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BEYOND FINGERPRINTING

INFERRING TOPOLOGICAL TRANSITIONS IN PATTERN-FORMING PROCESSES VIA SELF-SUPERVISED LEARNING

SIAM CONFERENCE ON MATHEMATICS OF DATA SCIENCE (MDS22)
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Classical Theories of Phase Transition Rely on Discontinuity

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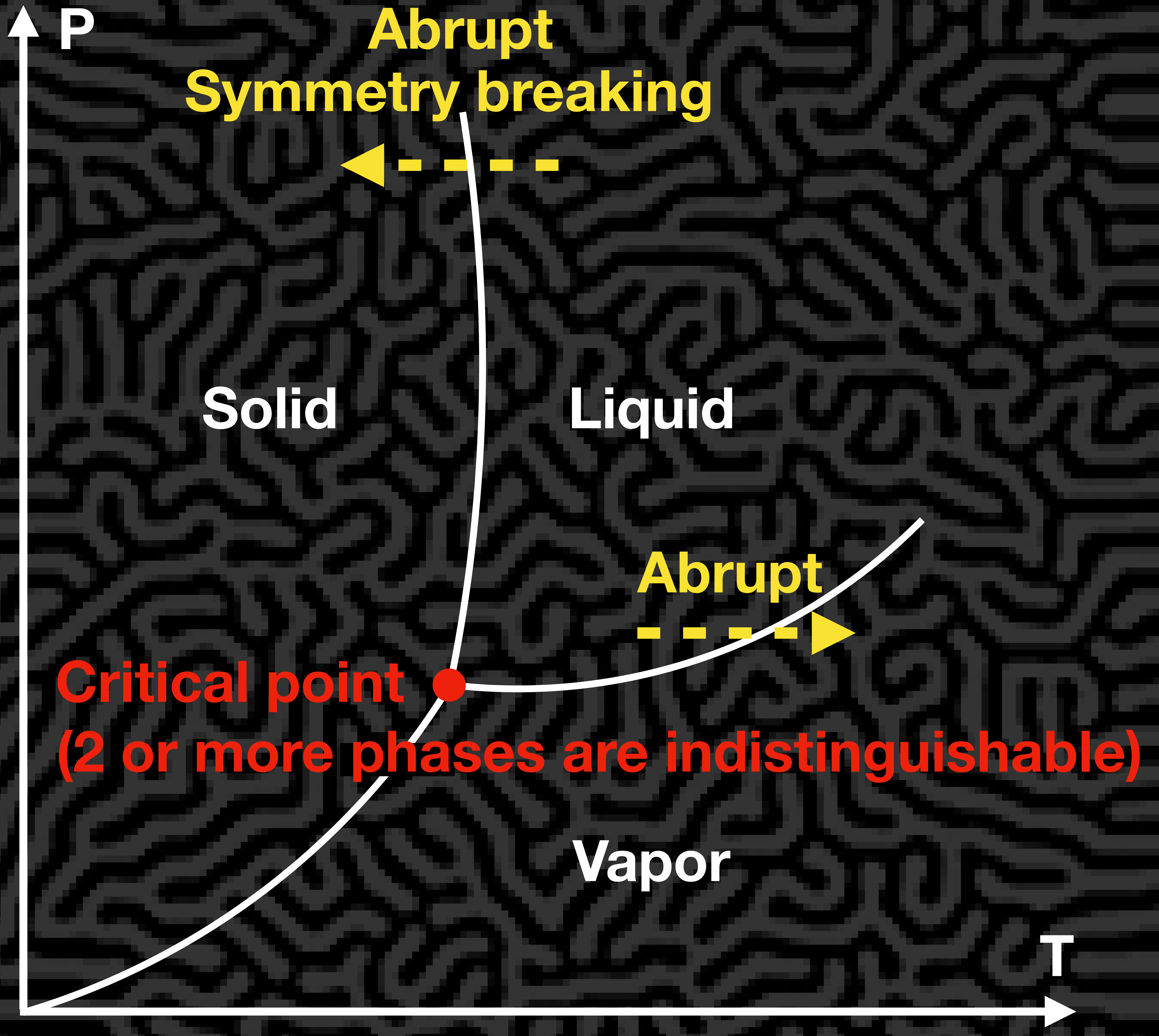
Landau Theory:
Transition described by an abrupt change in order parameter (or its derivative)

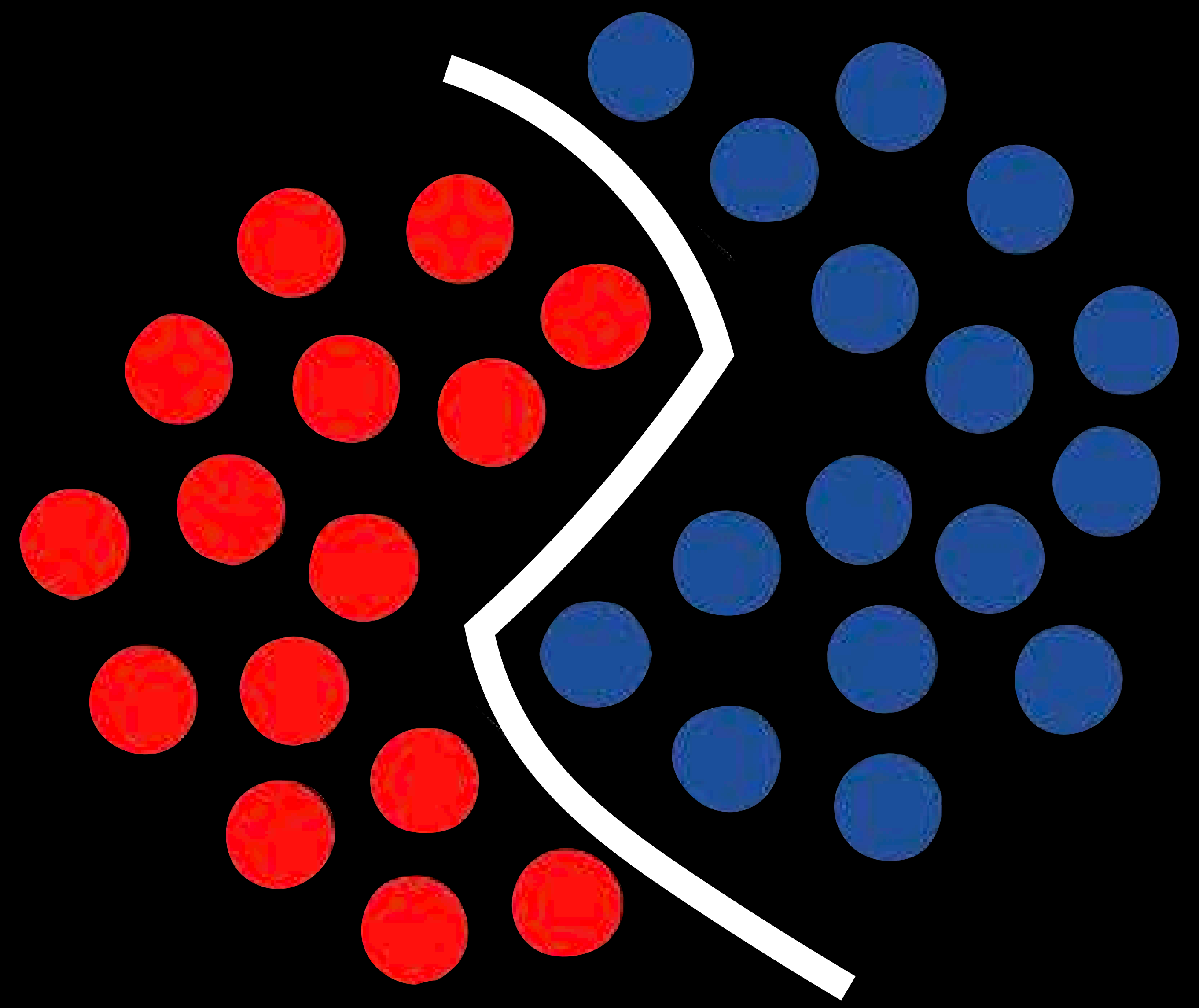
Phase transition	Order parameter
paramag↔ferromag	magnetization
liquid↔gas	density
liquid↔solid	shear modulus



Many Pattern-Forming Processes are Gradual and Cannot Be Described by Classical Transition Theories

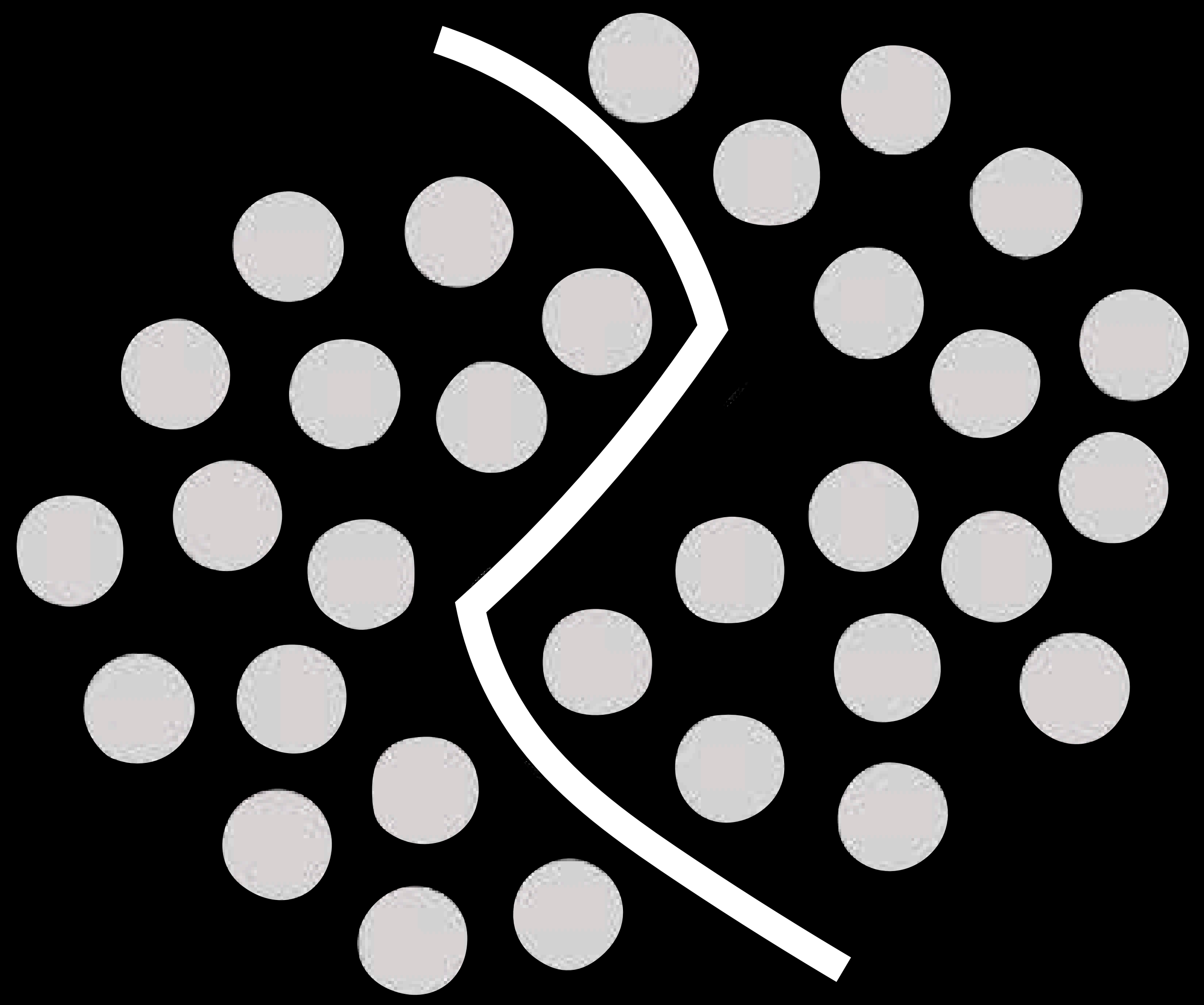
From a Machine Learning Perspective: This is a Classification Problem

Supervised



- Need labels to learn
- Requires prior knowledge

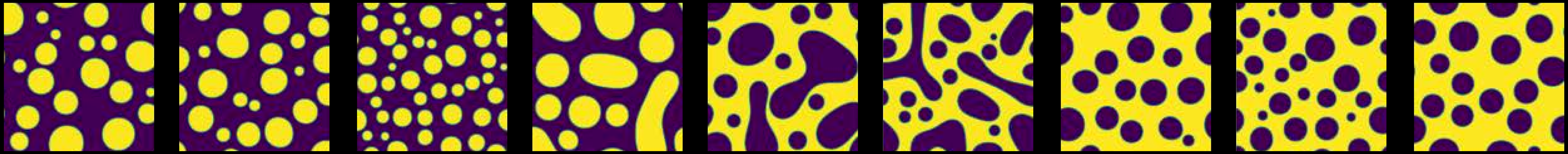
Unsupervised



- Does not need labels
- Use clustering for classification

Examples of Pattern-Forming Processes

- **Spinodal decomposition**
  - Process parameters: mobility of phase A and B, phase fraction
  - Transition expected to occur for 50% phase fraction (A-rich vs. B-rich)



- **Physical vapor deposition**
  - Process parameters: deposition rate, deposition angle, phase mobility
  - vertical-oriented, horizontal-oriented, random-oriented

The Ambiguity Of Identifying Topological Transitions For High-Order & Dynamic Transitions

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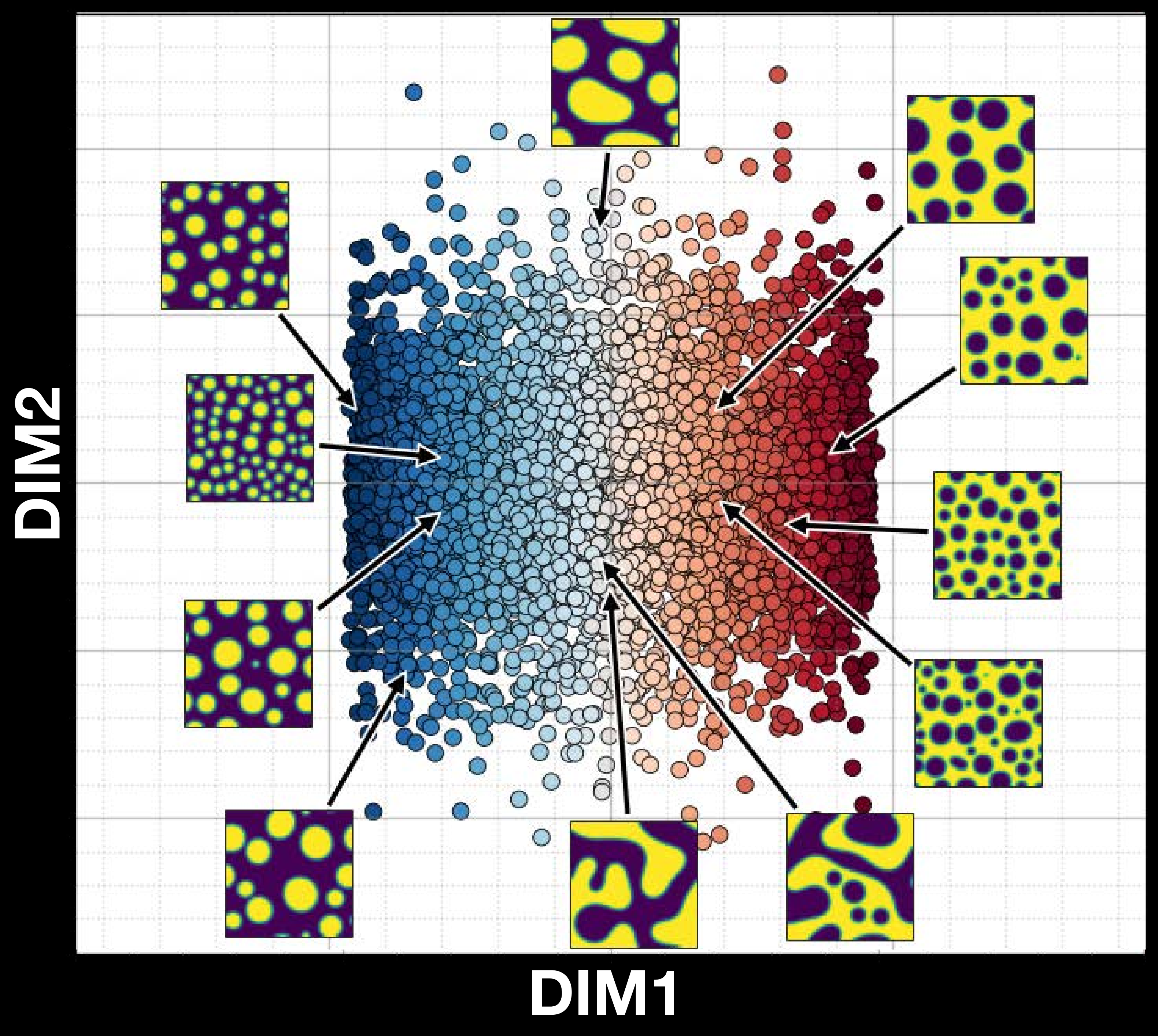
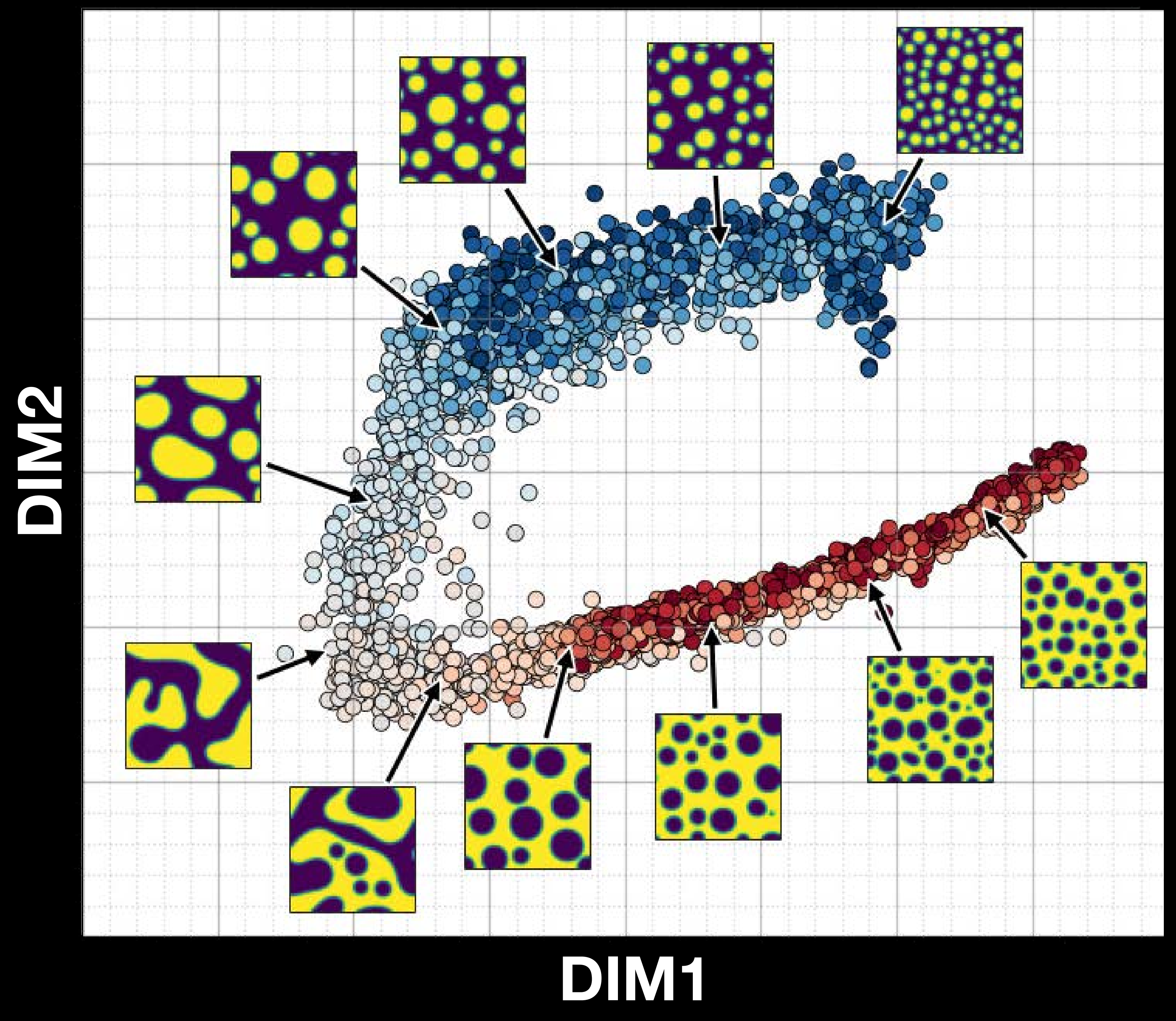
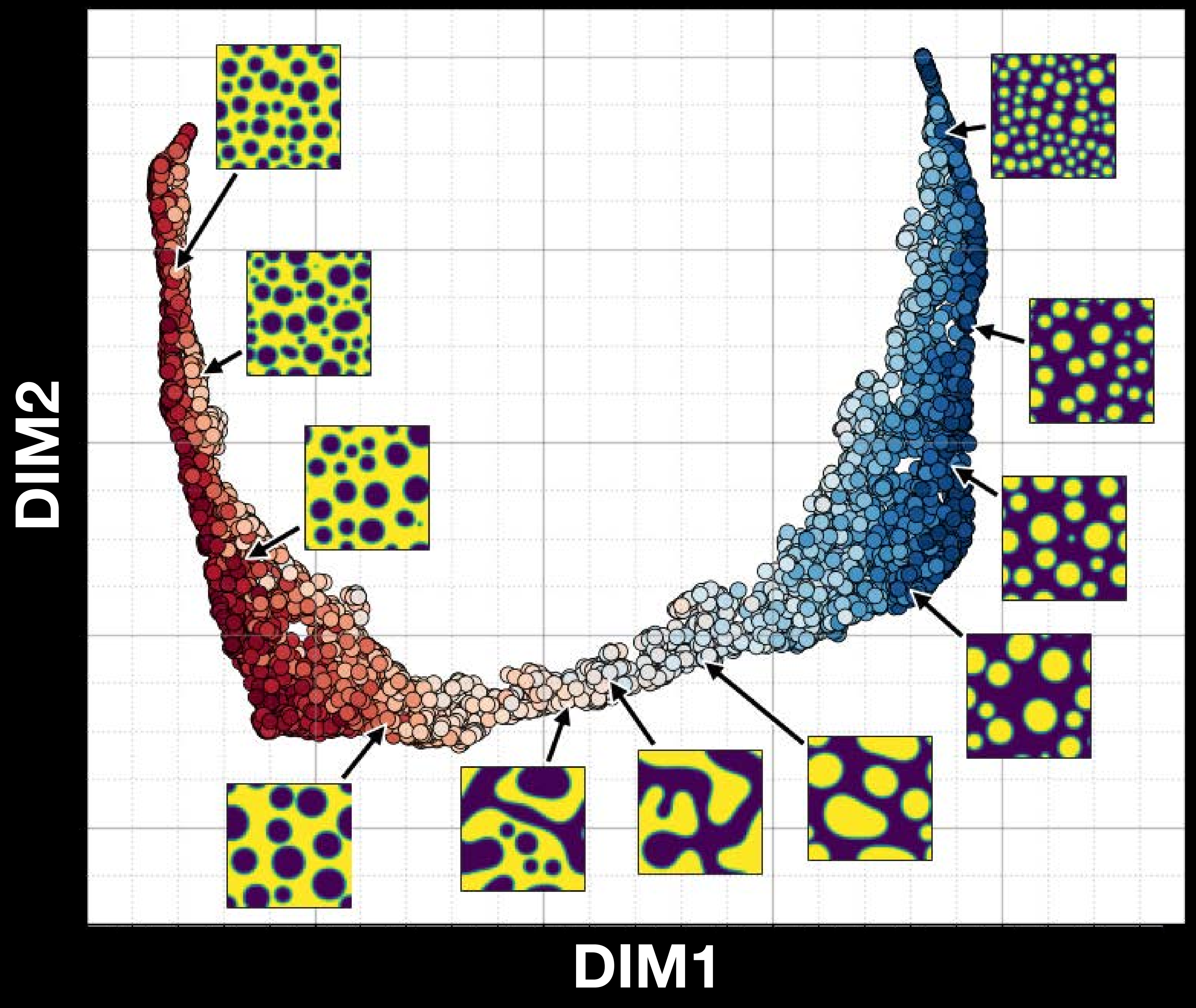
PCA on microstructure image



PCA + ResNet on microstructure image

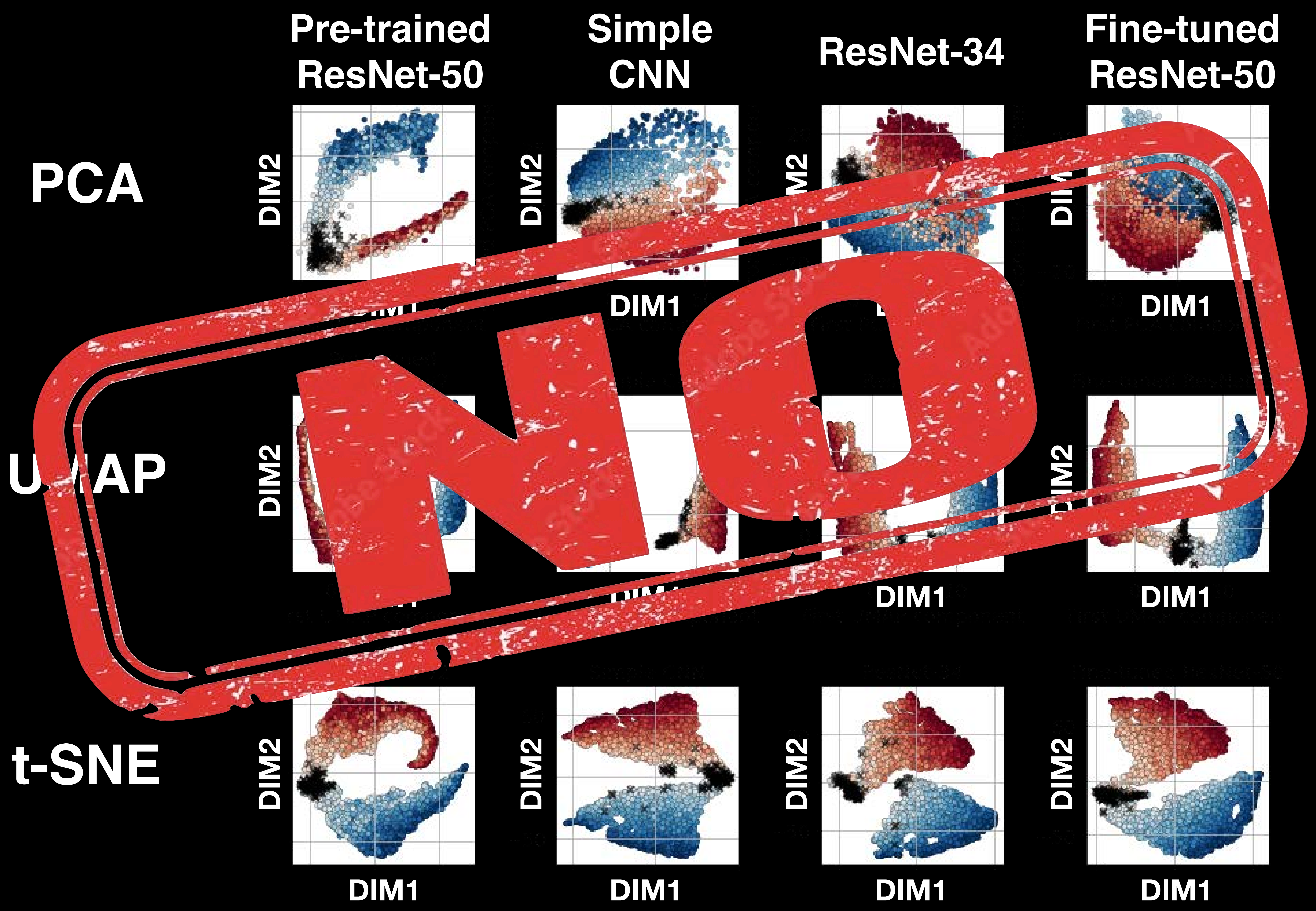


UMAP + ResNet on microstructure image



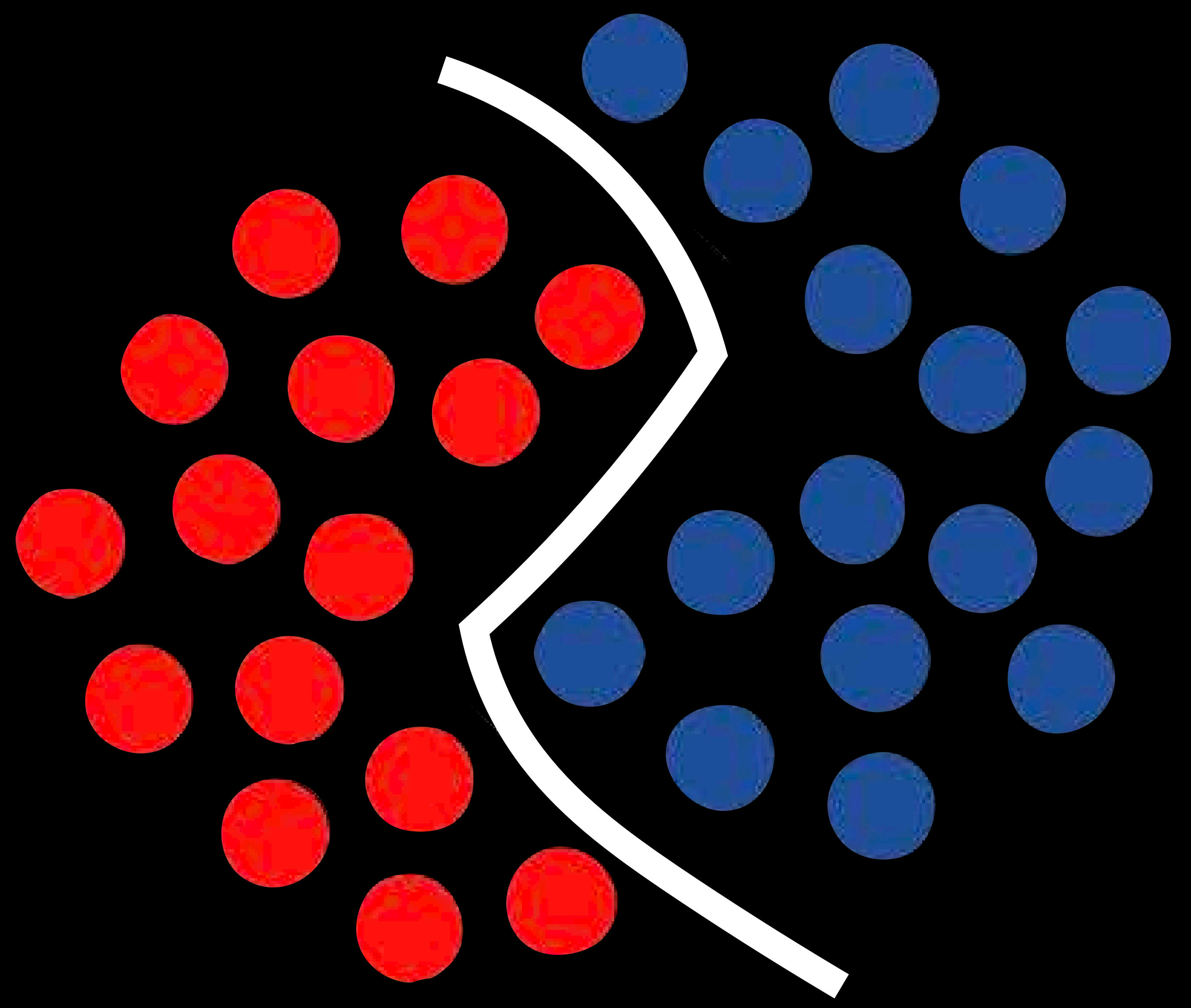
- Gradual changes in microstructure patterns when process parameters vary
- No clear clustering in low-dimensional space

Does the Choice of Projection Method Matter?



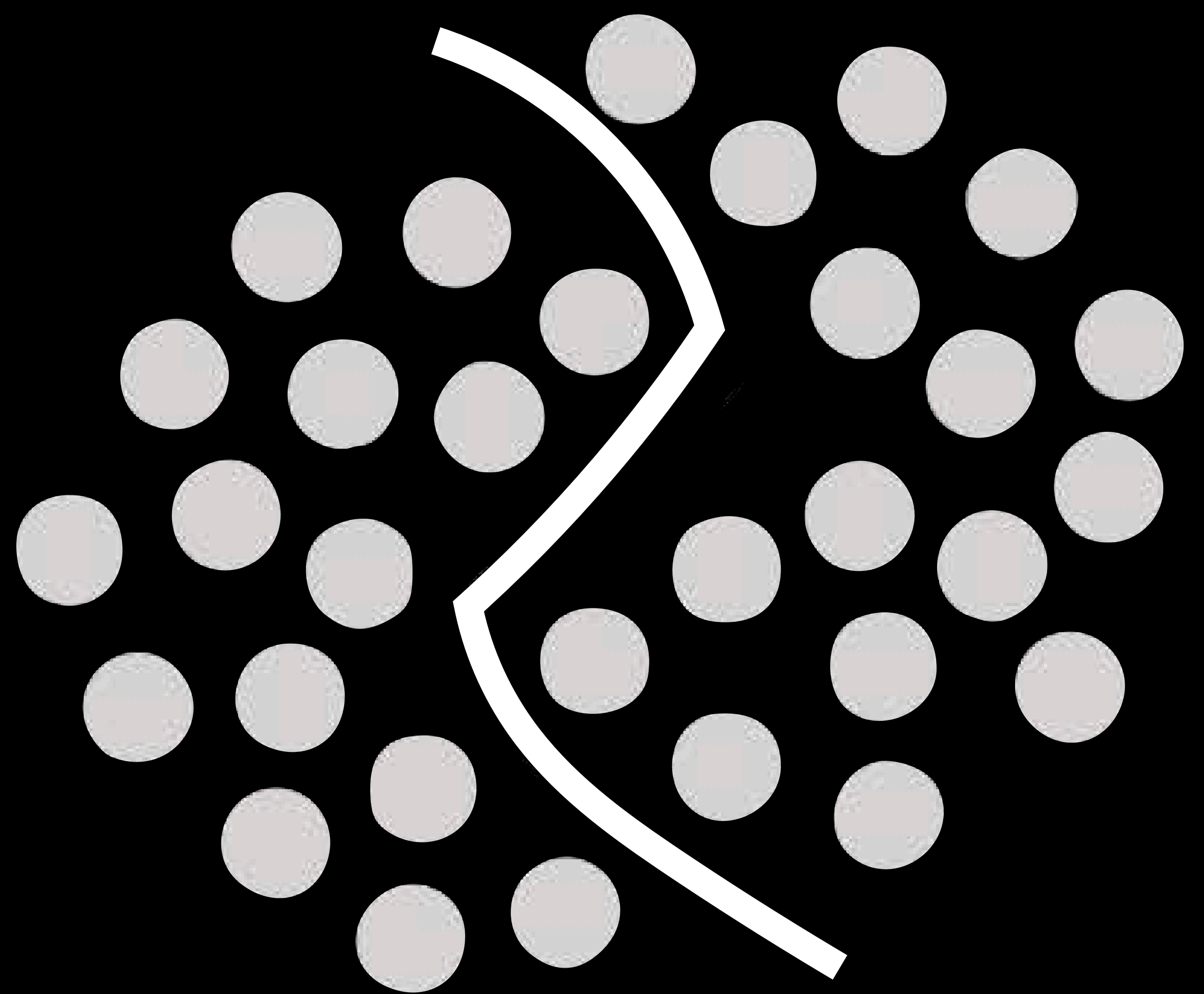
SOLVING AN AUXILIARY PROBLEM INSTEAD

Supervised



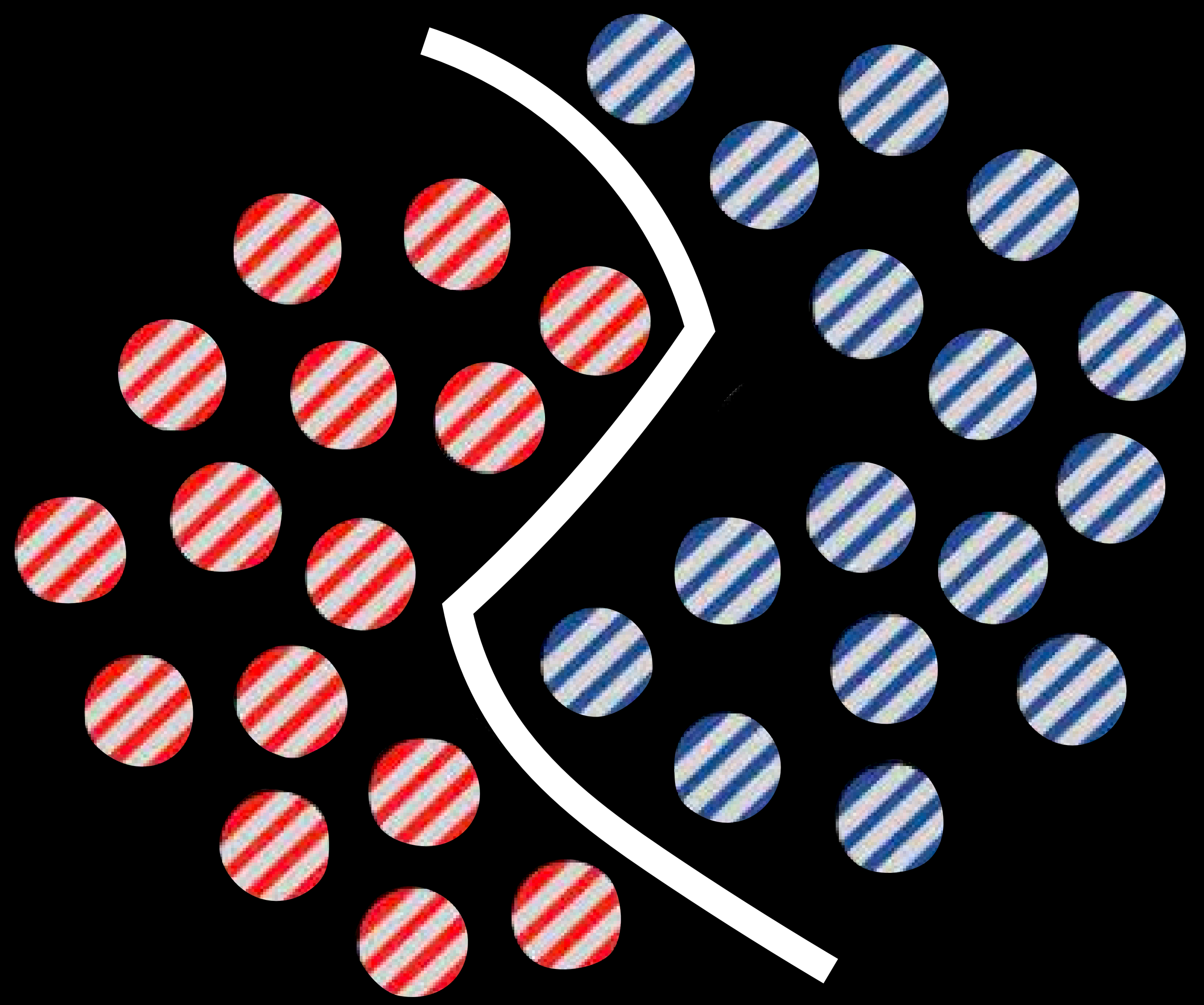
- Need labels to learn
- Requires prior knowledge

Unsupervised



- Does not need labels
- Use clustering for classification

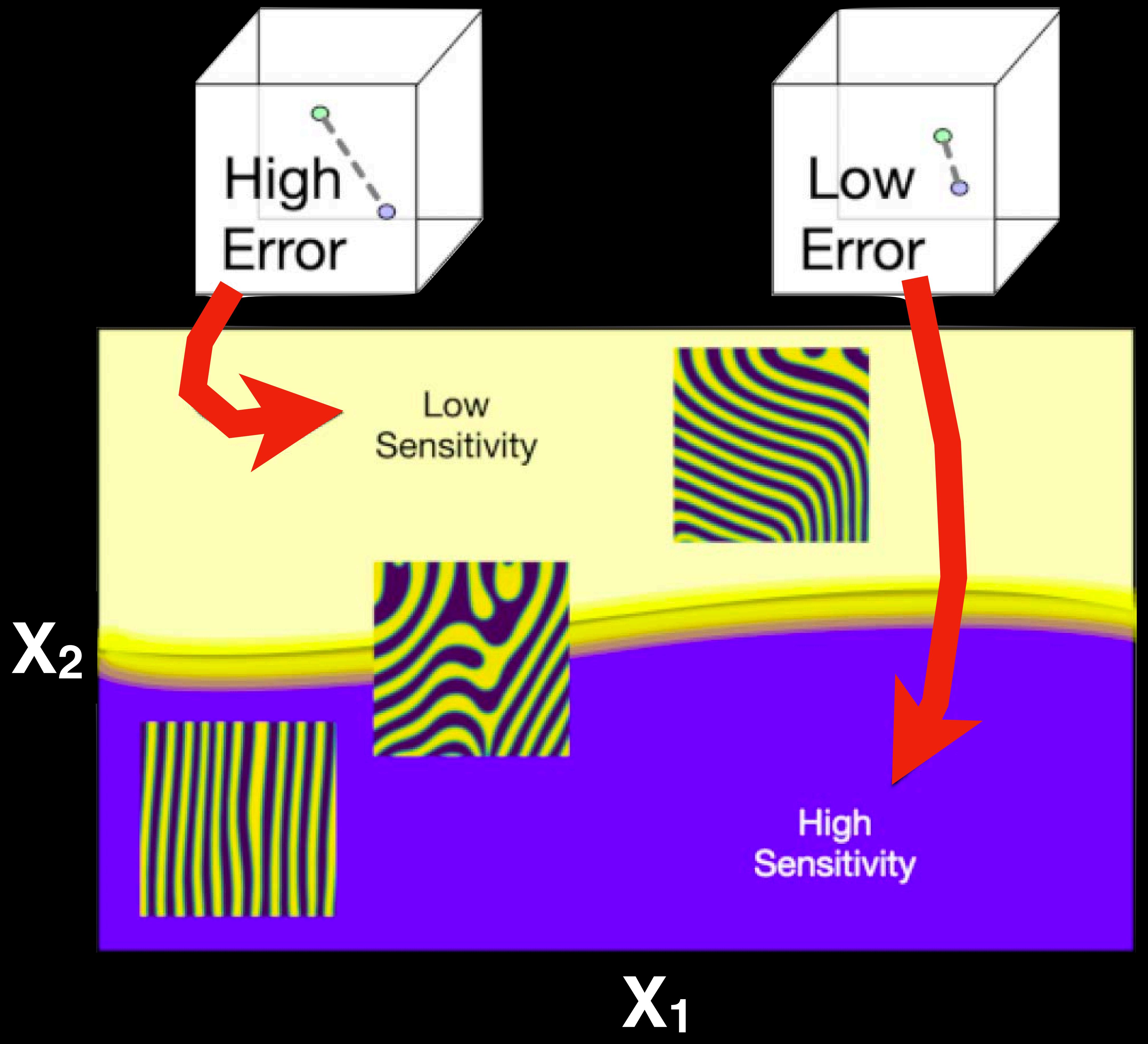
Self-supervised



- Does not need labels
- Solve an auxiliary (easier?) problem closely related and semantically connected

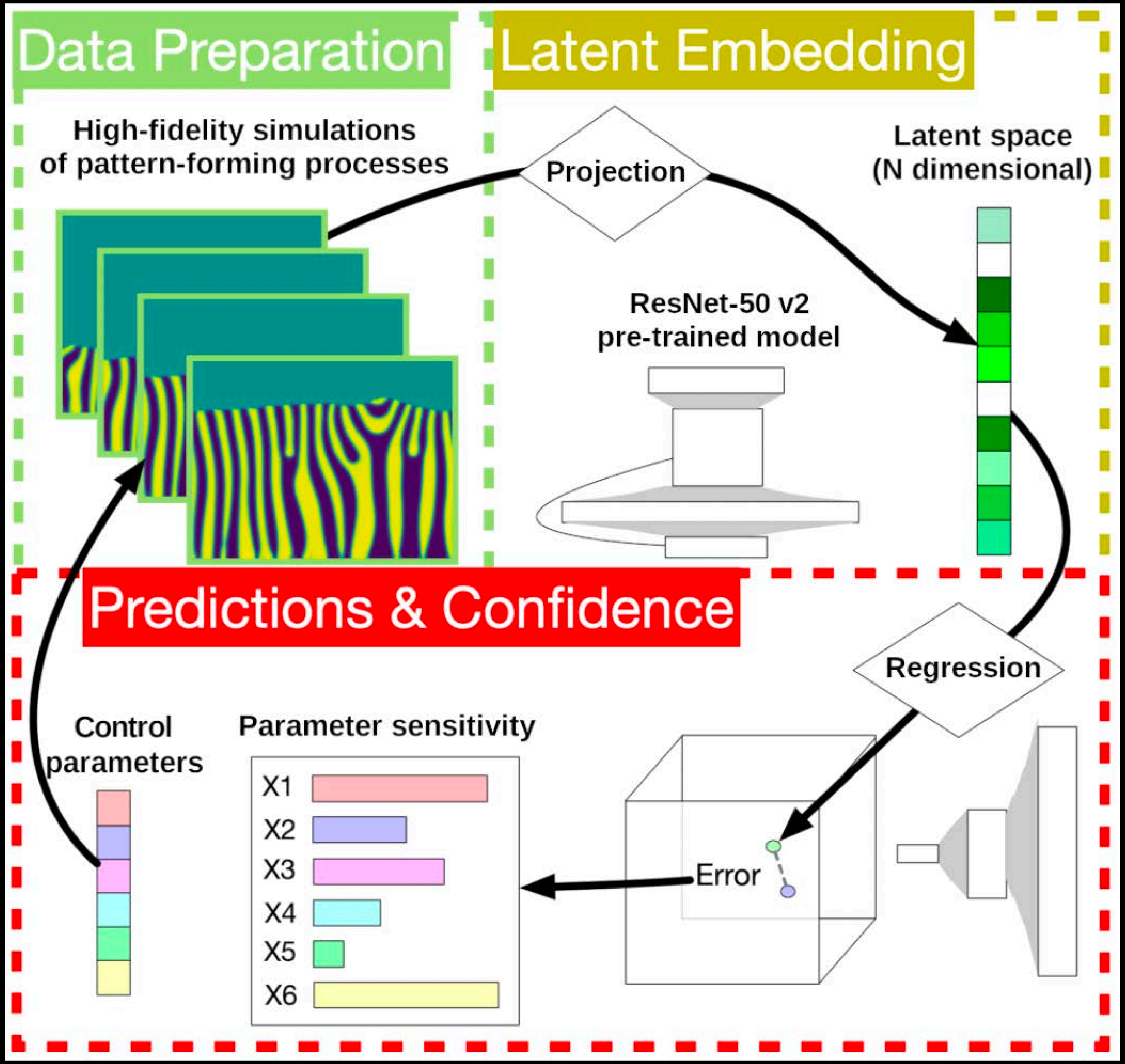
Re-Discovering The Critical Point (Universality)

Predicting process parameters from observed patterns



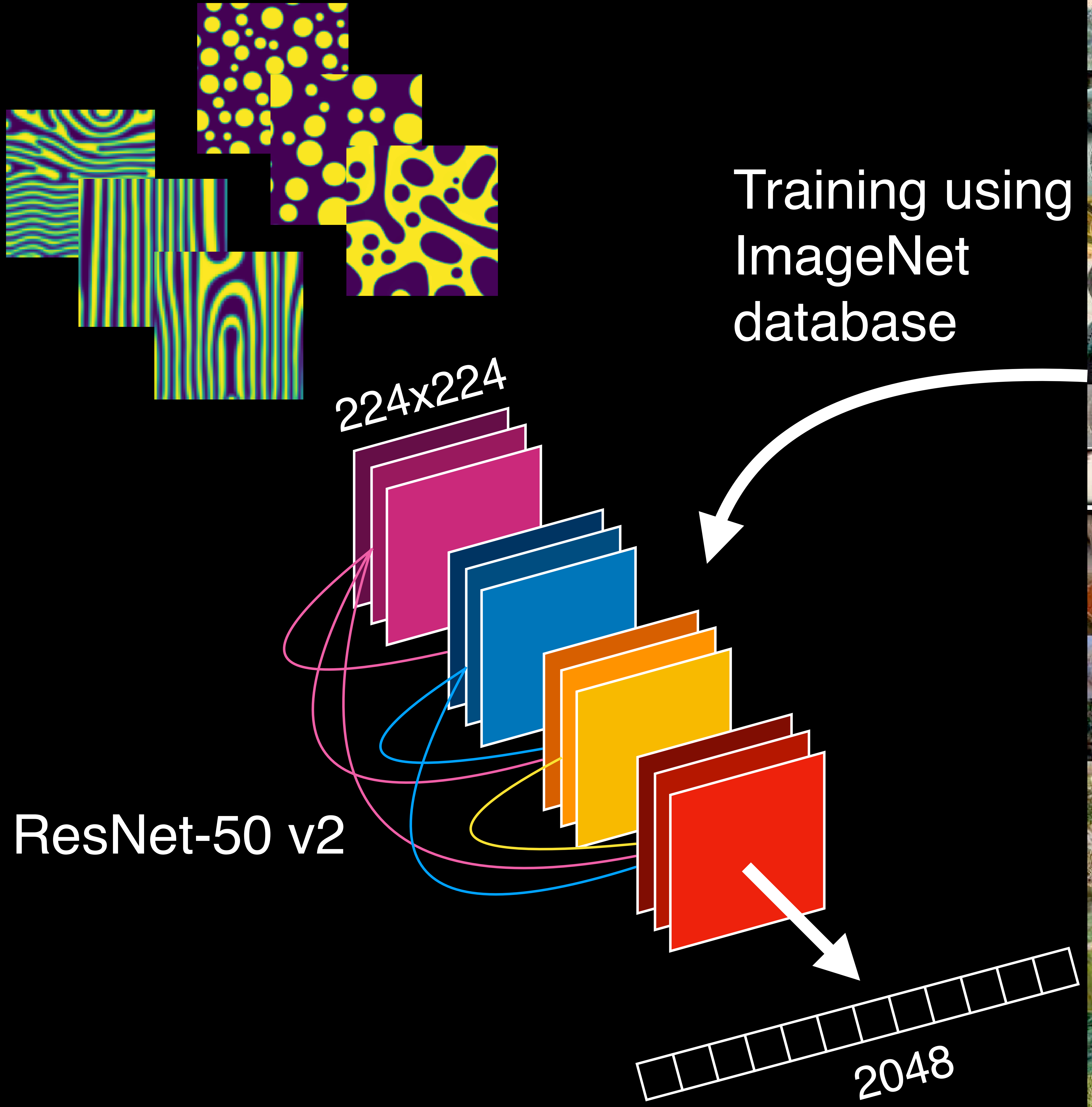
- **High sensitivity:** we are able to predict the input process parameter accurately
- **Low sensitivity:** relation between input process parameter and pattern is weak
- **When score changes** from low to high or high to low, may indicate a transition
- Analogy to critical point and **universality** in dynamical systems

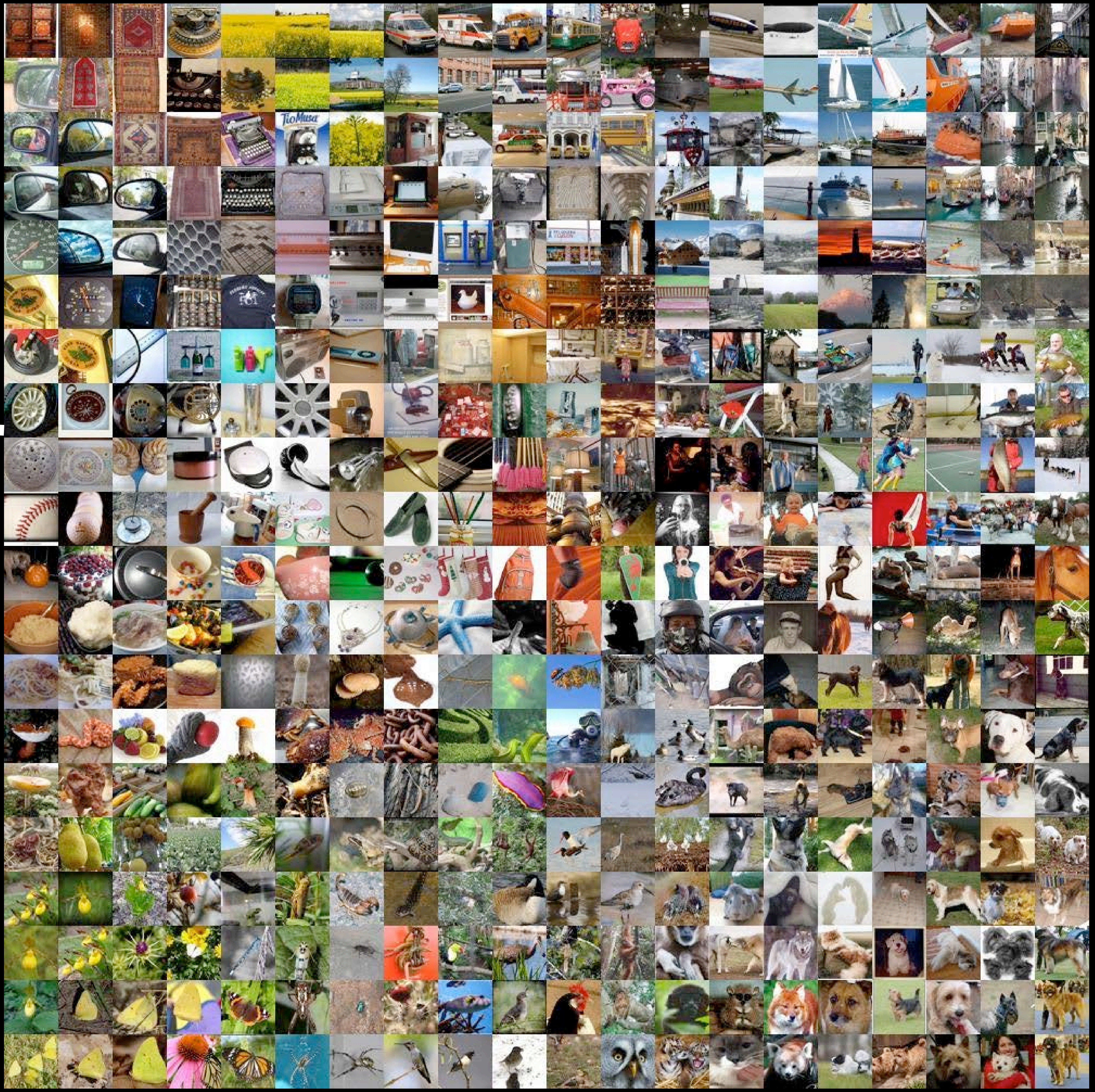
Embed, Predict, Evaluate



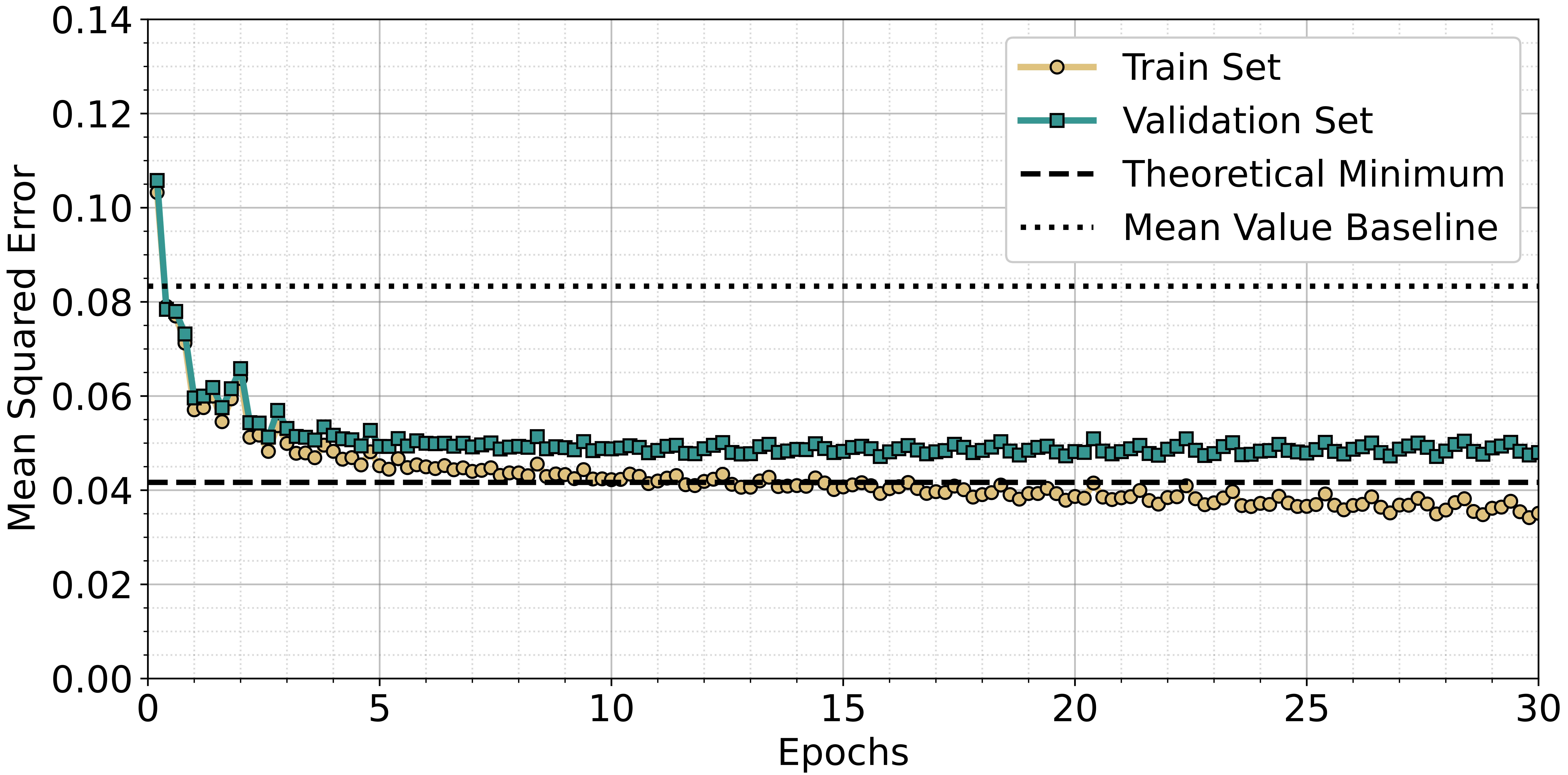
1. Large and diverse set of pattern regimes
2. Pre-trained CNN (ResNet-50 v2 model) to represent microstructure in latent space
3. Use feed-forward NN to regress input process parameters from observed microstructures
4. Evaluate errors between predictions and ground truth

EMBED:


224x224
ResNet-50 v2
2048
Training using
ImageNet
database



PREDICT:



Train Set
Validation Set
Theoretical Minimum
Mean Value Baseline
Mean Squared Error
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0
5
10
15
20
25
30
Epochs

Evaluate:

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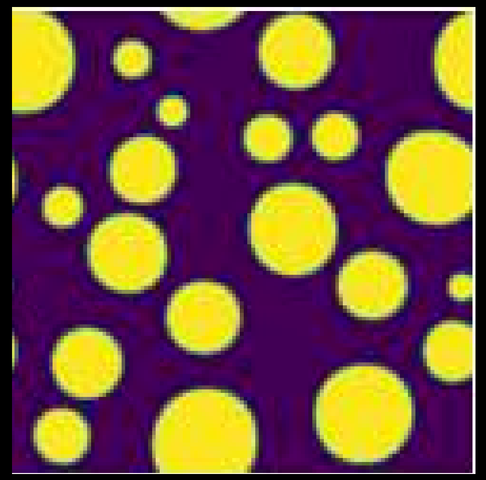
$$S = N / \sum_{i}^{N} \left| \overset{\text{Predicted}}{\hat{y}_i} - \overset{\text{True}}{y_i} \right|$$

- **High *S*:** we are able to predict the input parameter accurately
- **Low *S*:** relation between input parameter and pattern is weak
- **When score changes** from low to high or high to low, may indicate a transition

1



2

3

Instance	Predicted/Target mobility A	Predicted/Target mobility B	Sensitivity score (Mobility A/B)
1	0.37/0.97	**0.44/0.50**	1.77/**15.53**
2	0.24/0.04	0.36/0.75	4.96/2.58
3	**0.41/0.51**	0.46/0.84	**10.16**/2.64

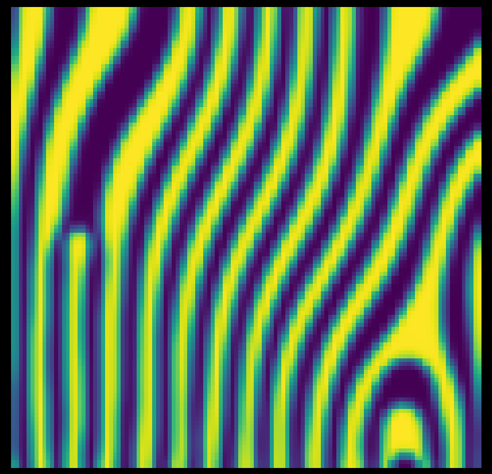
EVALUATE:

Predicted True

$$S = N / \sum_{i}^{N} |\hat{y}_i - y_i|$$

- **High *S*:** we are able to predict the input parameter accurately
- **Low *S*:** relation between input parameter and pattern is weak
- **When score changes** from low to high or high to low, may indicate a transition

1



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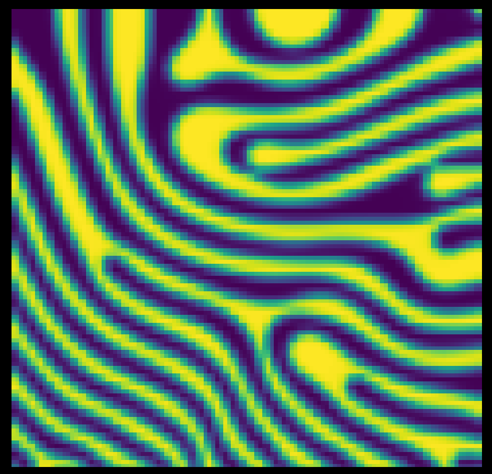
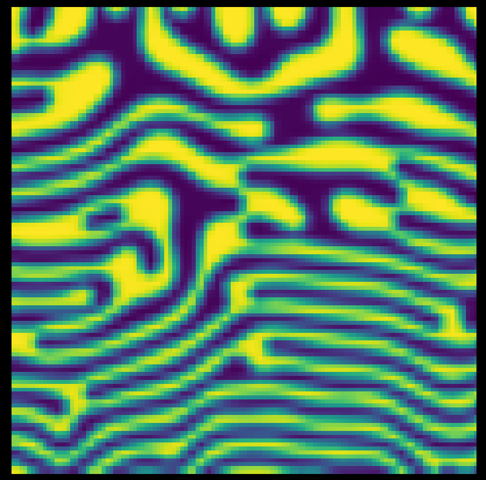


3



Instance	Predicted/Target deposition rate	Predicted/Target bulk mobility	Sensitivity score (deposition rate/mobility)
1	0.32/0.26	**4.09/4.68**	19.31/**1.68**
2	0.77/0.96	3.51/5.40	5.15/0.53
3	**0.75/0.79**	1.96/2.22	**20.58**/7.01

IDENTIFYING TOPOLOGICAL TRANSITIONS: REGIMES & COMPLEXITY

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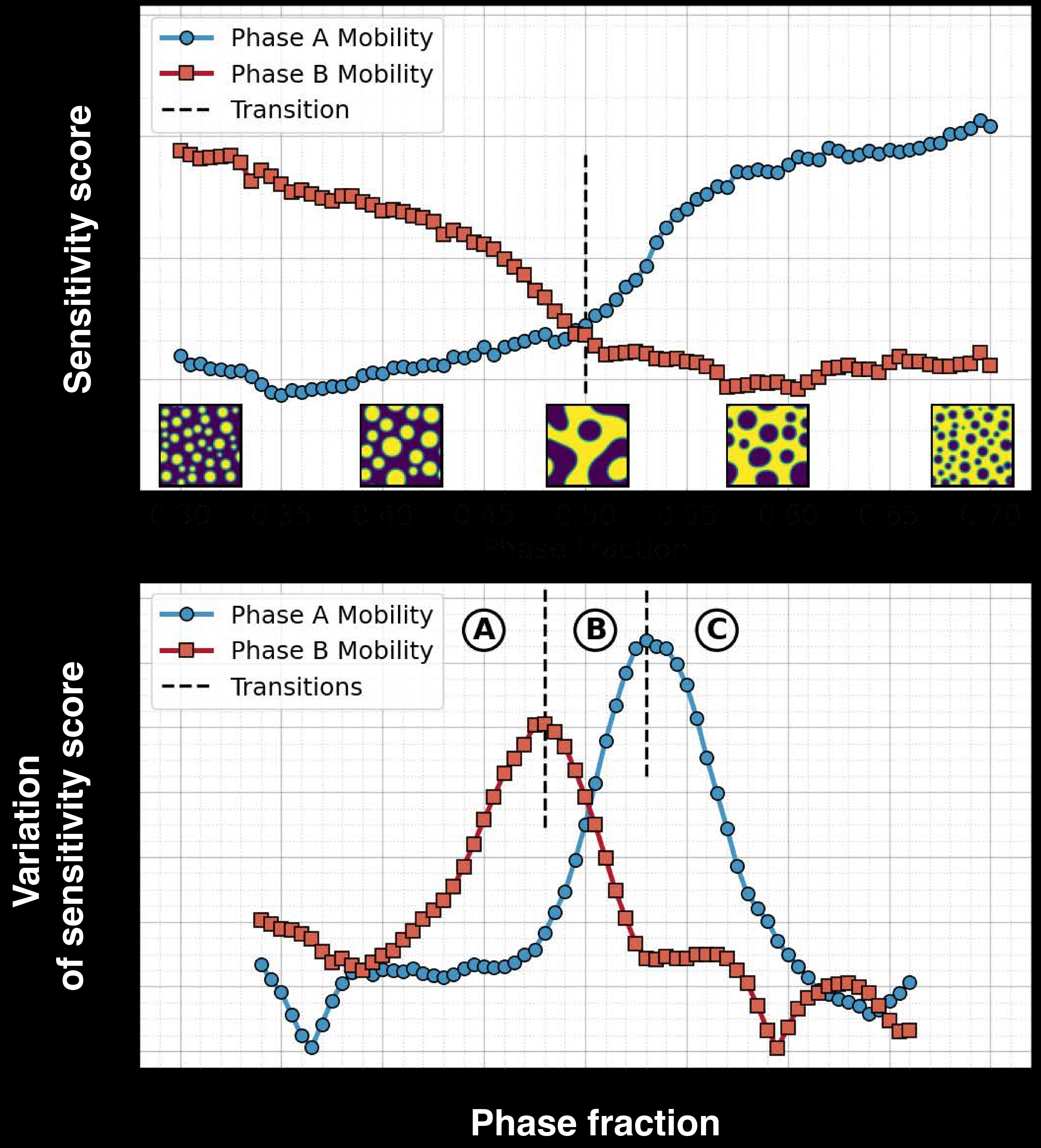
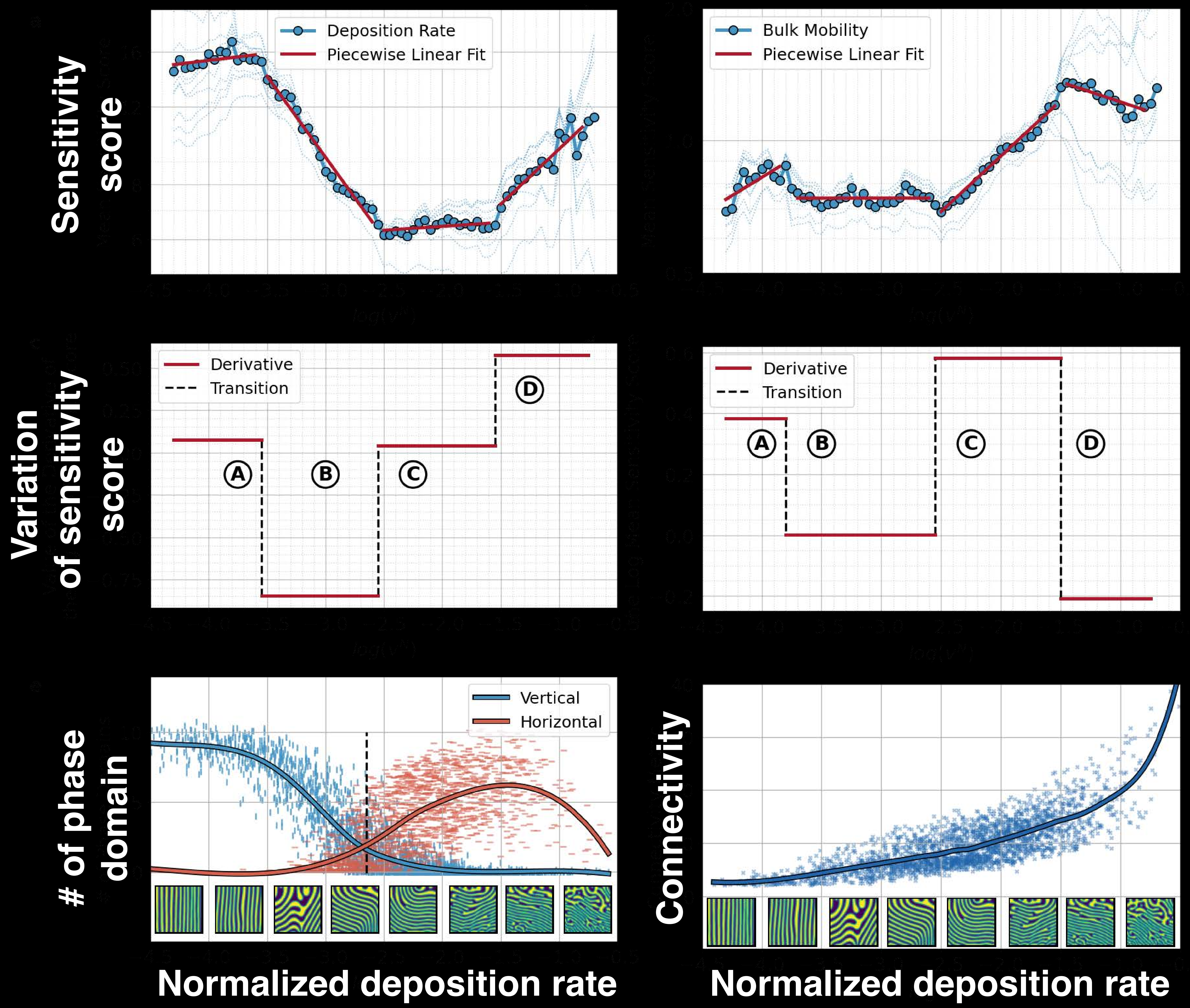


- **Qualitative changes** in microstructural patterns correspond to **changes in uncertainty** for our self-supervised prediction problem
- Detect major topological transitions (A => C)
- Detect intermediate regime (B)

Identifying Topological Transitions: Regimes & Complexity

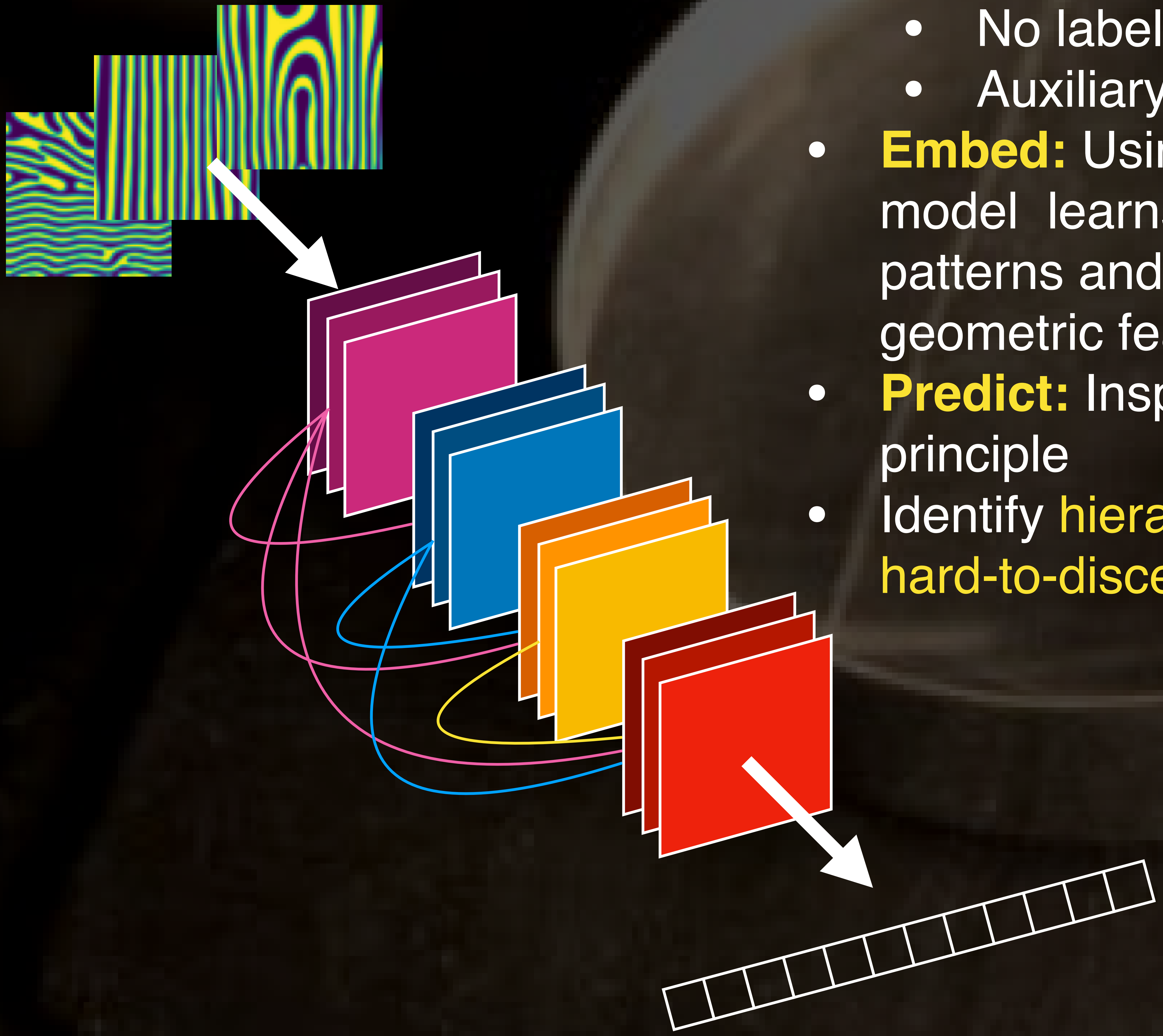
Predicting deposition rate from microstructures

Predicting bulk mobility from microstructures

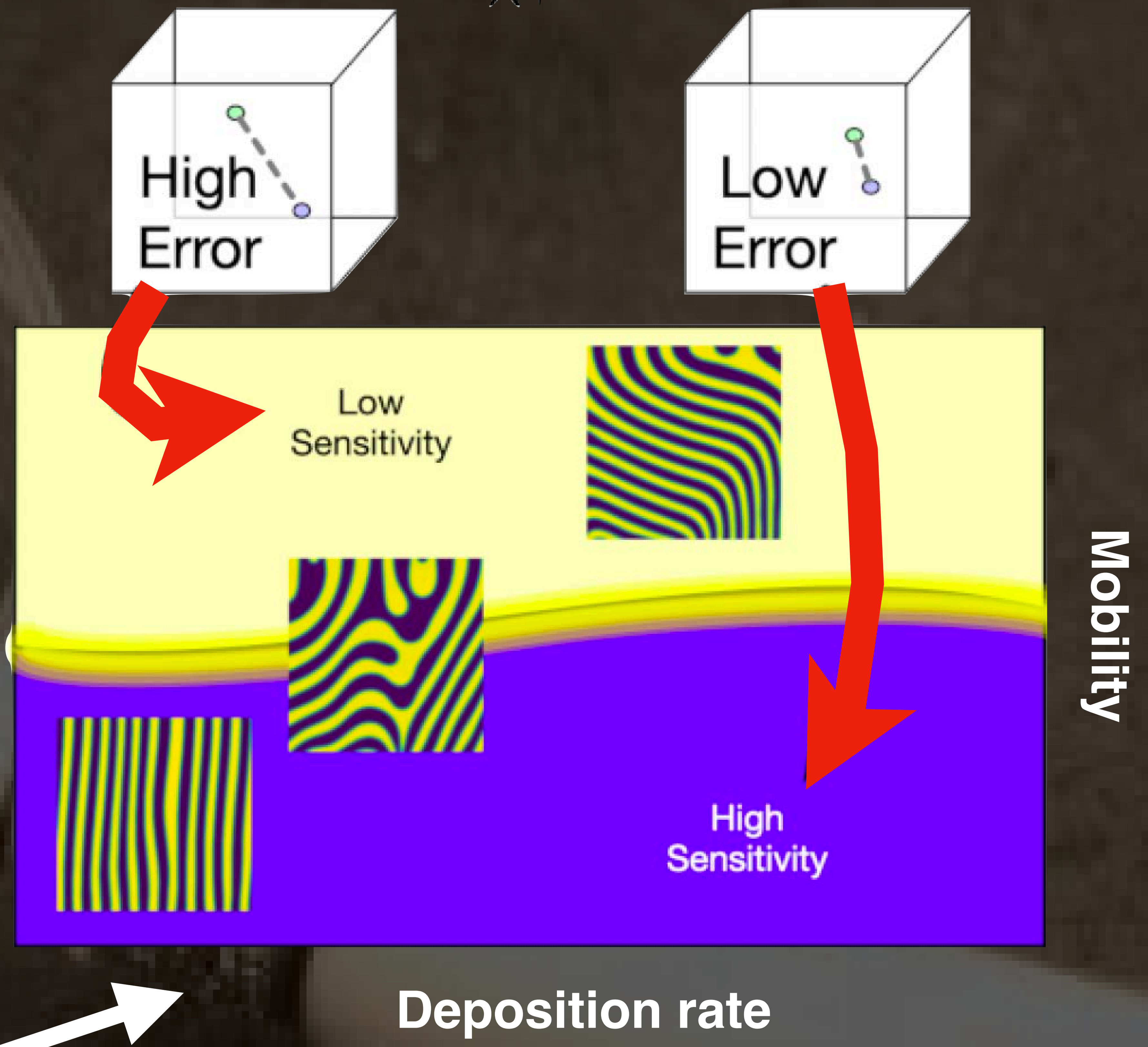


- **Qualitative changes** in microstructural patterns correspond to **changes in uncertainty** for our self-supervised prediction problem
- Detect major topological transitions (A => C)
- Detect intermediate regimes (A=>B; C=>D)
- Pattern orientation vs. pattern complexity (monomodal/multimodal patterns)

DETECTING HARD-TO-DISCERN TRANSITIONS IN PATTERN-FORMING PROCESSES BEYOND



- **Self-taught:**
  - No label needed
  - Auxiliary problem
- **Embed:** Using pre-trained CNN model learns to recognize basic patterns and more complicated geometric features
- **Predict:** Inspired by universality principle
- Identify hierarchy of hard-to-discern transitions



Abram et al., npj Computational Materials, 2022