Teaching AI Agents to See: Geometric Machine Learning for Single-Cell Data

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WHY AGENTS NEED TO SEE

Complex biological data needs more intelligent analysis

Embeddings reveal cell relationships:
- ➢ Clusters → Different kinds of cells
- ➢ Trajectories → Cell Development
- ➢ Branching → Cells "choosing" a path

Current agents describe structure in word, losing geometric information

We teach agents to "see" structure through quantitative metrics.

KEY FINDINGS

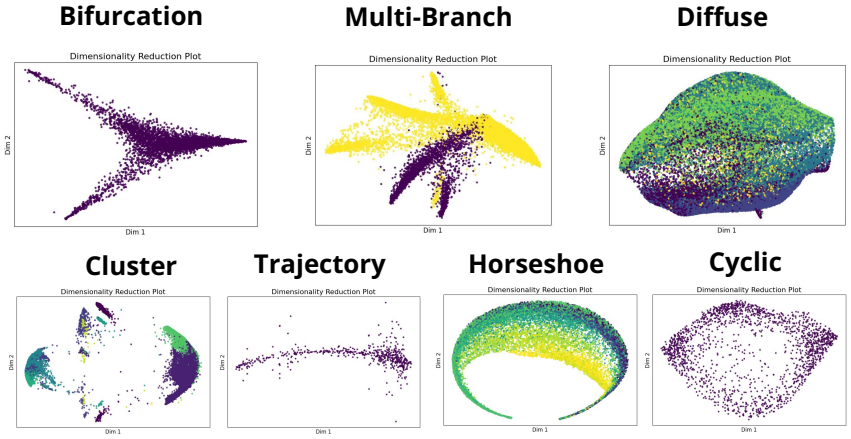
- **> 40.43%** accuracy on 7-class classification
- **> 2.9x** improvement over random baseline
- **> 53** geometric metrics extracted per embedding
- **> Spatial Entropy features are most predictive**
- > Distinctive shapes (horseshoe) classified well
- > Similar structures need more features (i.e., Clusters vs Multi-Branch)

LEARNING TO SEE

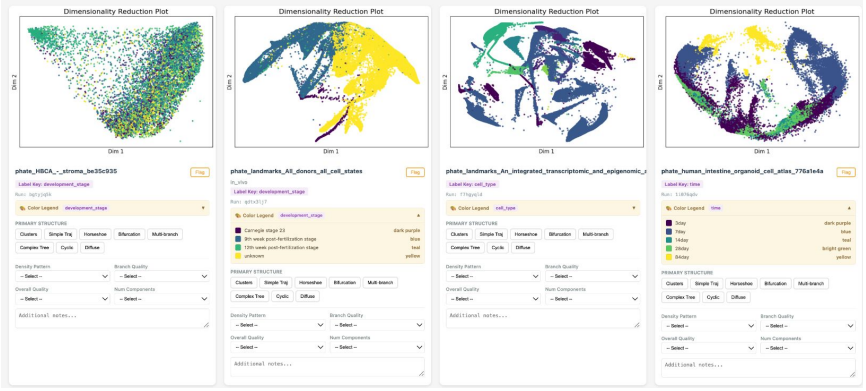
Data Pipeline:
- ➢ 100 datasets from CELLxGENE (Chan Zuckerberg Institute)
- ➢ PHATE embeddings (2D projections)
- ➢ 100 expert-labeled structures

Machine Learning Model:
- ➢ 53 geometric features (density, entropy, topology)
- ➢ ML classifier (SVM with RBF kernel)
- ➢ Leave-one-out validation

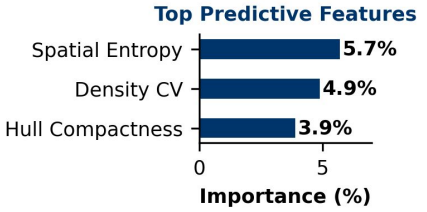
7-CLASS TAXONOMY

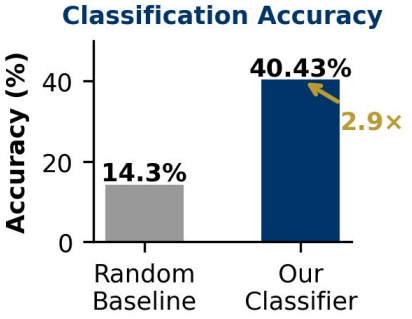


MANUAL CLASSIFICATION WEBSITE



RESULTS





NEXT STEPS

- ➢ Scale labeled data
- ➢ Integrate with multi-agent orchestration