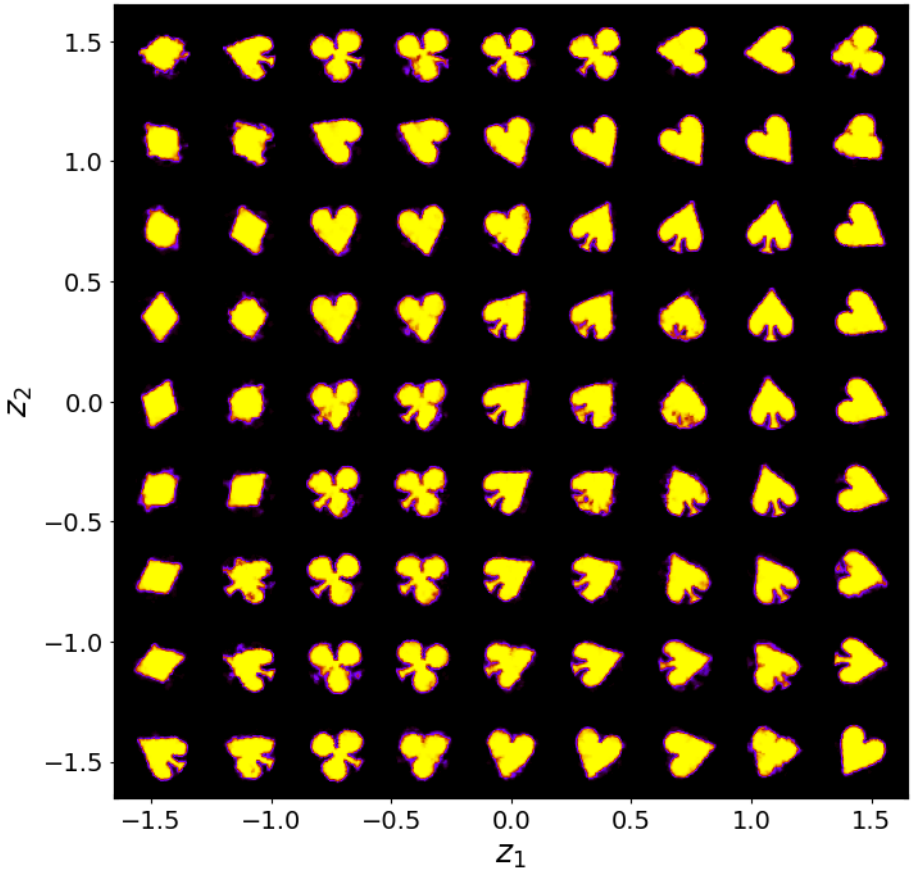

**Cards 2:** Low rotation (12 deg) and high shear (20 deg)

# VAE on Cards

**Example of data**

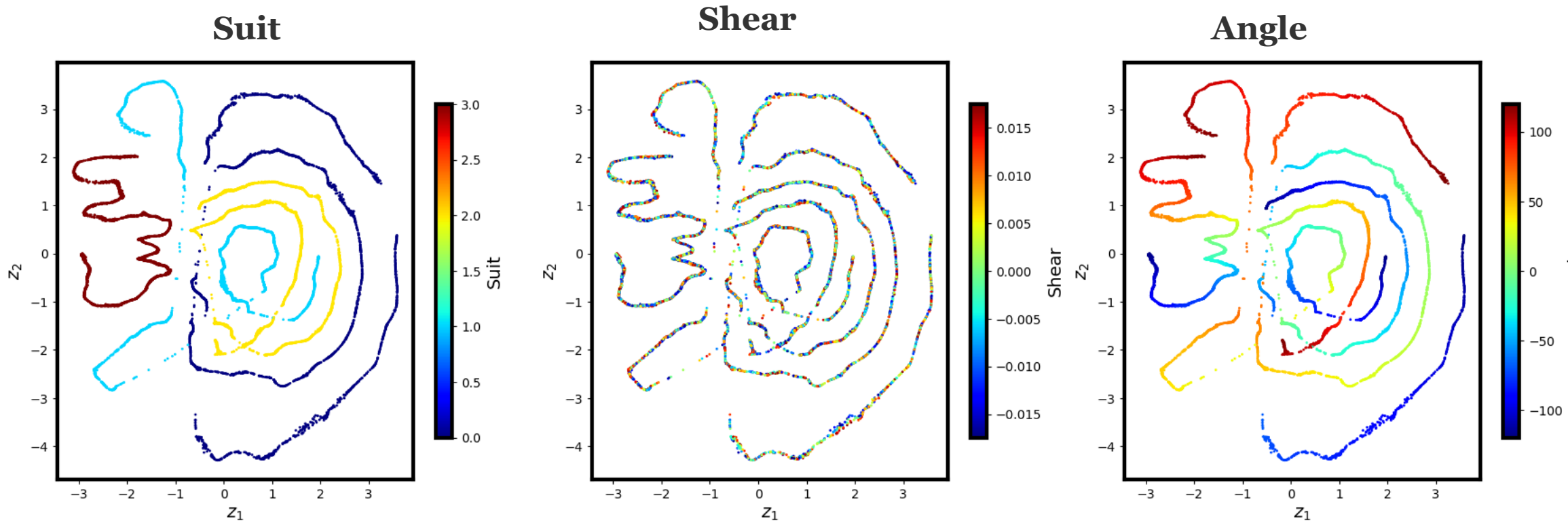


**Latent representation**




**Cards 3:** High rotation (120 deg) and low shear (1 deg)

# VAE on Cards

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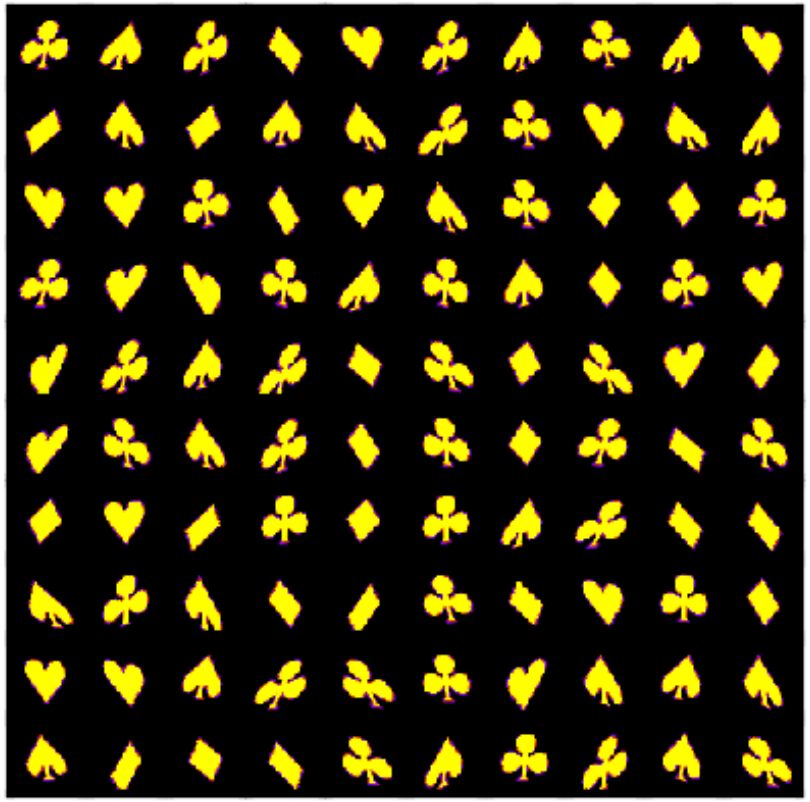
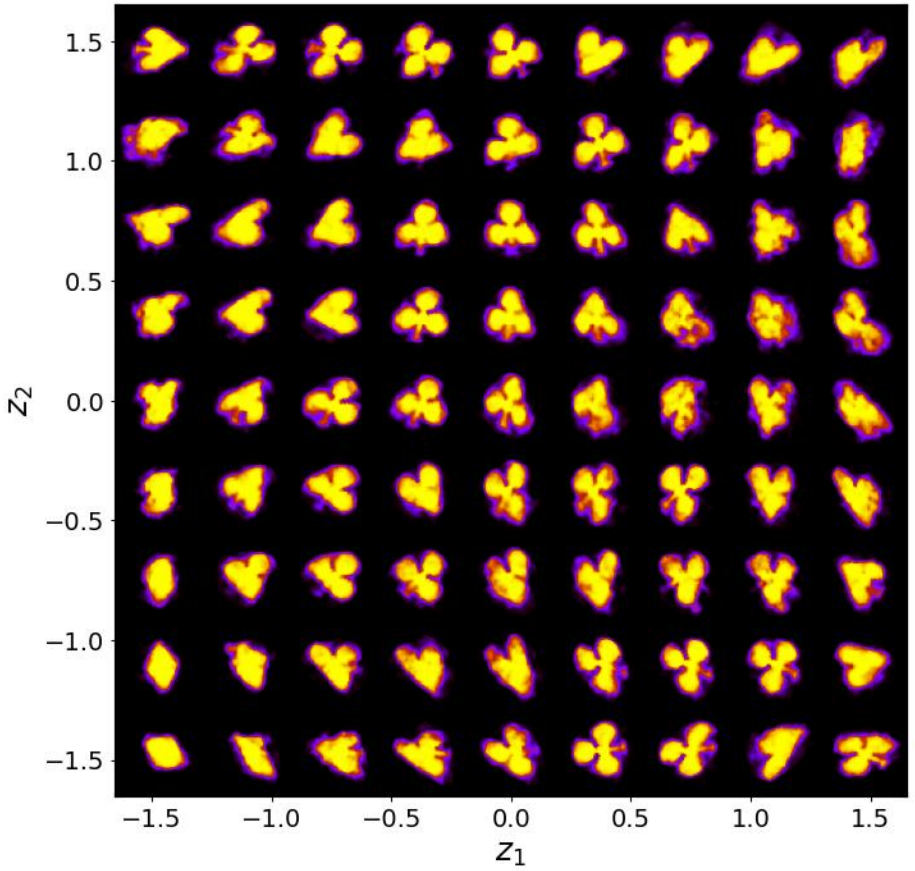
# VAE on Cards

**Example of data**

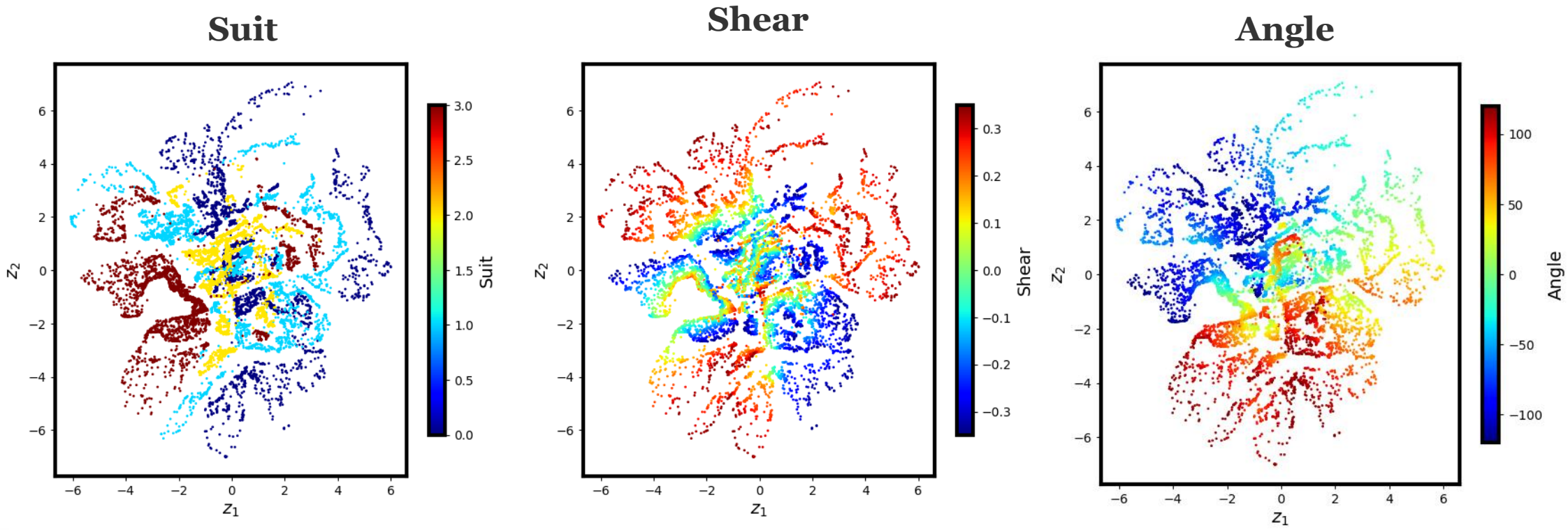


**Latent representation**




**Cards 4:** High rotation (120 deg) and high shear (20 deg)

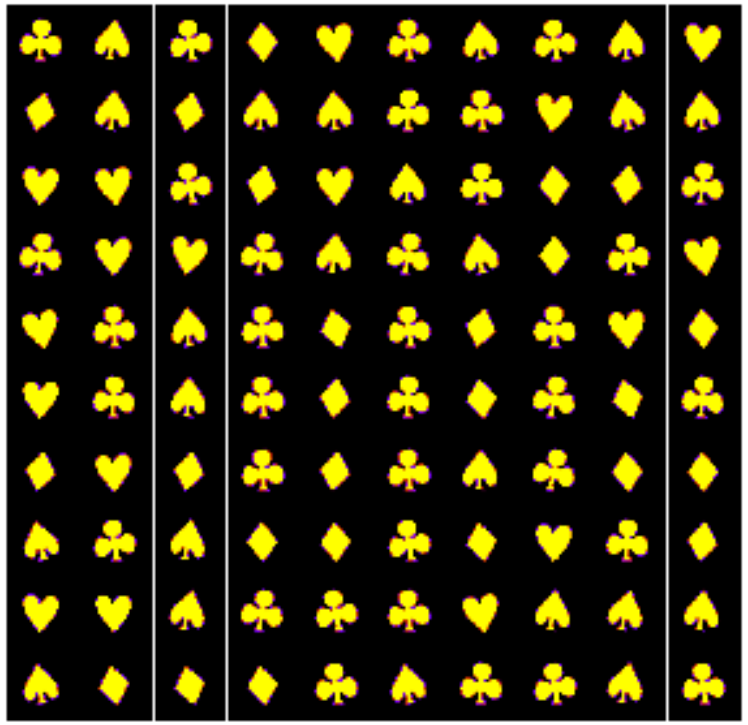
# VAE on Cards



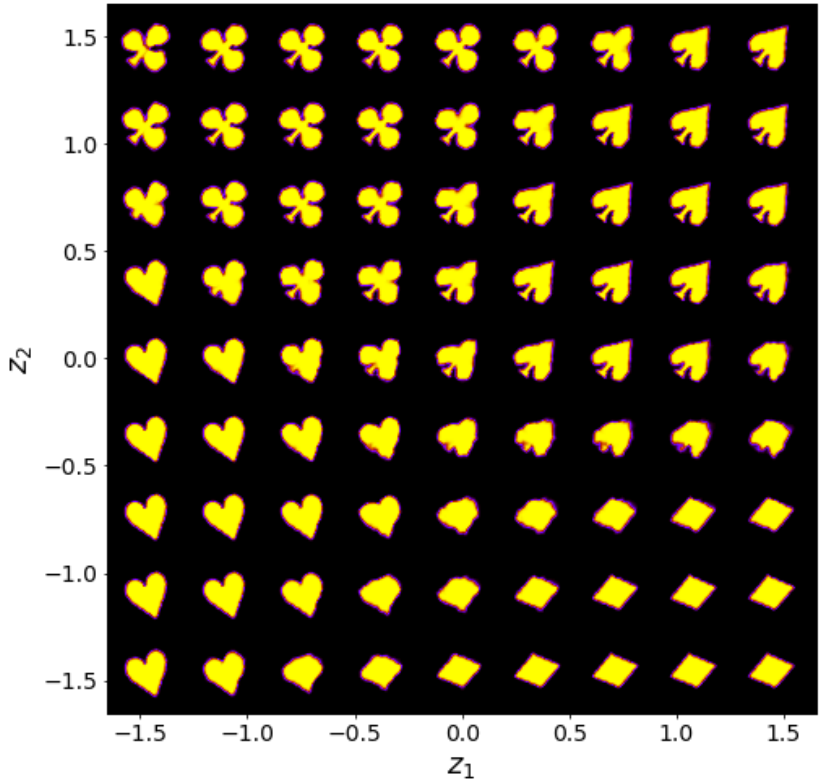

**Cards 4:** High rotation (120 deg) and high shear (20 deg)

# rVAE on Cards

**Example of data**

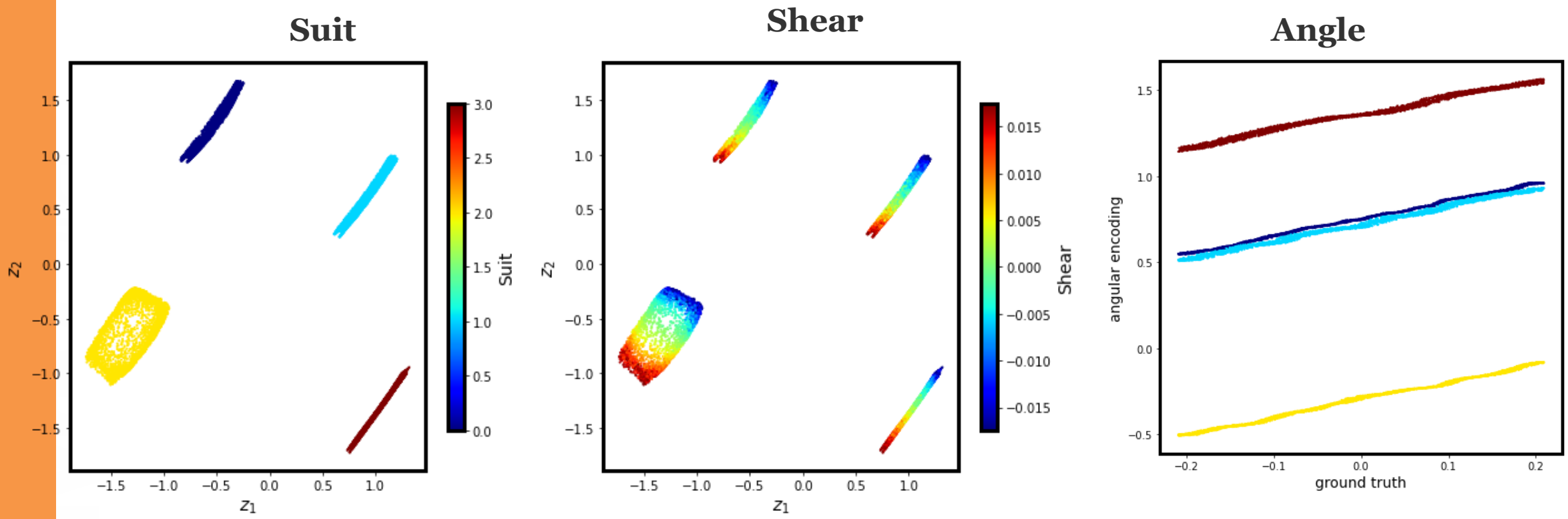


**Latent representation**




**Cards 1:** Low rotation (12 deg) and low shear (1 deg)

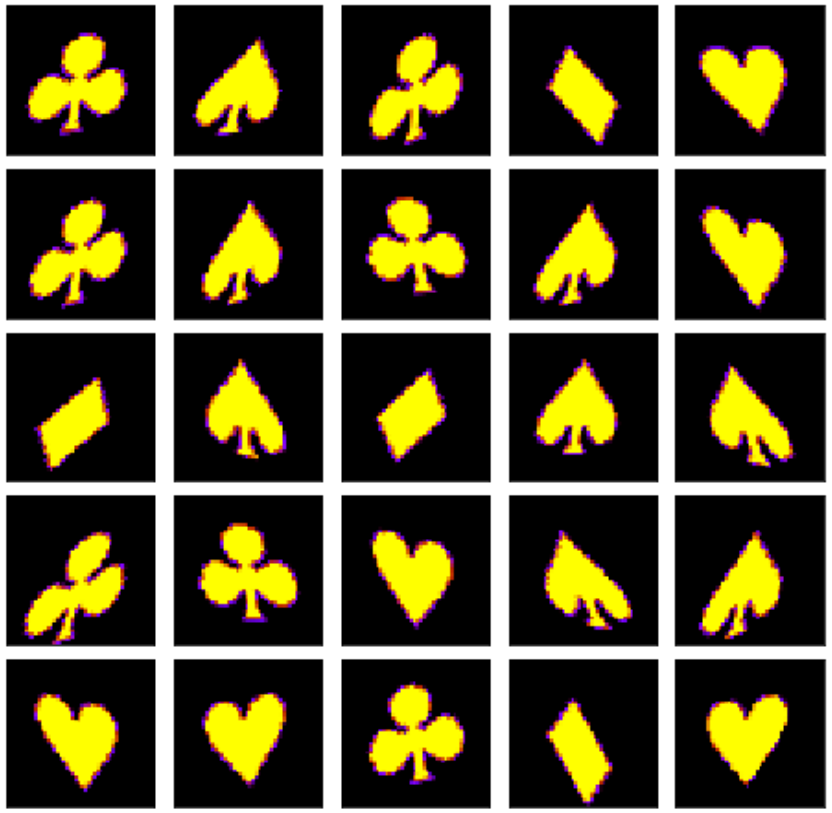
# rVAE on Cards



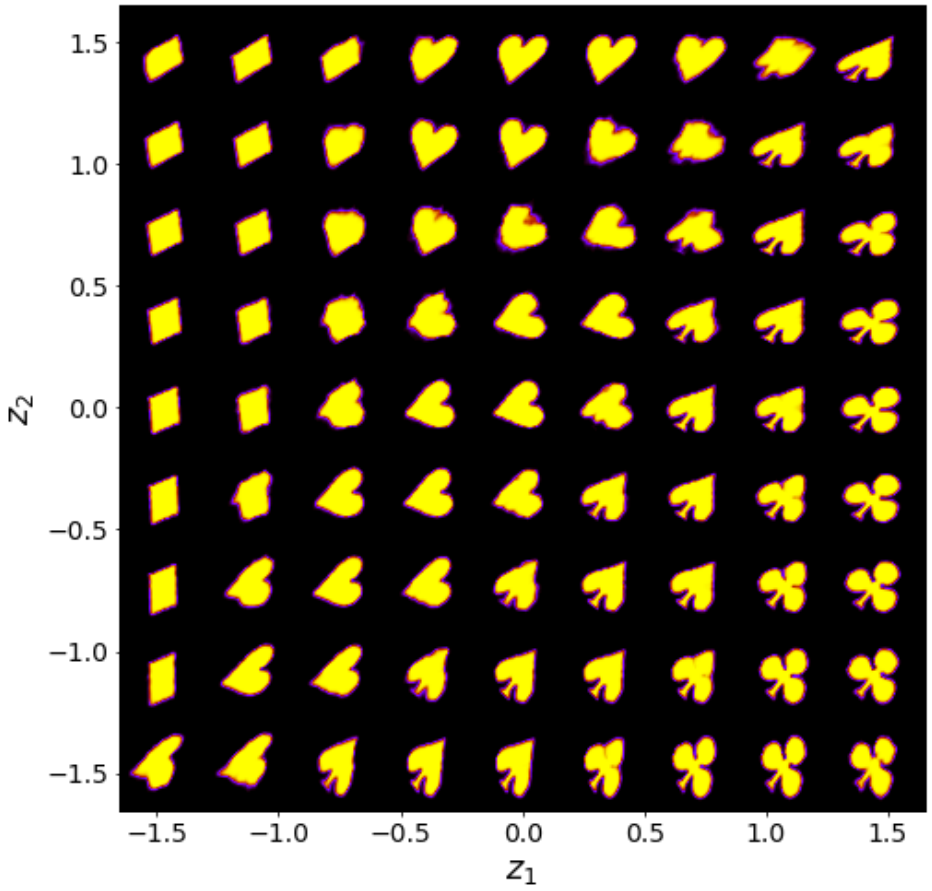

**Cards 1:** Low rotation (12 deg) and low shear (1 deg)

# rVAE on Cards

**Example of data**

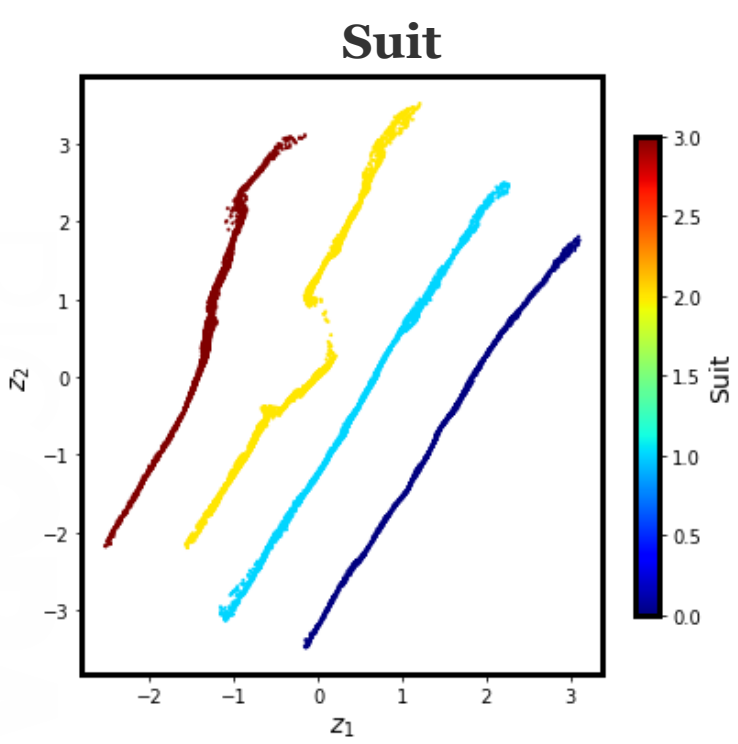


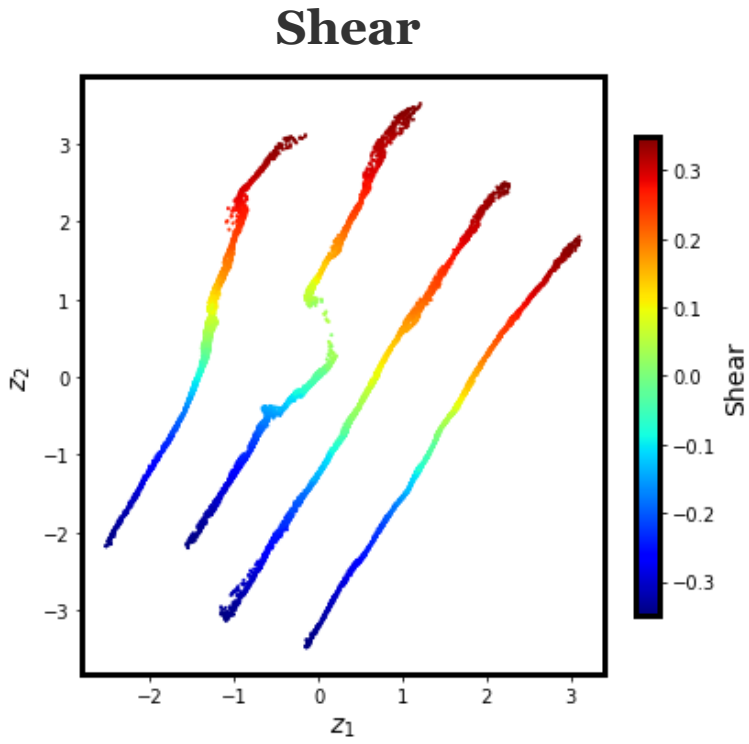
**Latent representation**

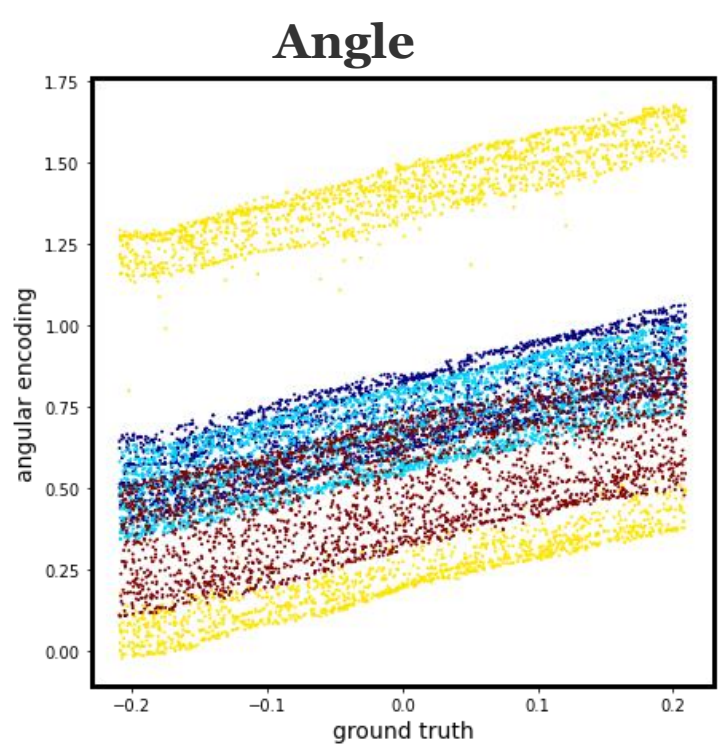



**Cards 2:** Low rotation (12 deg) and high shear (20 deg)

# rVAE on Cards

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# rVAE on Cards

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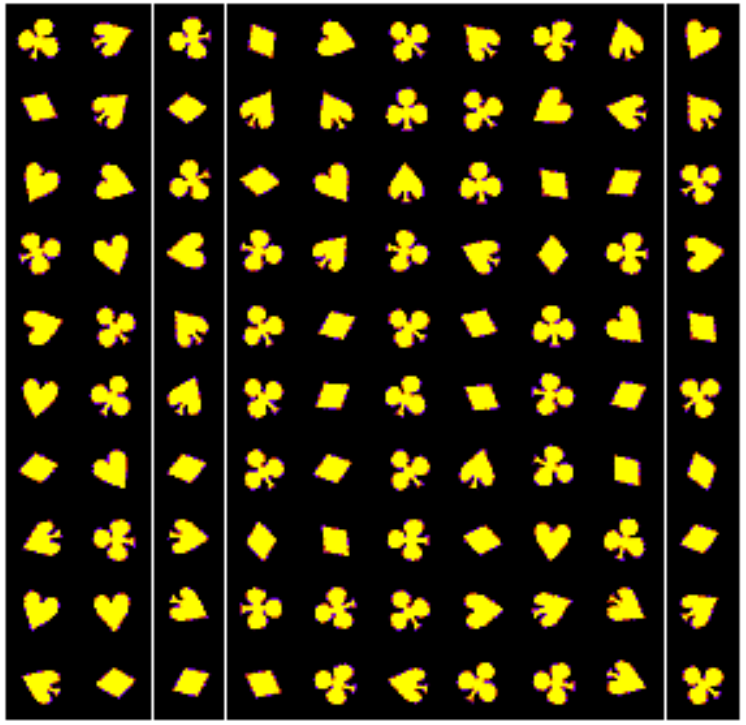
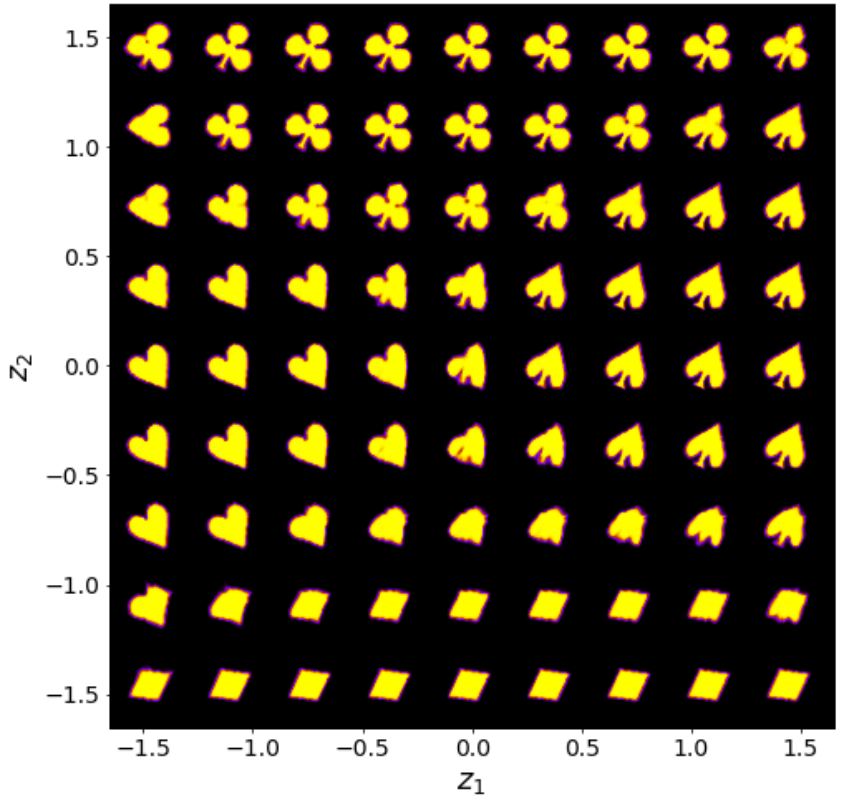
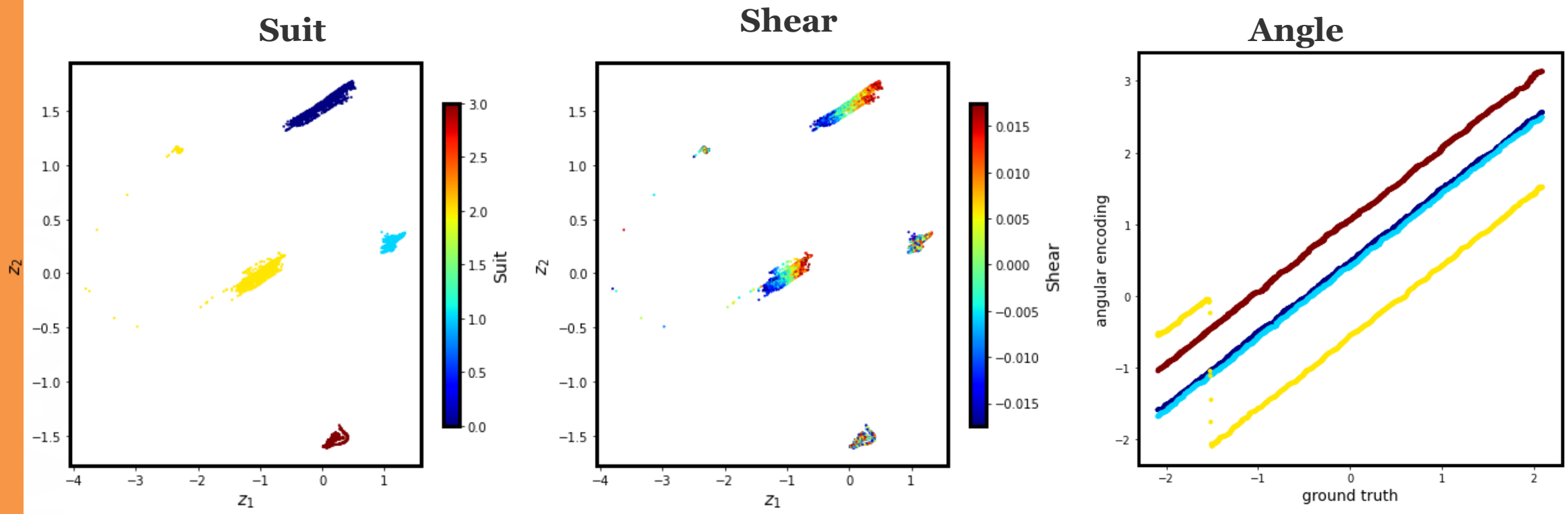


**Latent representation**




**Cards 3:** High rotation (120 deg) and low shear (1 deg)

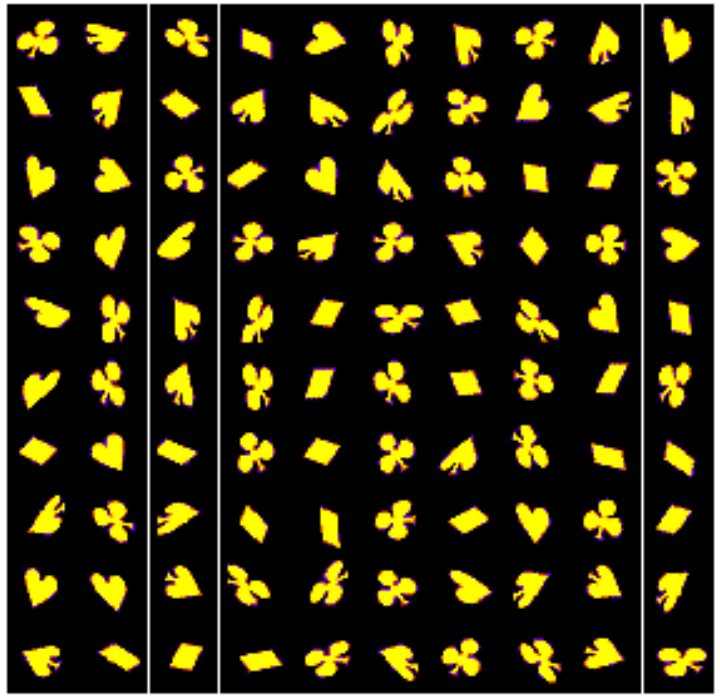
# rVAE on Cards



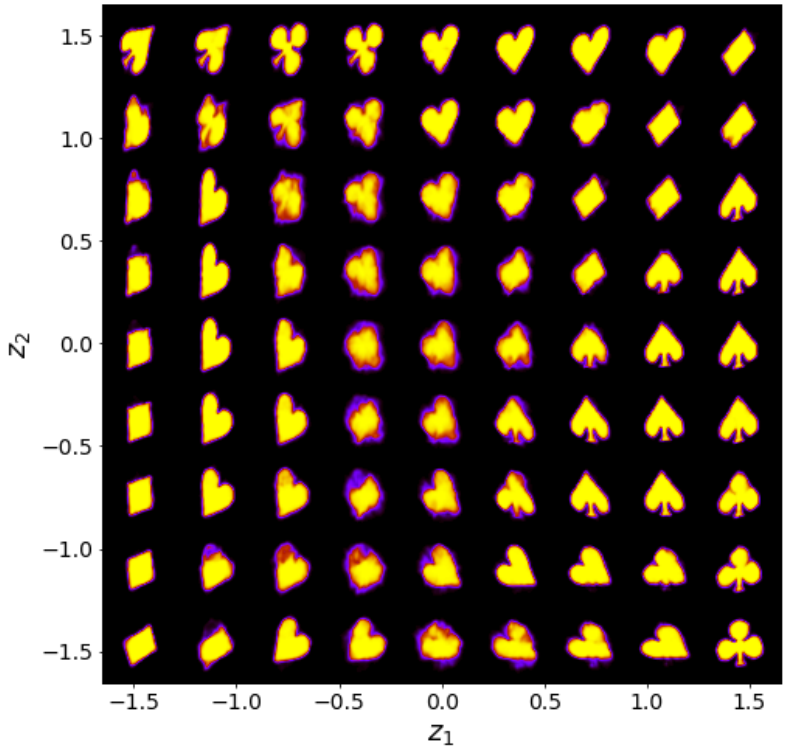

**Cards 3:** High rotation (120 deg) and low shear (1 deg)

# rVAE on Cards

**Example of data**

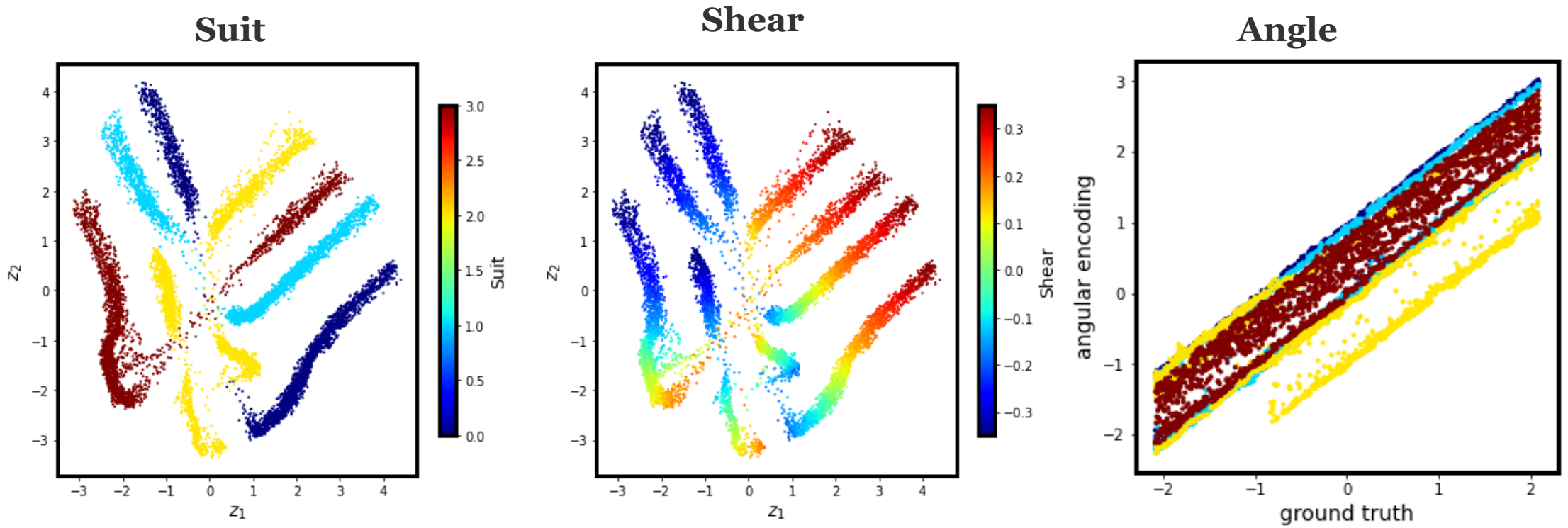


**Latent representation**




**Cards 4:** High rotation (120 deg) and high shear (20 deg)

# rVAE on Cards

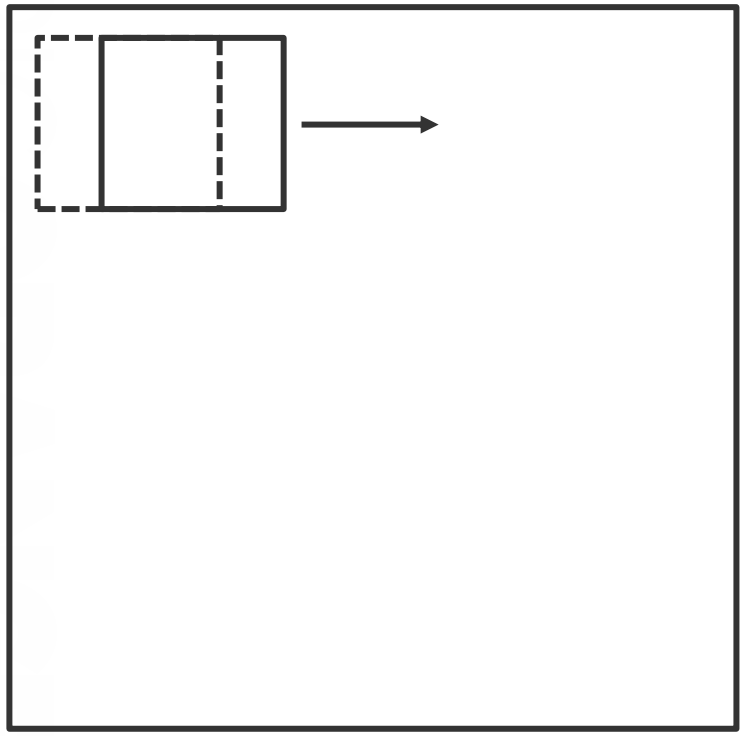



**Cards 4:** High rotation (120 deg) and high shear (20 deg)

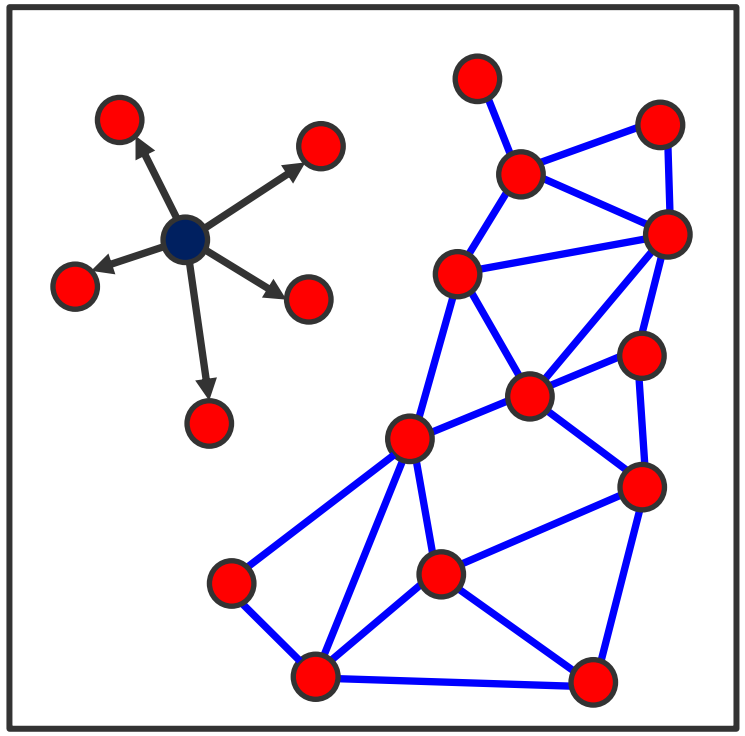
# Describing the building blocks

- The classical physical descriptions (symmetry, etc) can be defined locally only in Bayesian sens
- We can argue that local descriptors are simple, if not necessarily known
- And the rules that guide their emergence are also simple, if not known

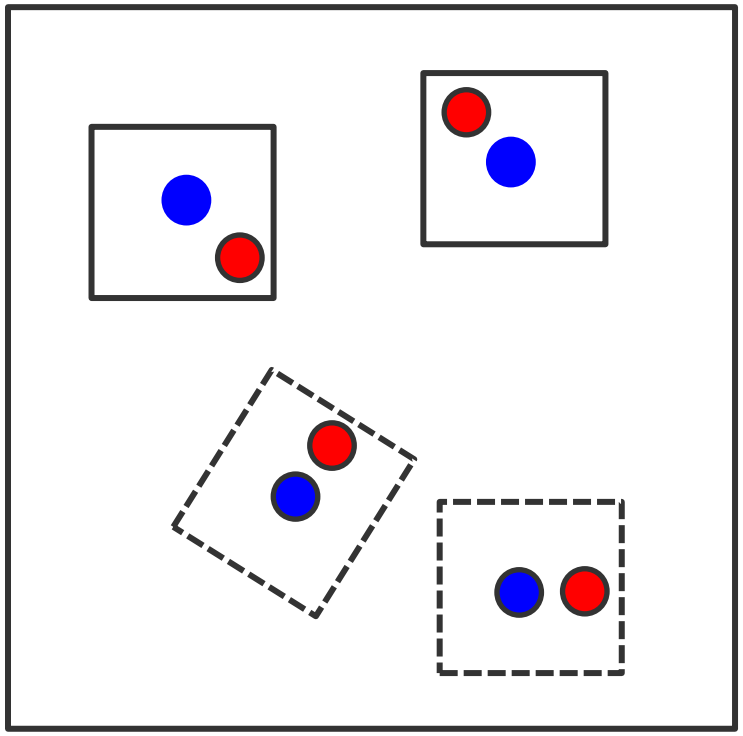
**Continuous translational symmetry**



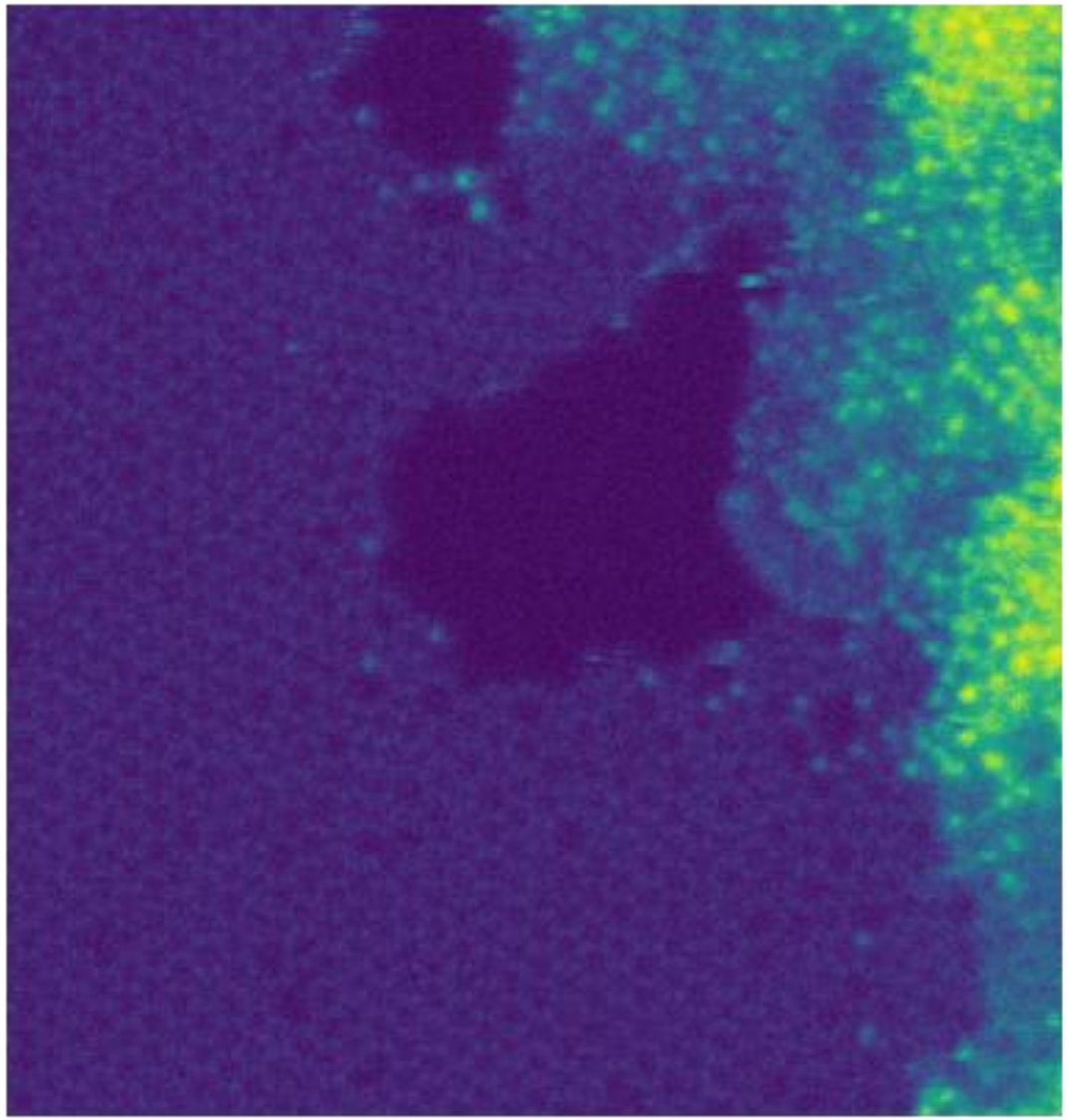
**Atom based descriptions**

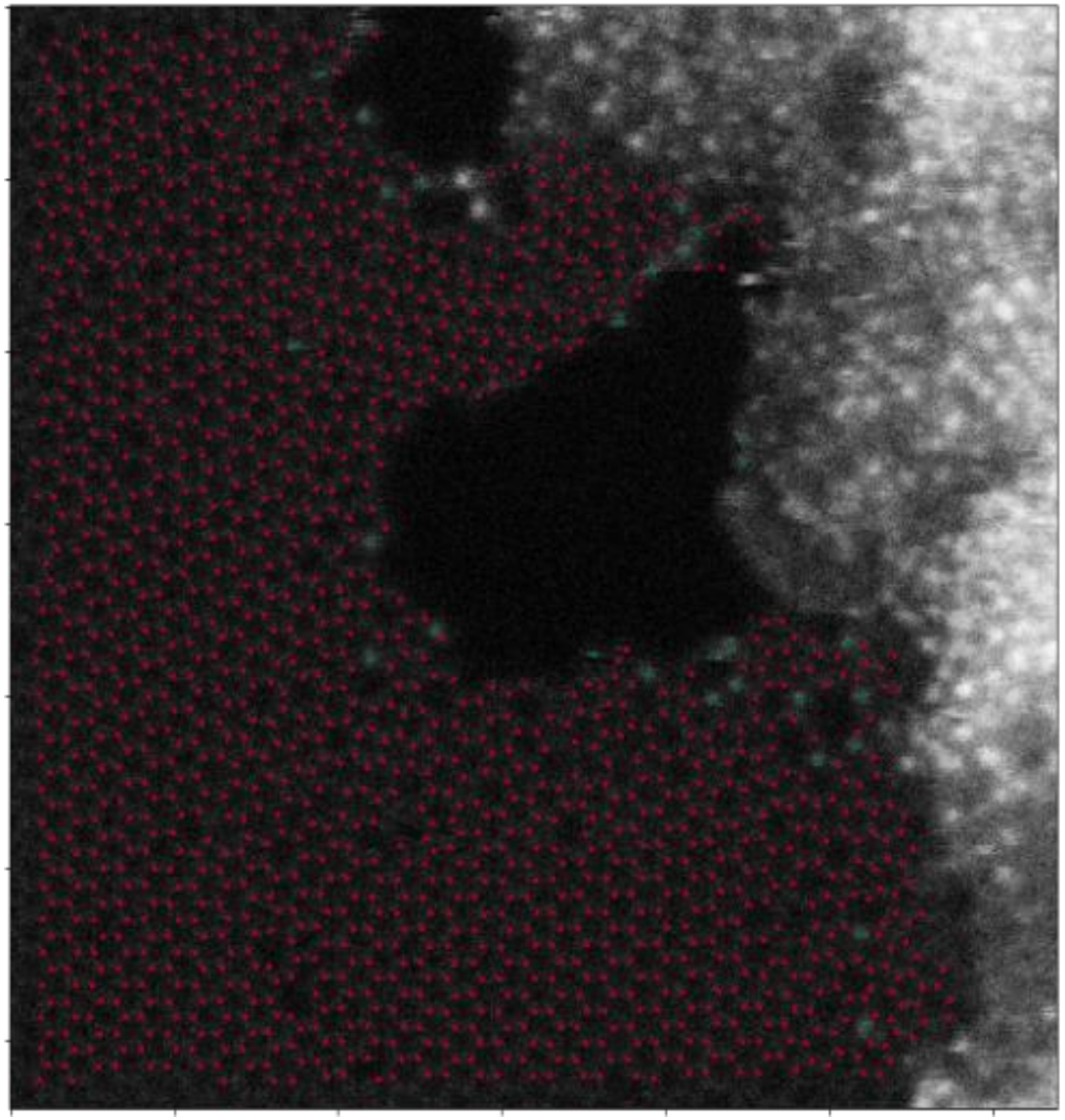


**Localized sub-images**

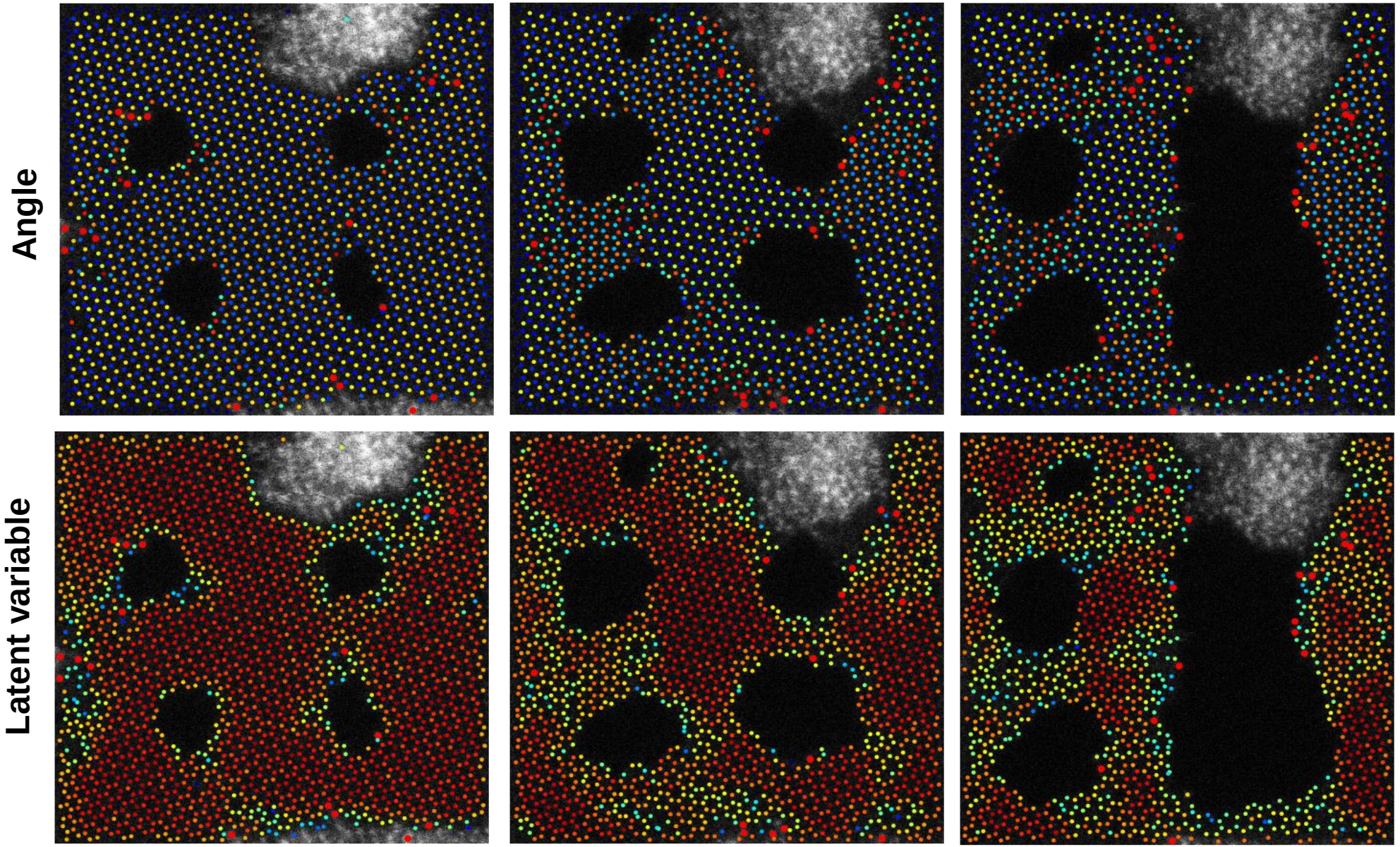


# Off to chemically-disordered systems

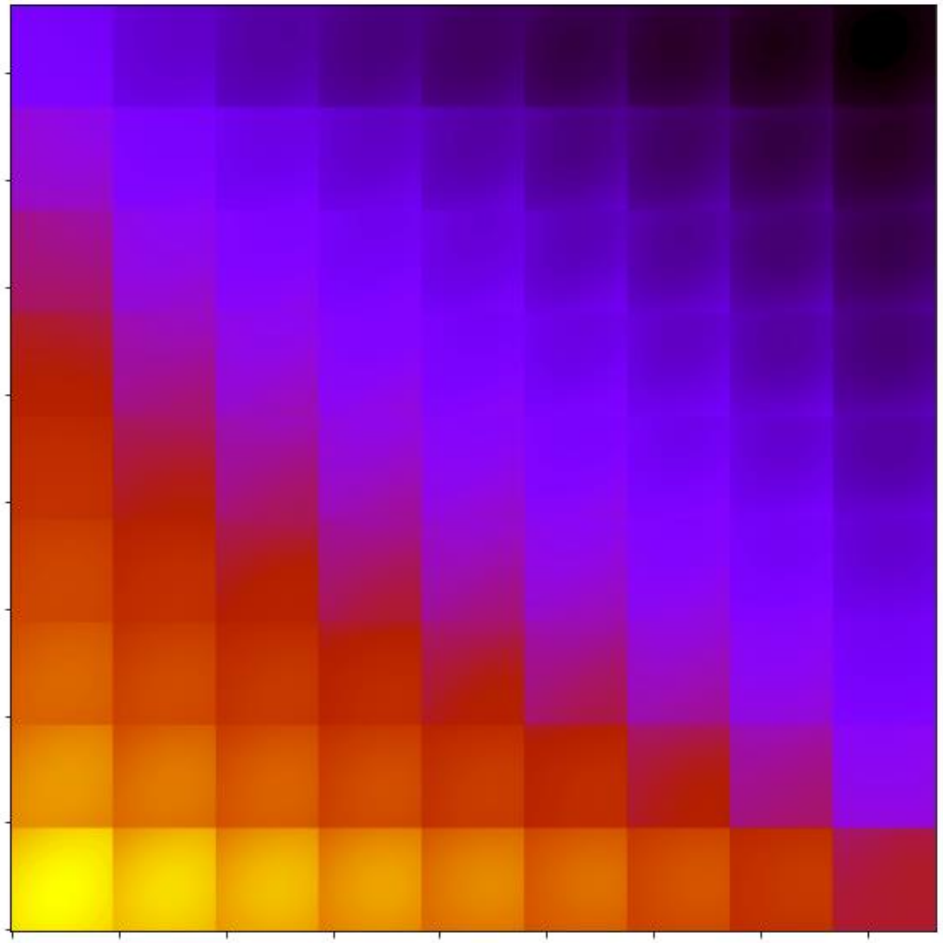


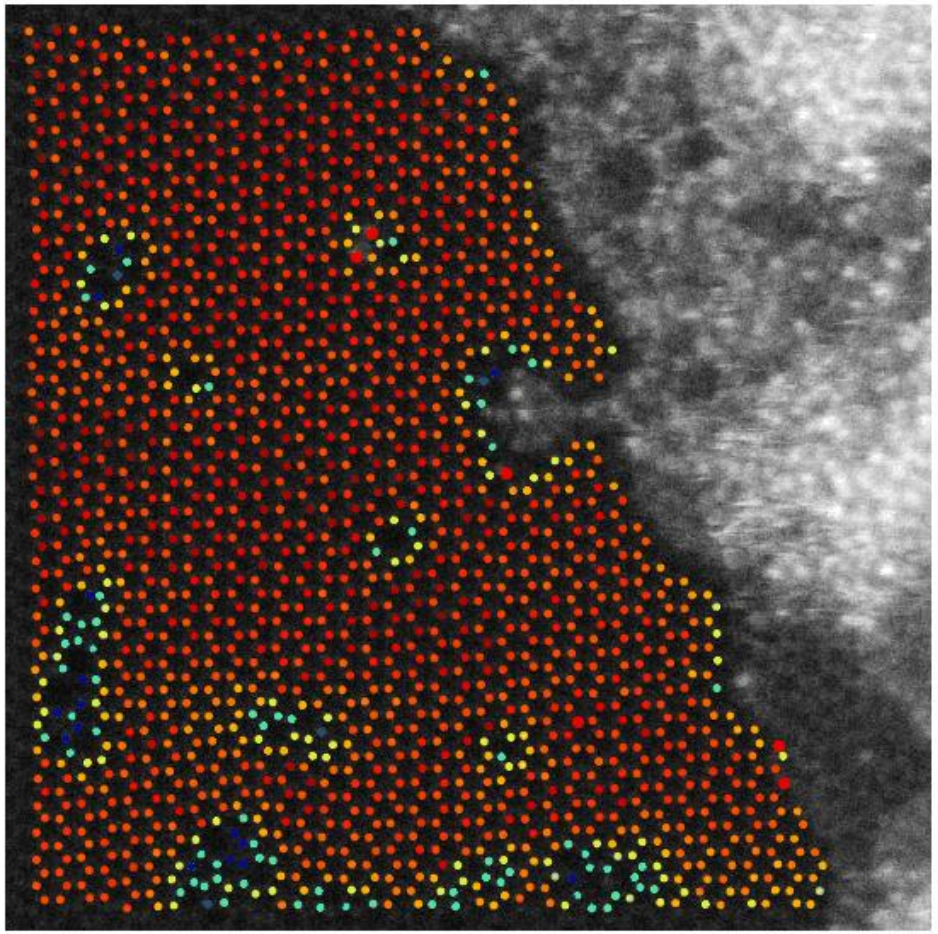


# rVAE analysis at different time steps



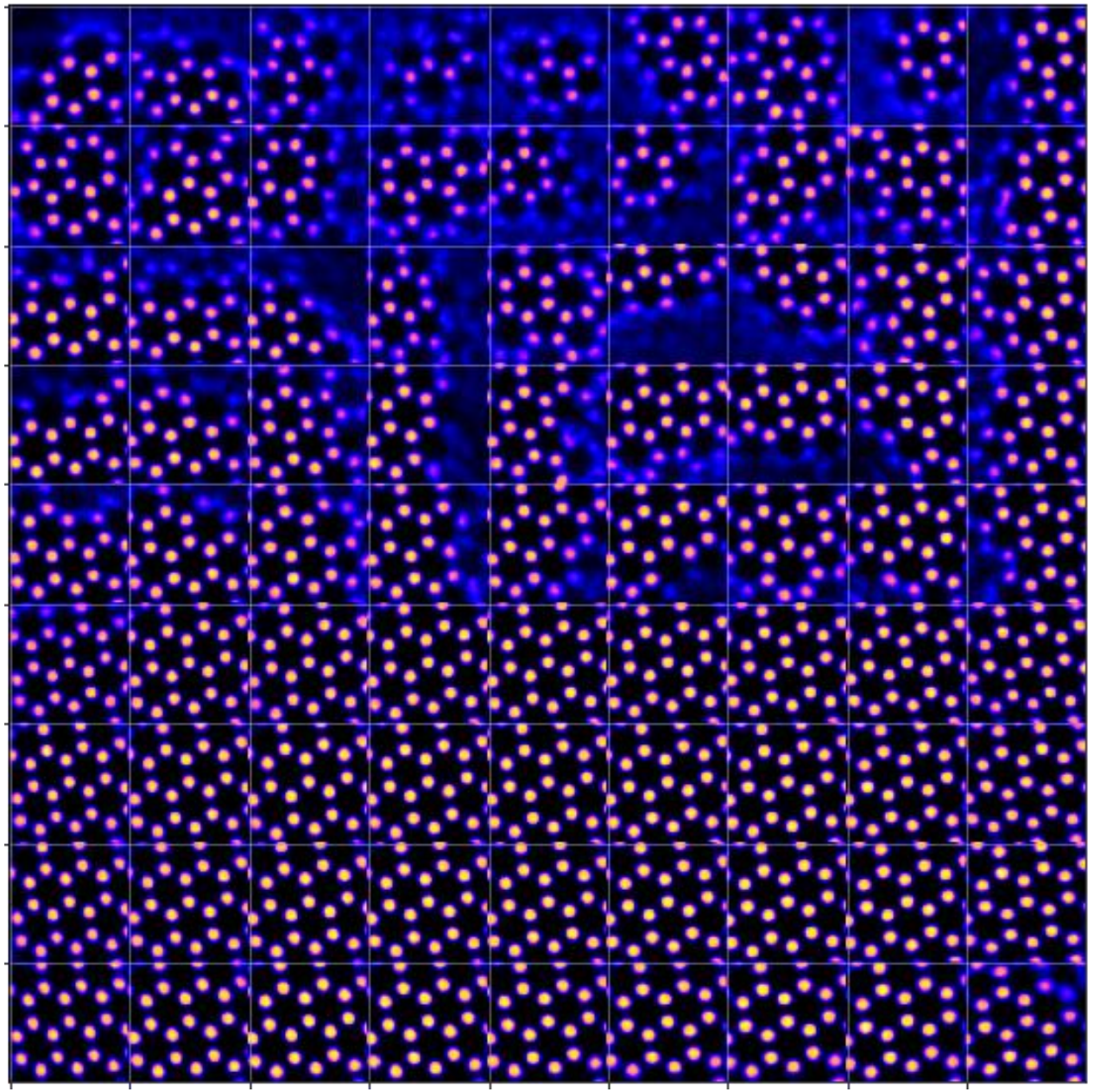
# There is nothing as beautiful as training VAE





# Next step: skip-rVAE



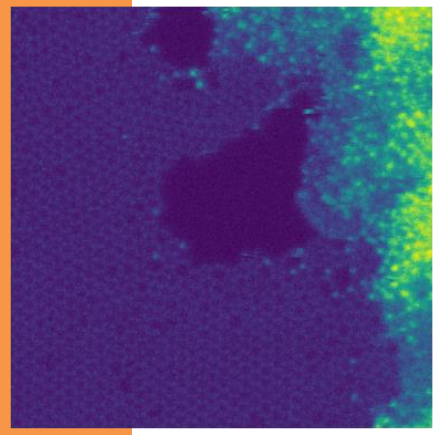


# Unsupervised discovery of molecules

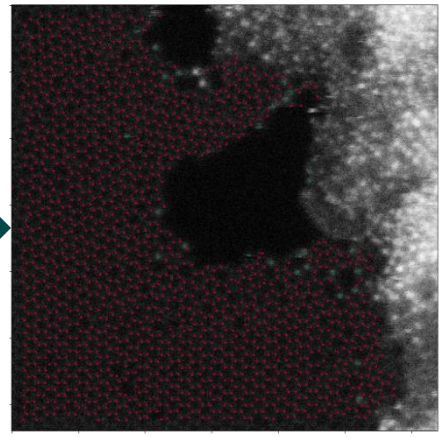
Atom exists, are discrete, and have known shape

Structures are parsimonious in nature

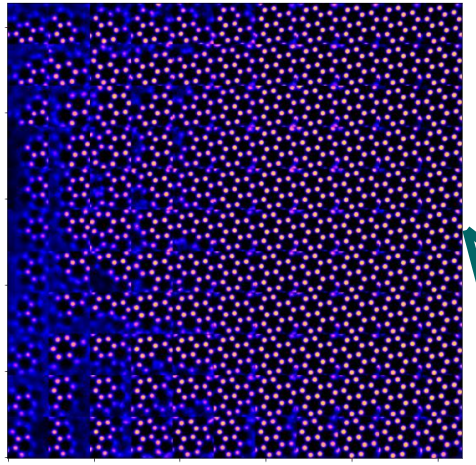
**Raw observation**



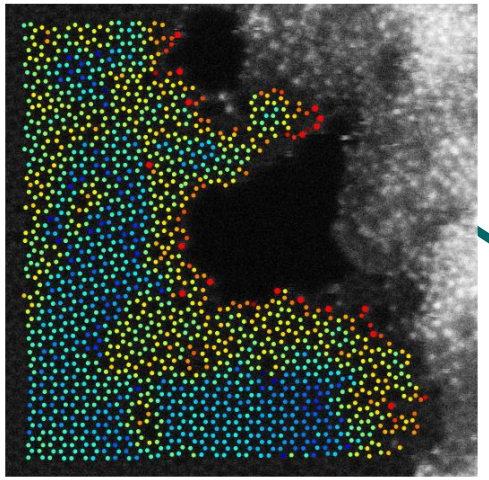
**DCNN decoded**



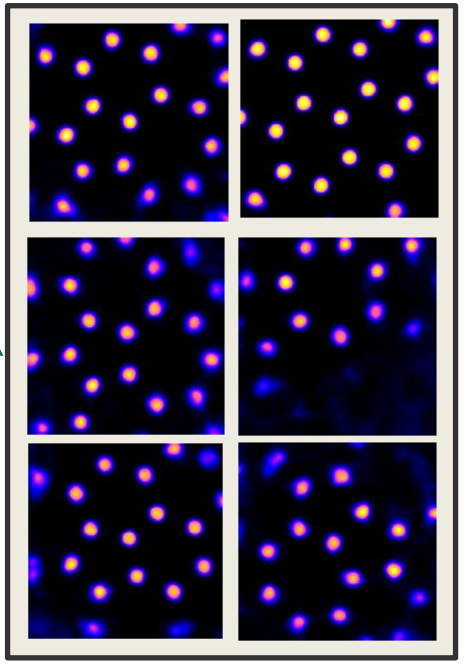
**Latent space of srVAE**



**Latent labels**



**I. Molecules**



**II. Reaction networks**

**A -> B -> C**

# Exploring the latent space structure