

Exploring Data Through Archetypal Representatives

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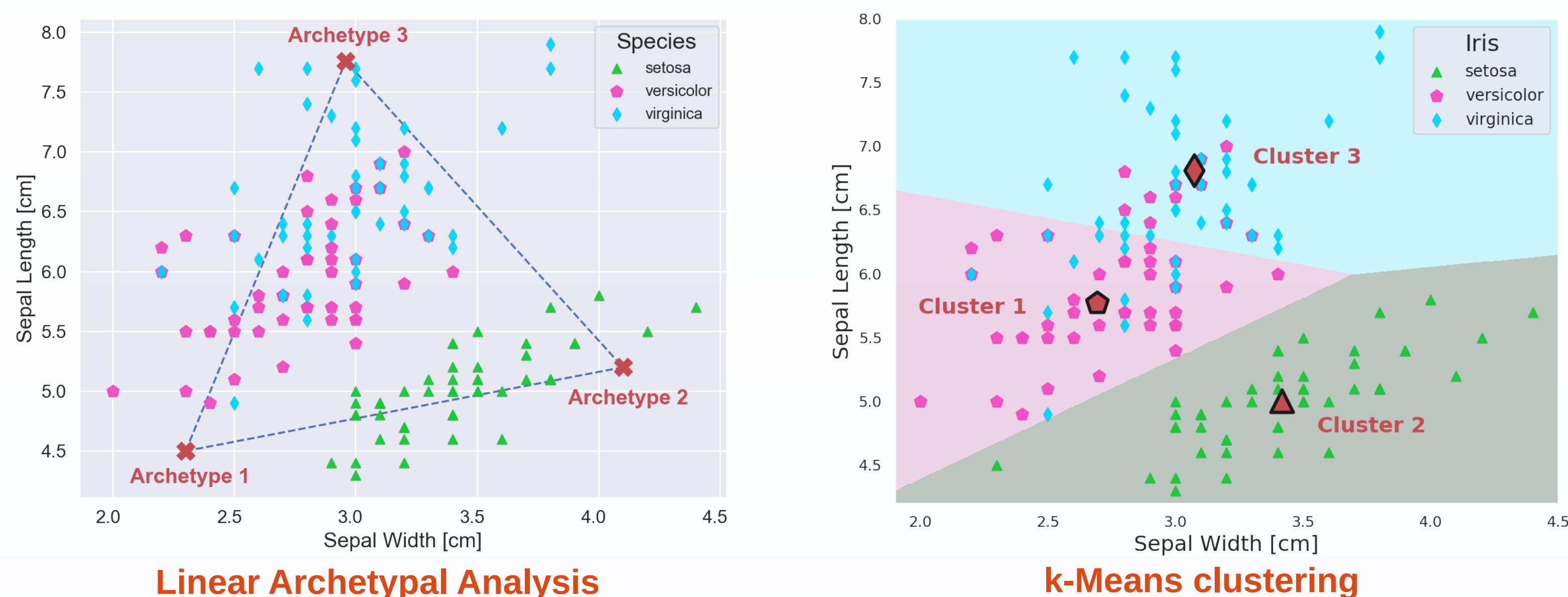
* equal contribution to poster/workshop

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Big Data
National Research Programme

FNSNF

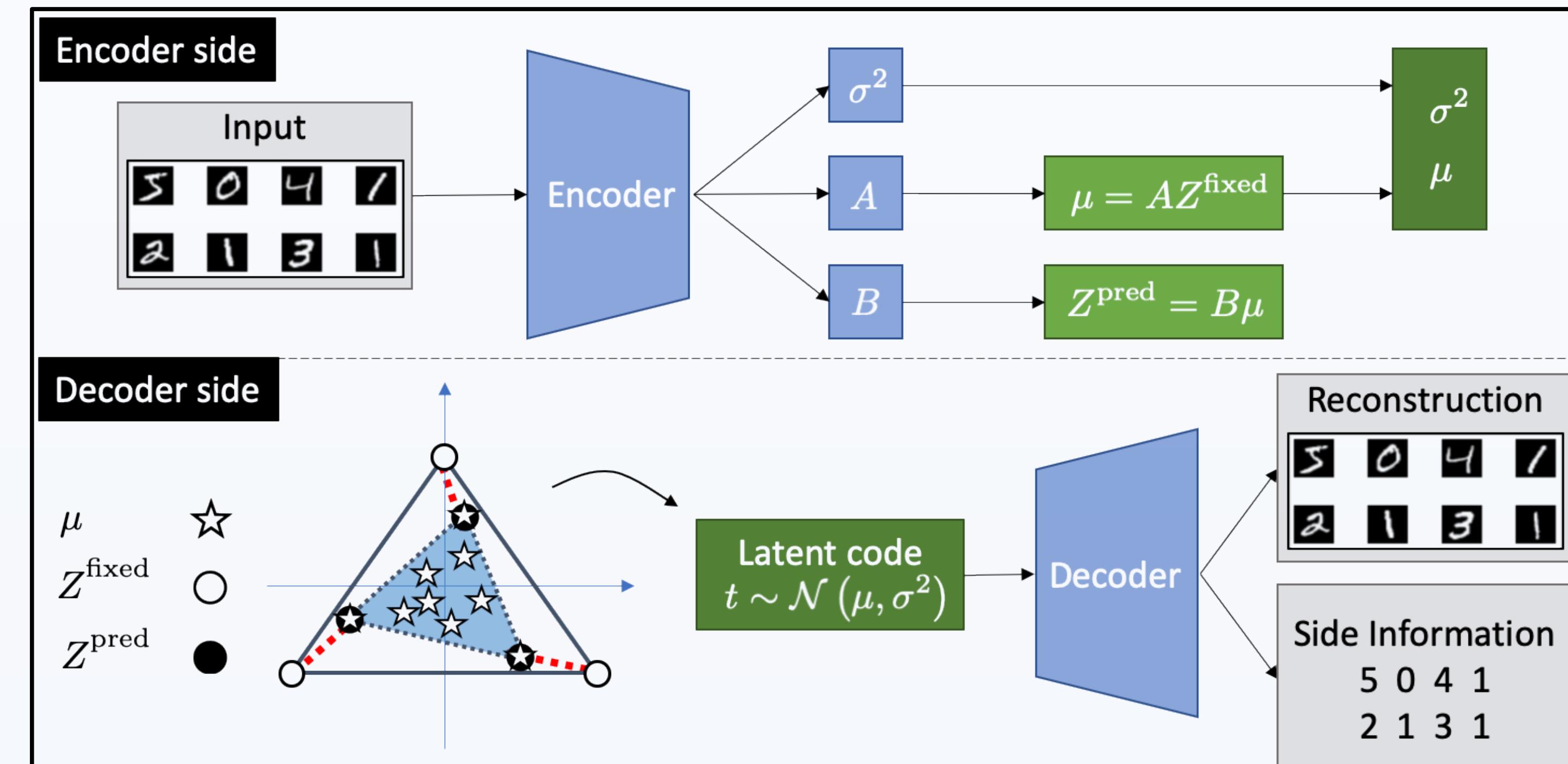
LINEAR ARCHETYPAL ANALYSIS [1]



- Represent data points X as convex mixtures of archetypes Z
- Represent archetypes Z as convex mixtures of data points X
- $\min ||X - AZ||^2 = ||X - ABX||^2$ with A, B : stochastic weight matrices

- Assign each data point x_i to the class of the closest prototype i
- Prototypes** are typical *mean* representative of their class
- Archetypes** are typical *extreme* representatives of the data

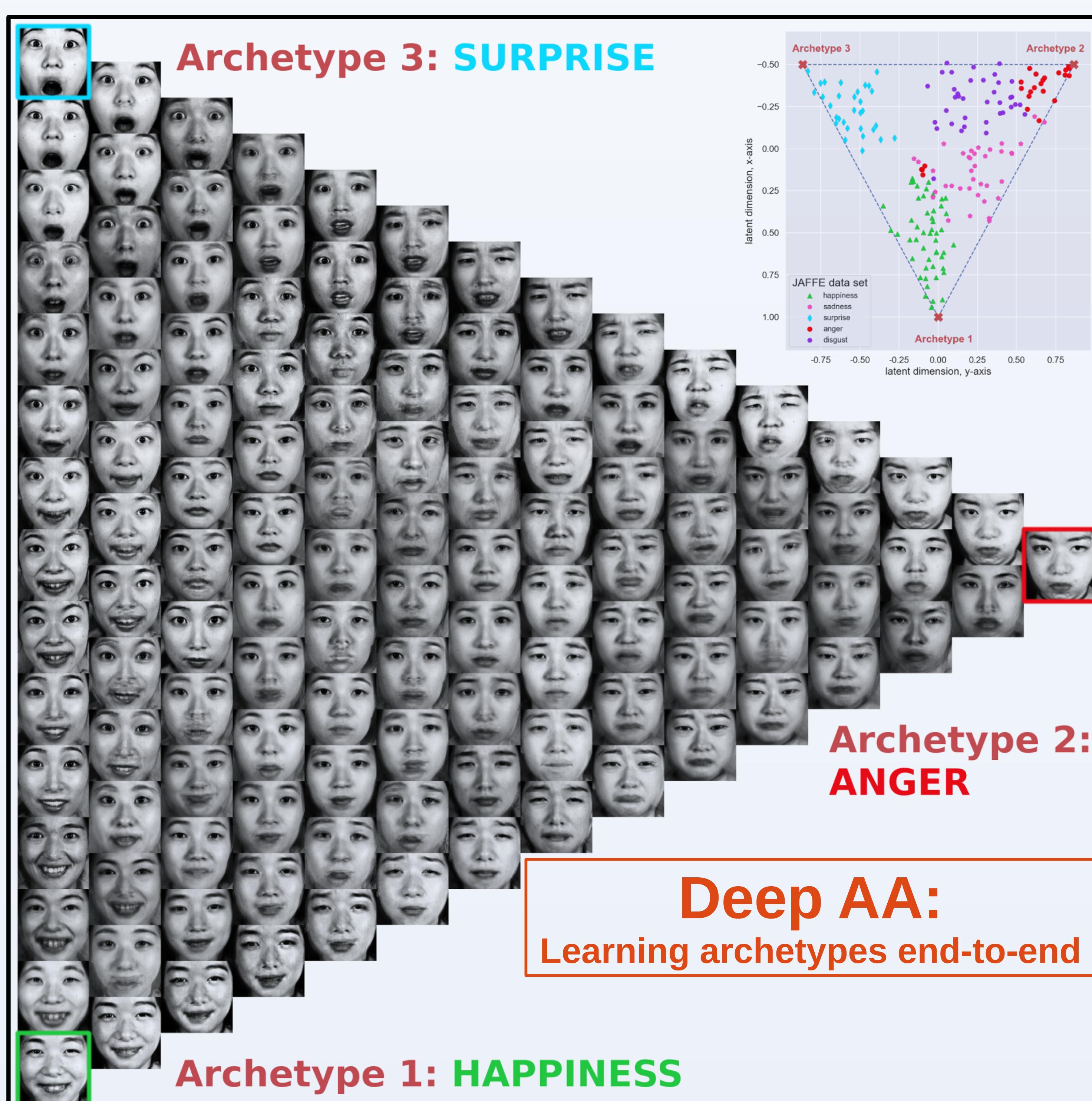
DEEP ARCHETYPAL ANALYSIS [2]: ARCHITECTURE



NEW ARCHETYPE LOSS: How well are A, B approximated?

EXPLORING JAFFE: SENTIMENT ANALYSIS WITH ARCHETYPES

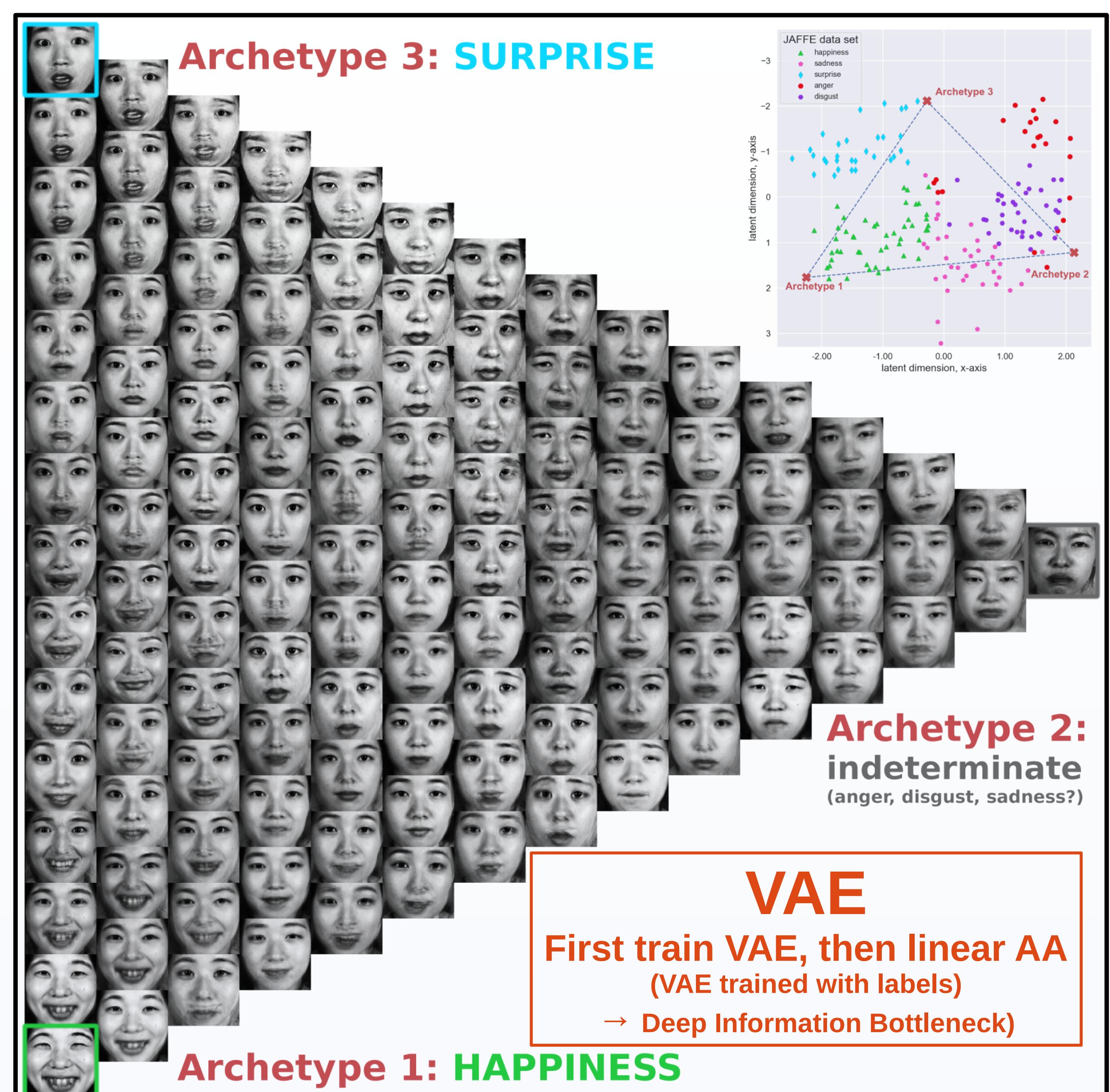
(Japanese Female Facial Expression, Lyons. M. J. et. al., 1998)



Deep AA:
Learning archetypes end-to-end

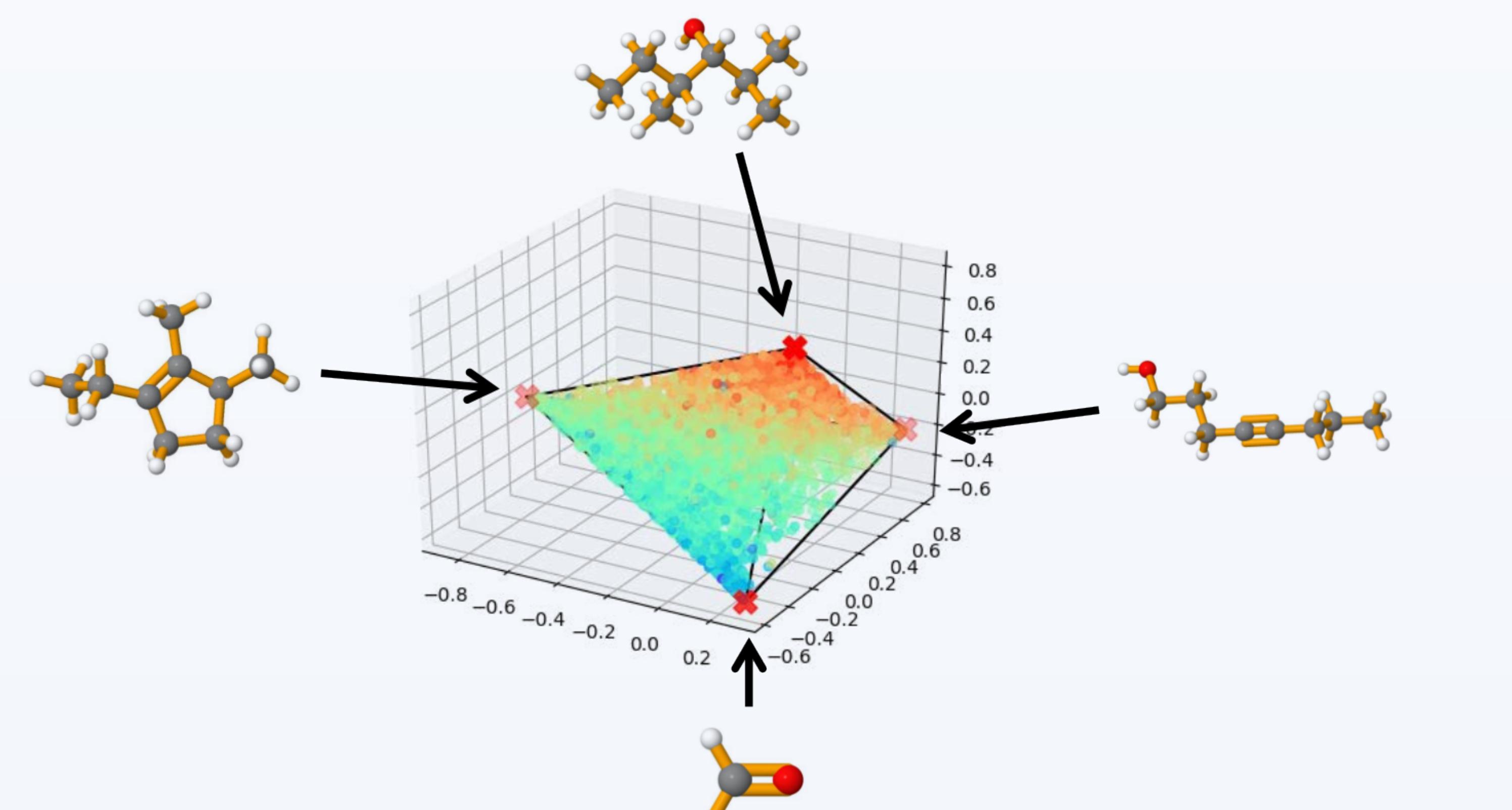
Archetype 1: HAPPINESS

Archetype 3: SURPRISE

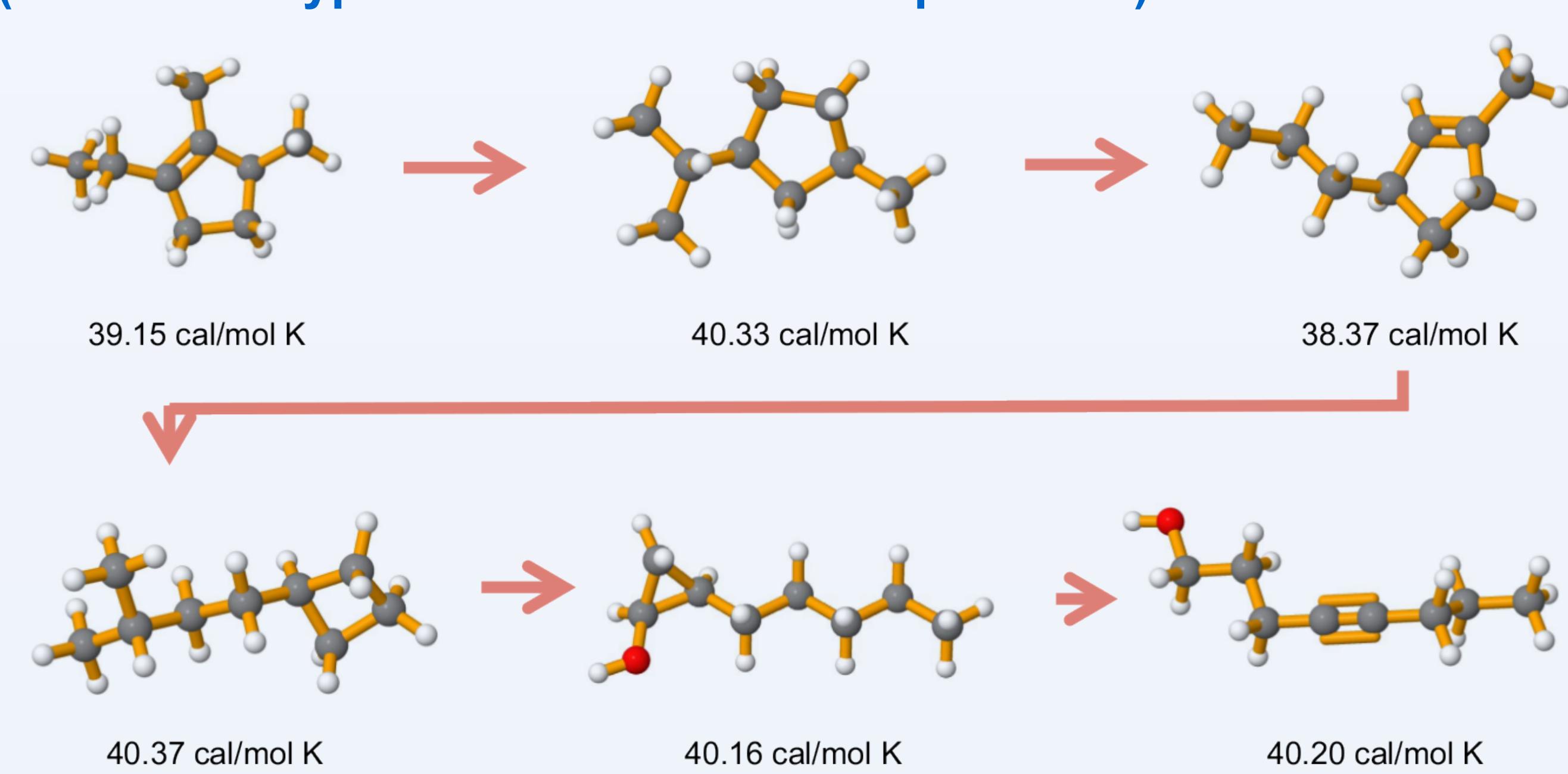


VAE
First train VAE, then linear AA
(VAE trained with labels)
→ Deep Information Bottleneck

EXPLORING CHEMICAL SPACES



DATA: QM9 data set – INPUT: Chemical Descriptors (Chem. Dev. Kit) – TARGET: Heat Capacity
Latent space traversal between archetypes
(both archetypes have similar heat capacities!)



BIOLOGICAL MOTIVATION FOR ARCHETYPES

Shoval et al., 2012, Evolutionary Trade-Offs, Pareto Optimality, and the Geometry of Phenotype Space, Science:
Archetypes in phenospace are interpreted as best adapted species.
→ Bats hunting high flying, large insects have high aspect ratios and medium bodies.

[1] Cutler, Adele, and Leo Breiman. Archetypal Analysis. Technometrics, vol. 36, no. 4, 1994, pp. 338–347.

[2] Keller S.M., Samarin M., Wieser M., Roth V. (2019) Deep Archetypal Analysis. In: Fink G., Frintrop S., Jiang X. (eds) Pattern Recognition. DAGM GCPR 2019. Lecture Notes in Computer Science, vol 11824. Springer, Cham