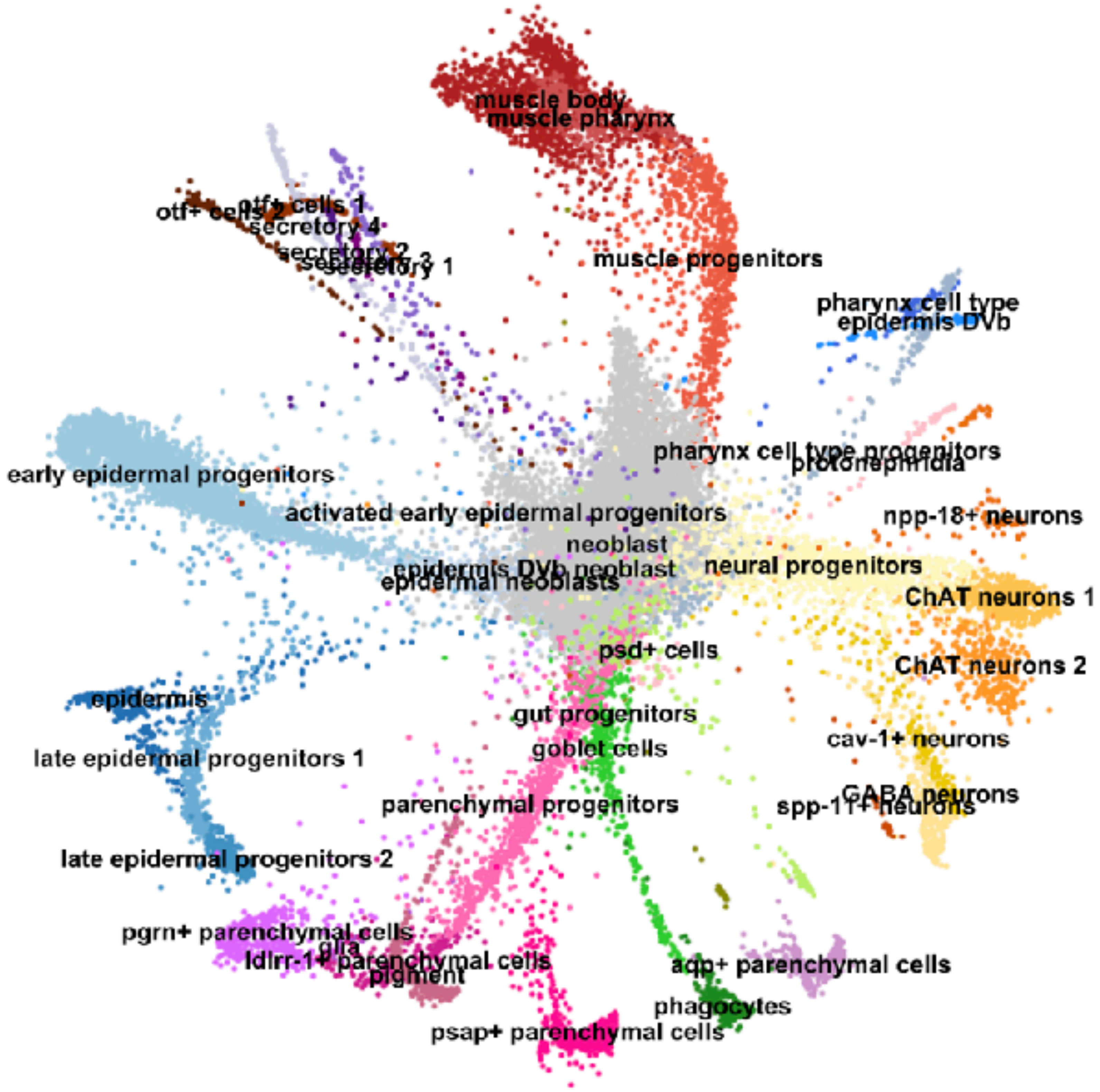
scverse

Scientific Python Sparse Summit

Isaac Virshup – 26th Sept. 2022

What is single cell RNA-seq?

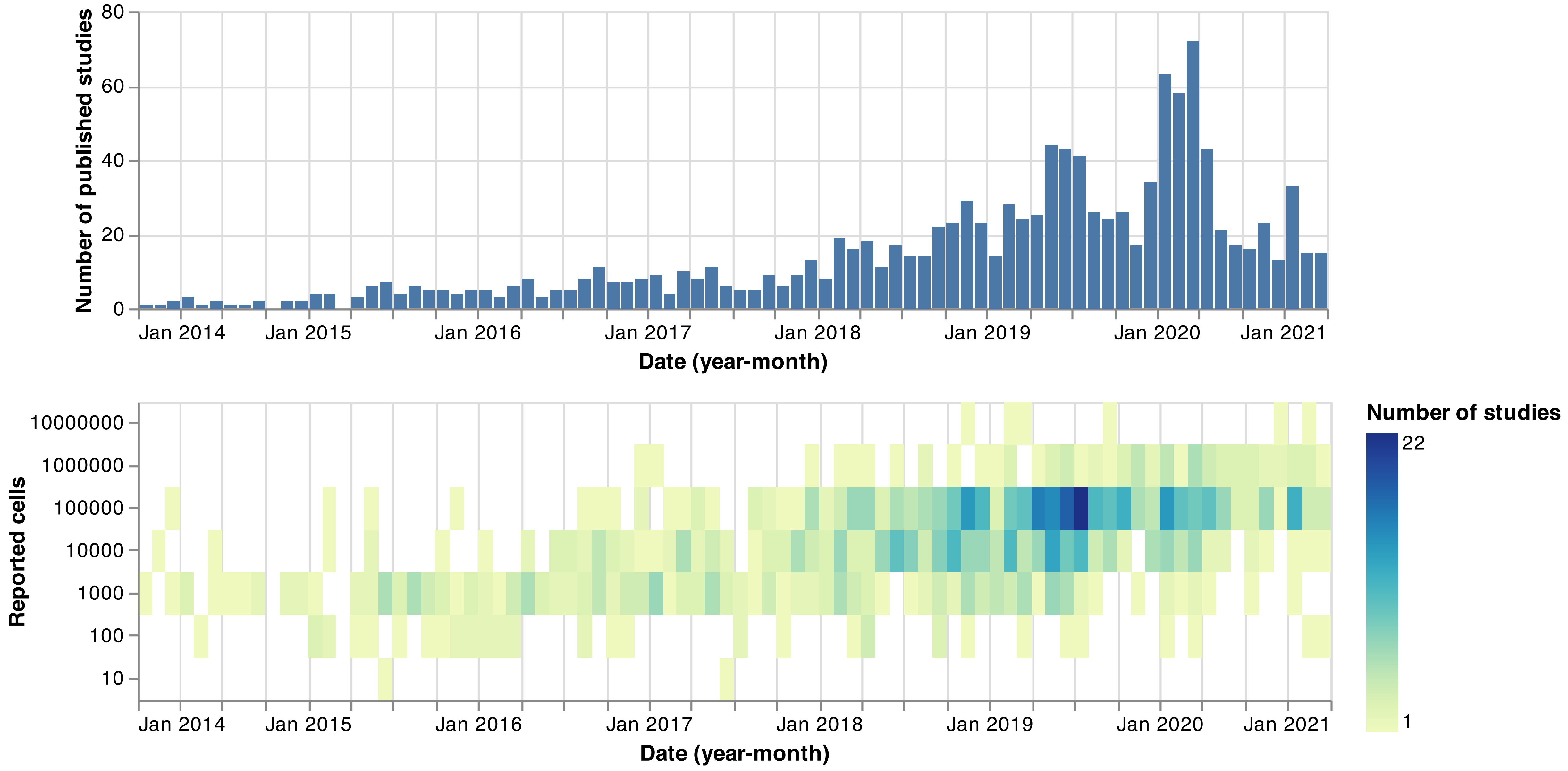
- High throughput assays on single cells
- Thousands to millions of observations (cells) on tens of thousands of variables (genes)
- Identify cell types, states, and dynamics



Wolf 2019, doi: 10.1186/s13059-019-1663-x

single cell data is sparse

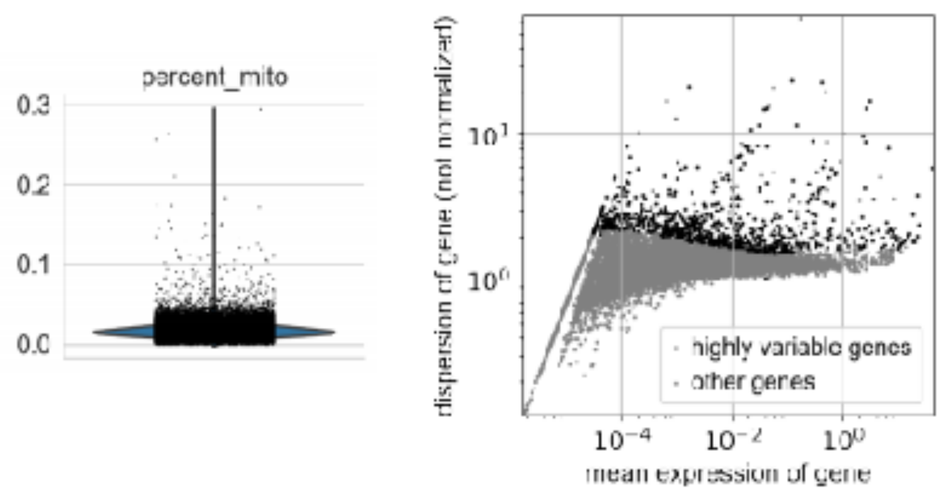
- The data is
  - ~20k possible genes
  - ~3-5k counts per cell
  - Increasing dataset sizes (1m+)
- Benefits of sparse representation
  - Memory usage
  - Compute time



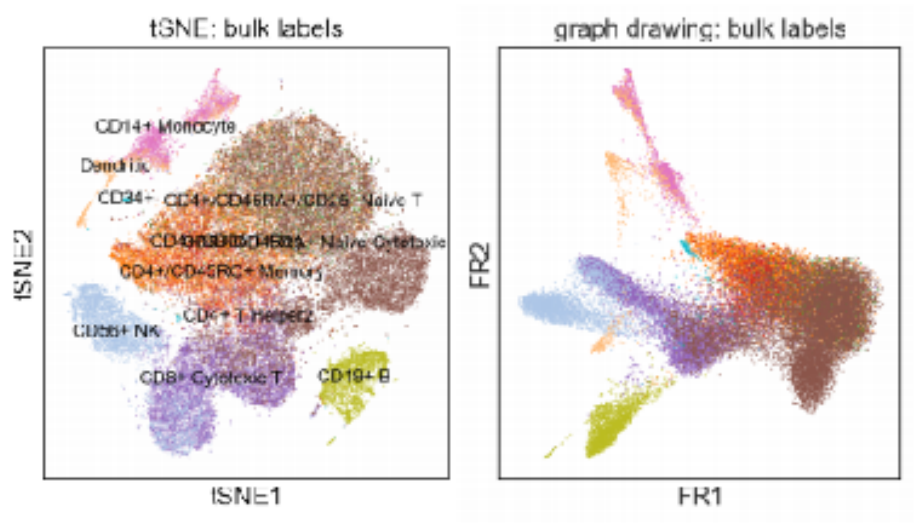
graphs are important in our domain

Normal Workflow

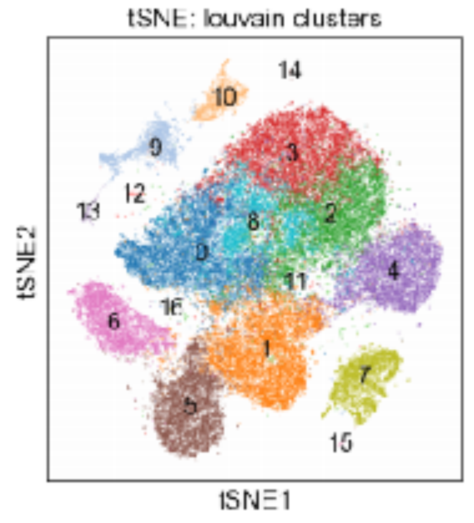
Preprocessing



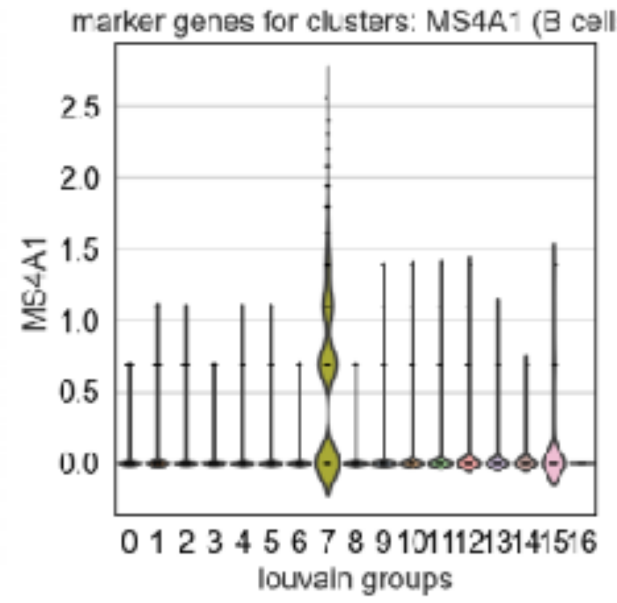
Viz via UMAP



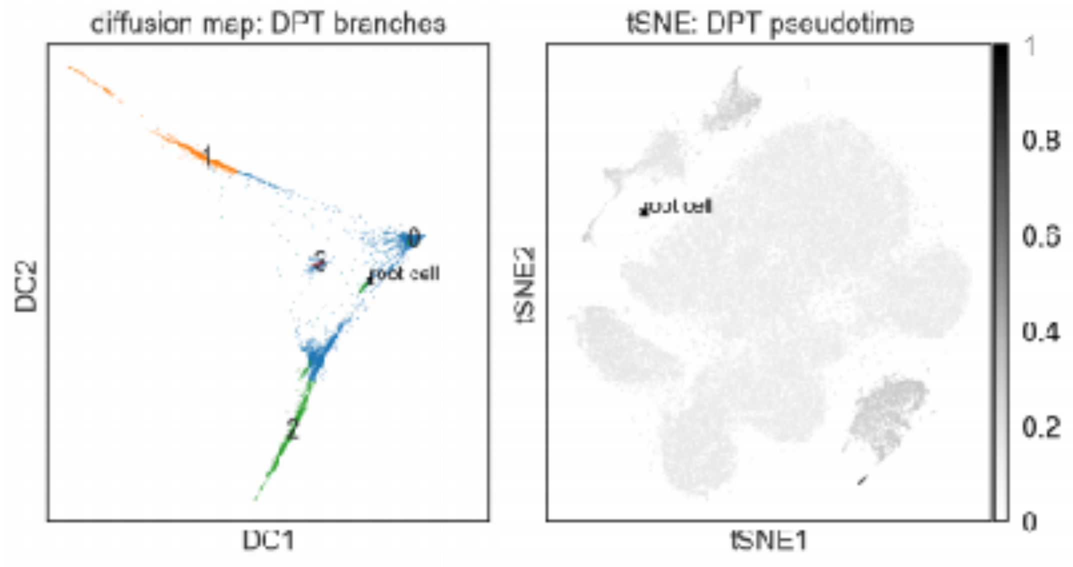
Clustering via
Community detection



Feature importance via
differential expression



Trajectory inference via
diffusion and optimal transport



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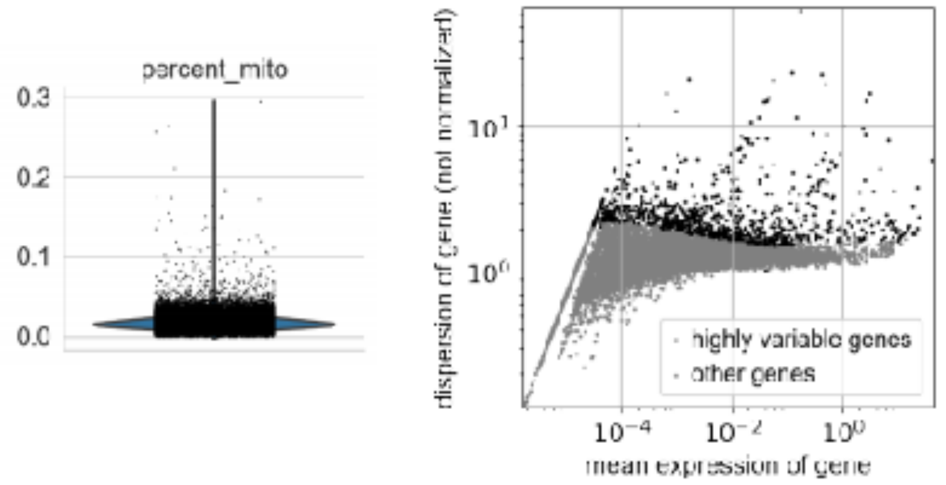
Normal Workflow

Graph based

Preprocessing



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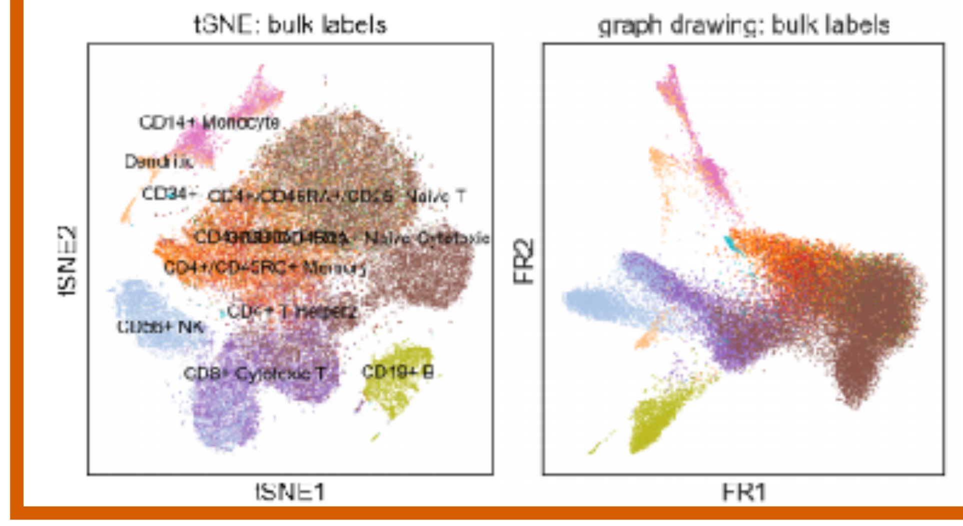
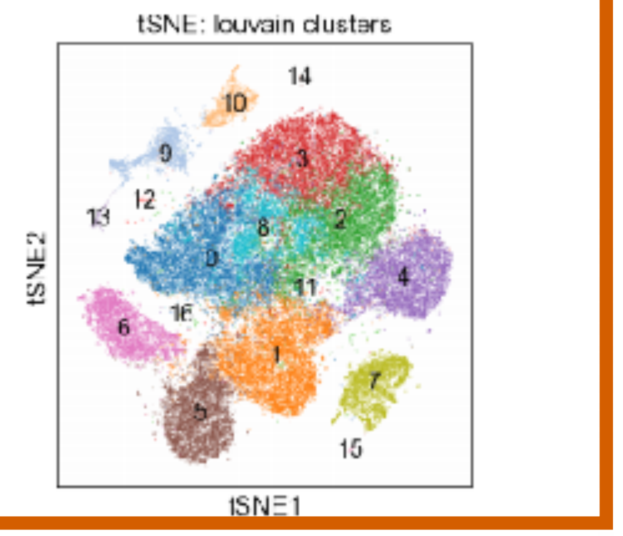
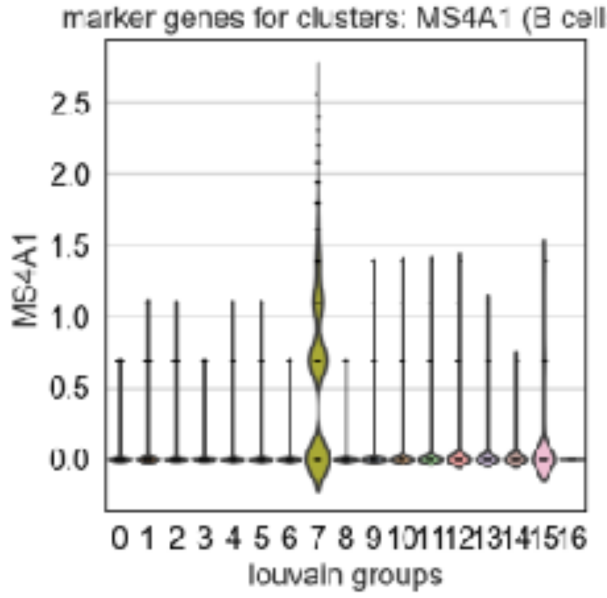


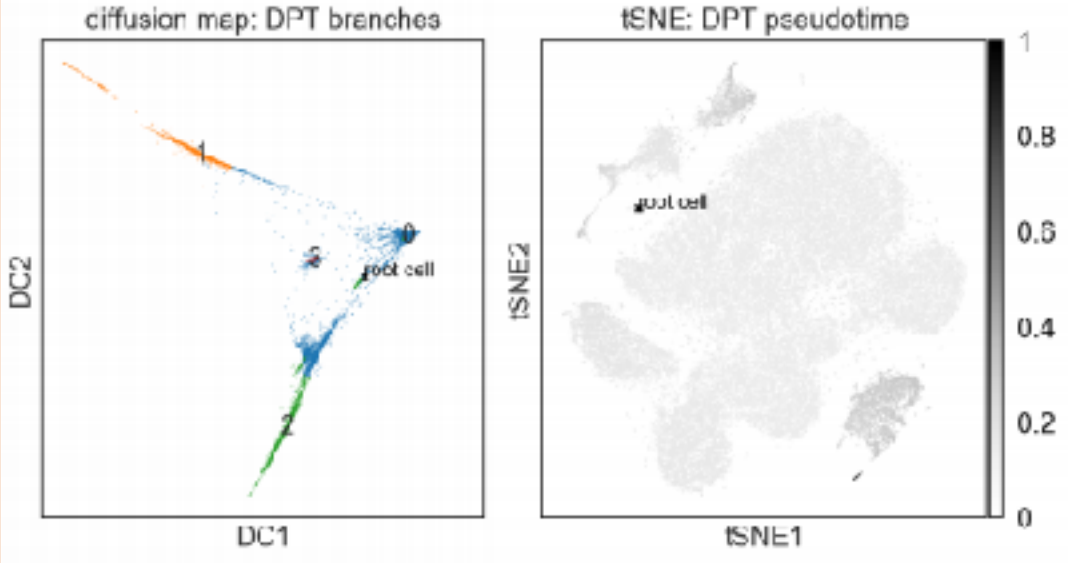
Clustering via Community detection



Feature importance via differential expression



Trajectory inference via diffusion and optimal transport



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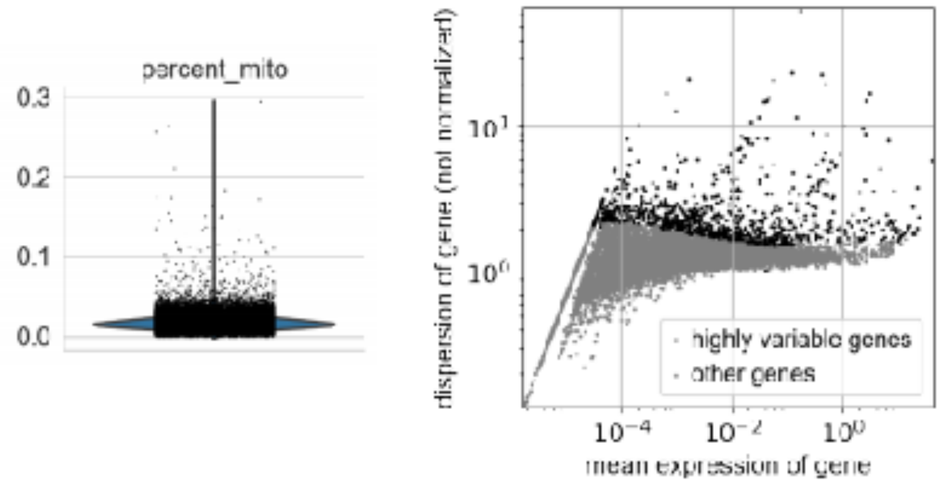
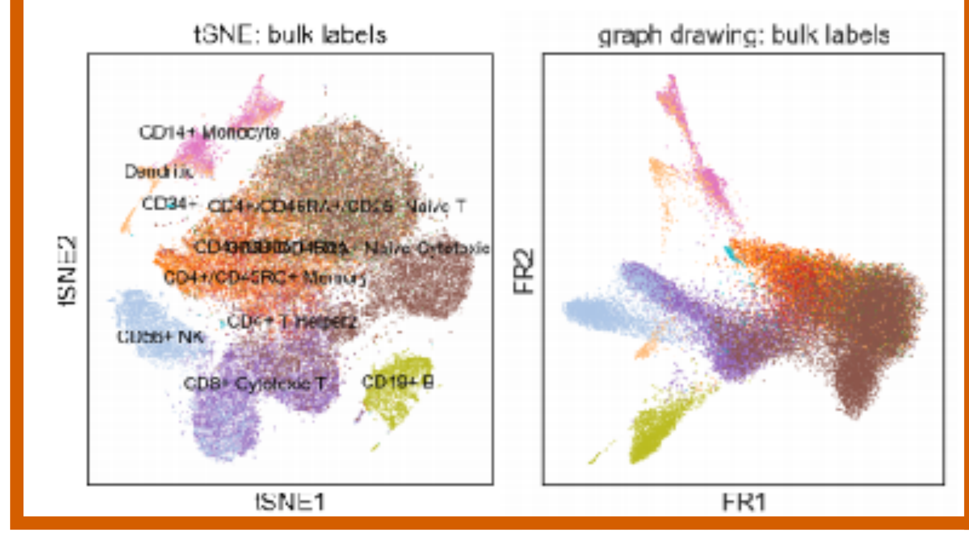
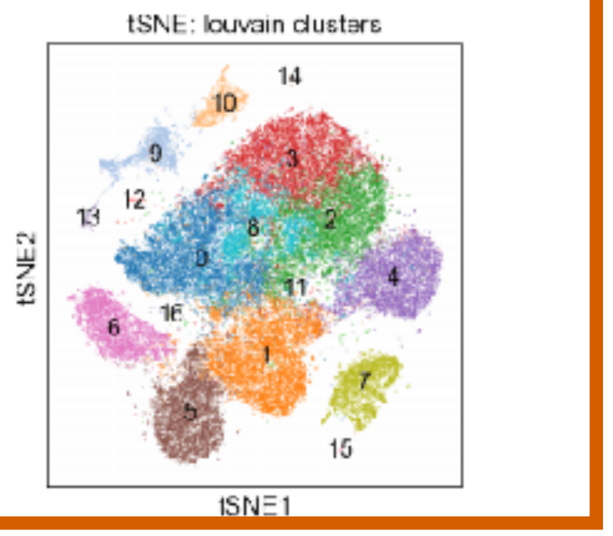


Viz via UMAP



Clustering via Community detection



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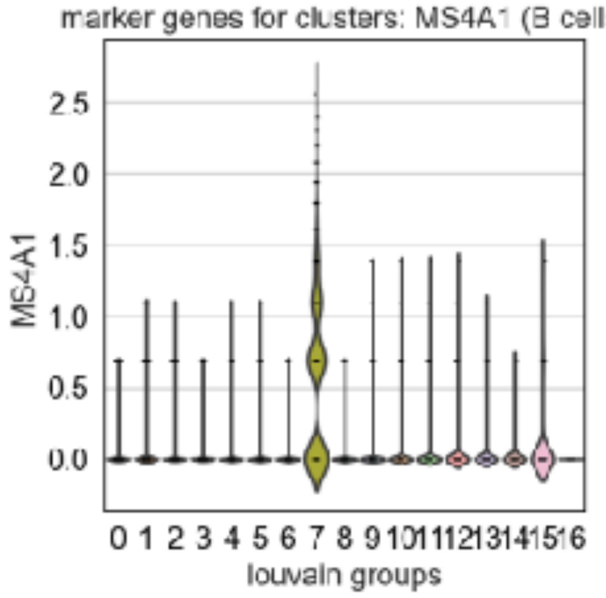

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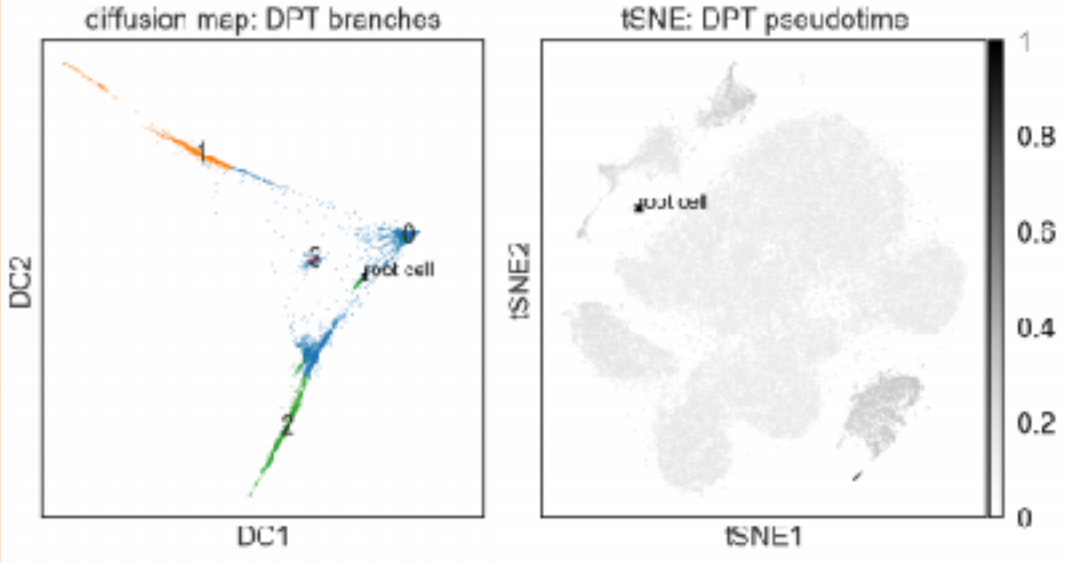
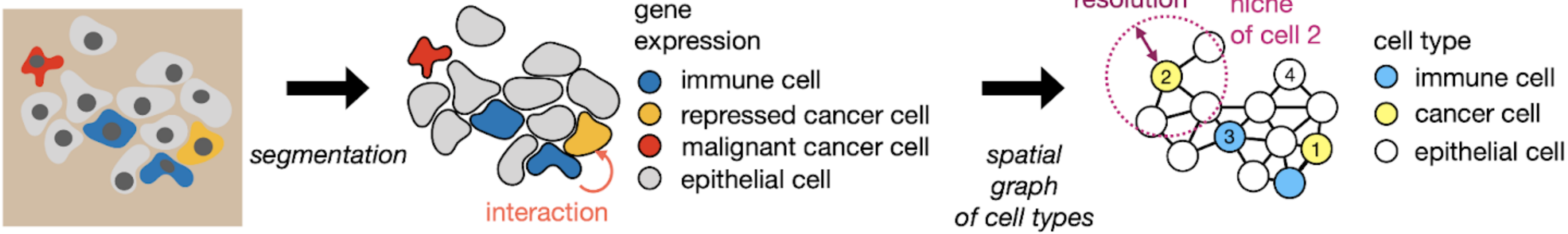


Spatial Graphs



gene expression

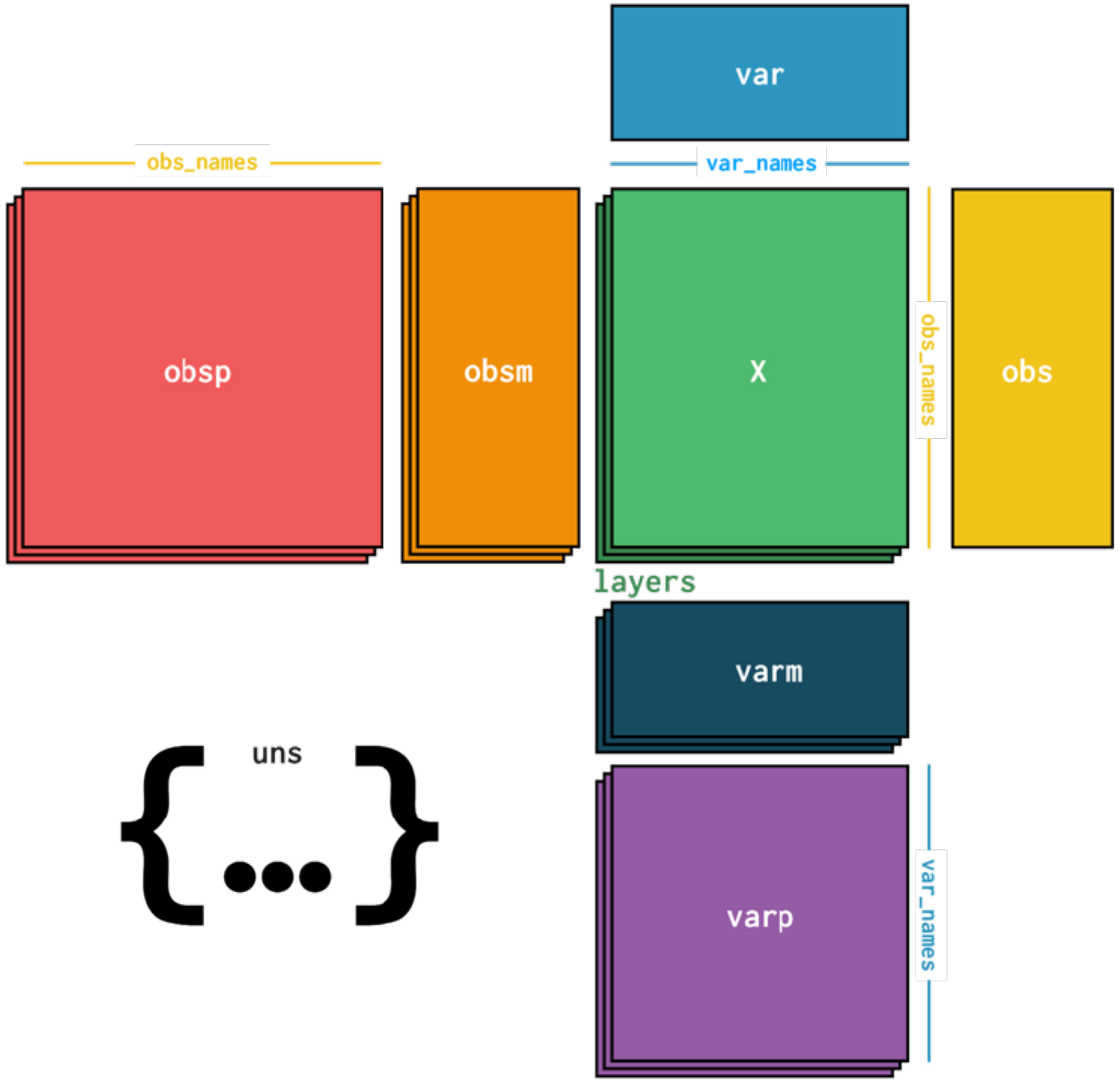
- immune cell
- repressed cancer cell
- malignant cancer cell
- epithelial cell

cell type

- immune cell
- cancer cell
- epithelial cell

How we handle sparse data

- AnnData container
  - Special casing sparse access
  - On disk representation (zarr, hdf5)
    - with out of core access (largely used for viz)
- Compute
  - PCA on sparse data
  - Fast sparse statistics (mean, var)
  - Fast Graph statistics (Morans I, etc)



What do we want

- Array API friendly sparse arrays
  - Eventual compatibility with xarray
  - Dask support (?)
- Consistent support throughout ecosystem (e.g. sklearn, pytorch-geometric)
- Out of core sparse arrays