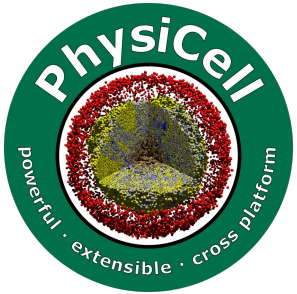
pcdl, pandas, and anndata data analysis plots

Elmar Bucher
PhD Student 2013-09-17
PhysiCell Project



PhysiCell data analysis with one lines

- PhysiCell sample project 2D: interaction.
- PhysiCell sample project 3D: cancer-immune.
- Tutorial: https://github.com/elmbeech/physicelldataloader/blob/master/man/TUTORIAL.md
- Jupyter notebook: https://github.com/elmbeech/physicelldataloader/blob/master/man/jupyter/pcdl_repl_programming.ipynb

pcdl dataset fetching functions

core python:

- mcdsts.get_cell_df_states() # python dictionary with **feature to states** or state count mapping.
- mcdsts.get_conc_df_states() # python dictionary with **feature to states** or state count mapping.

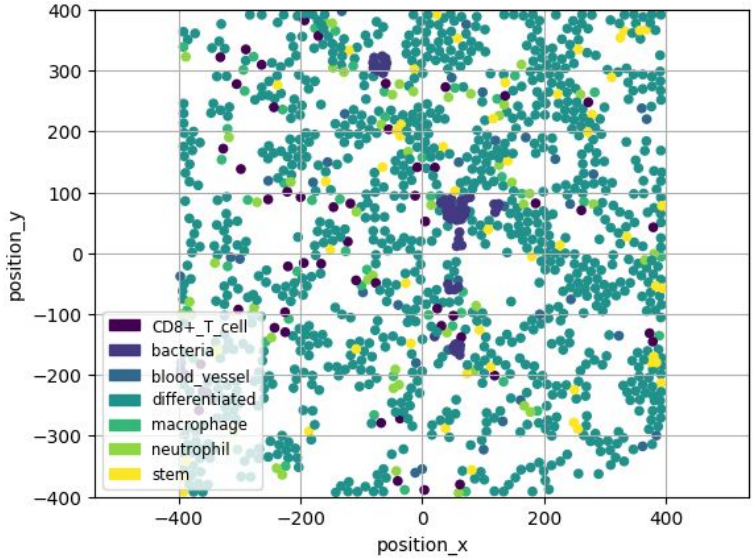
pandas:

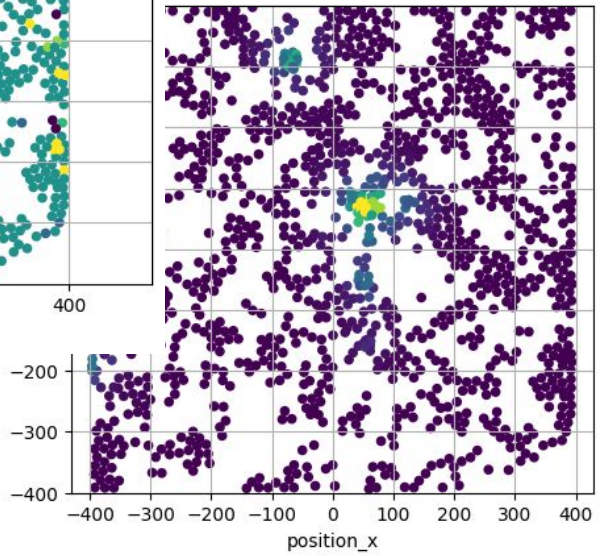
- mcds.get_cell_df() # pandas DataFrame with **cell agent to categorical and numerical data** mapping.
- mcds.get_conc_df() # pandas DataFrame with **voxel to substrate concentration** mapping.
- mcds.get_unit_se() # pandas Series with **parameter to unit** mapping.

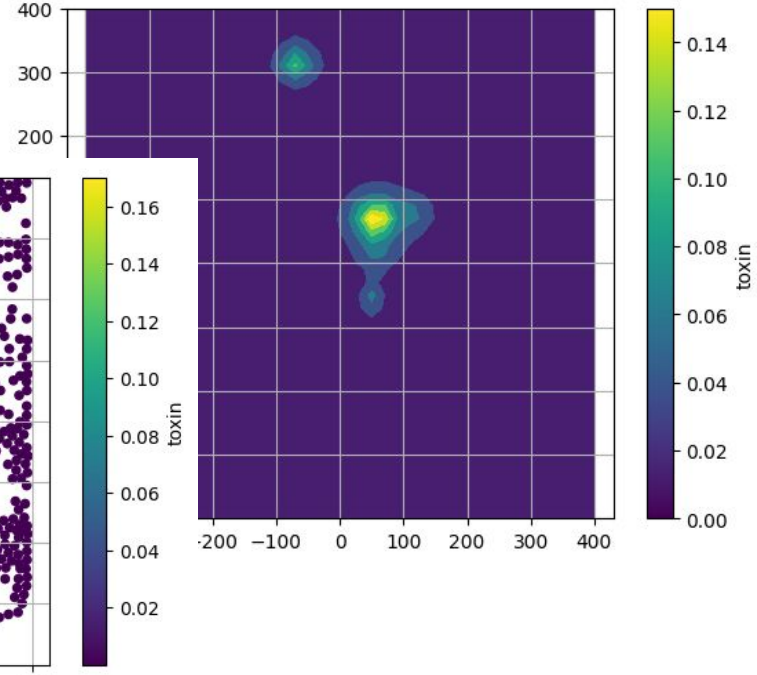
scverse:

- mcds.get_anndata() # transform PhysiCell **TimeStep into anndata** object.
- mcdsts.get_anndata() # transform PhysiCell **TimeSeries into anndata** object.

TimeStep pcdl: get_scatter() & get_contour()





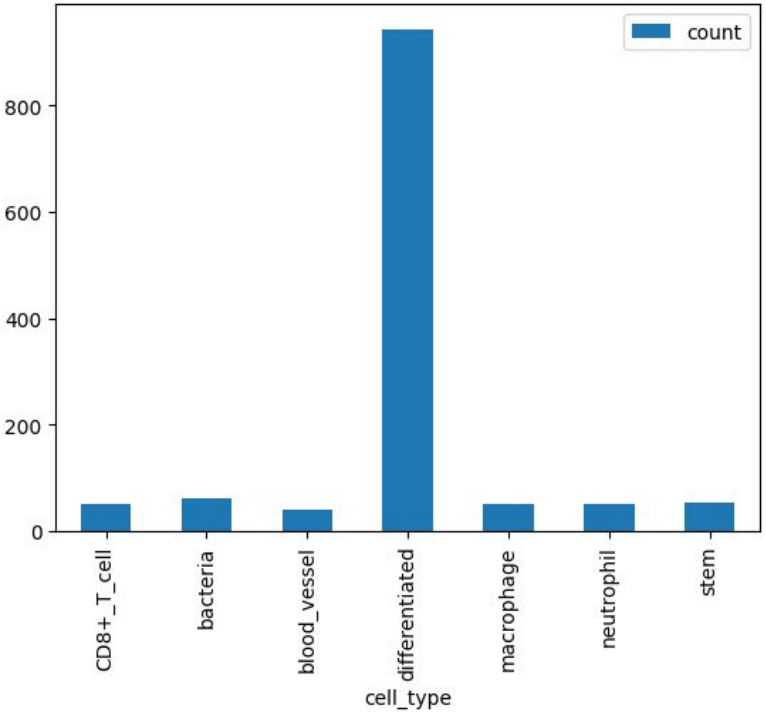


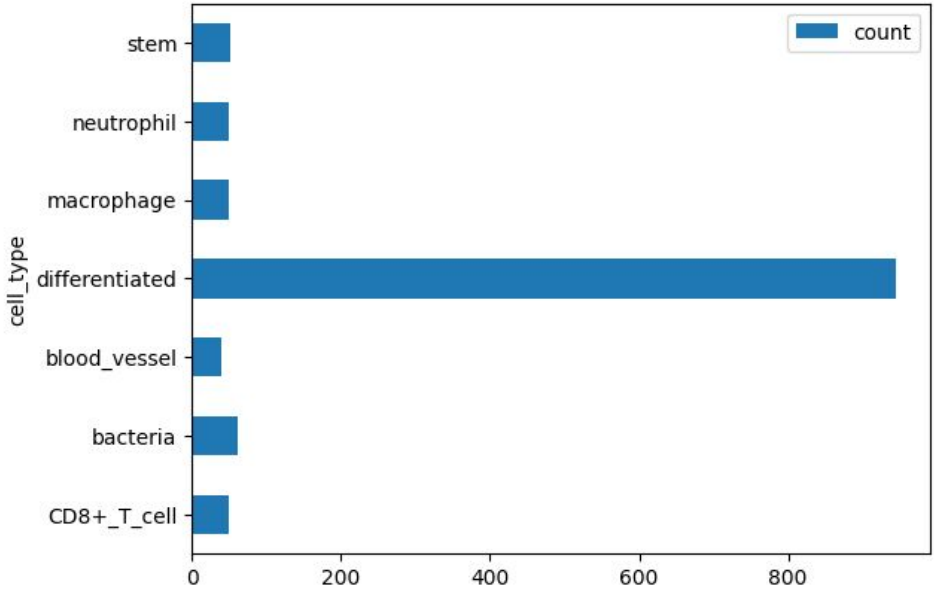
pcdl TimeSeries plotting functions

- mcdsts.make_imgcell()
- mcdsts.make_imgconc()
- mcdsts.make_gif()
- mcdsts.make_movie()

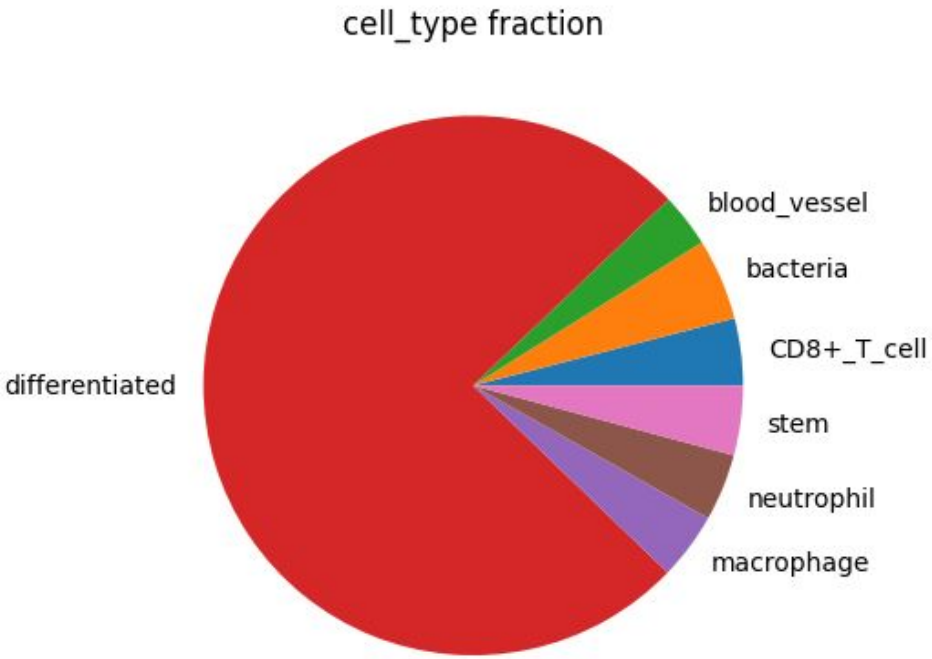
pandas

TimeStep pandas: bar & barh

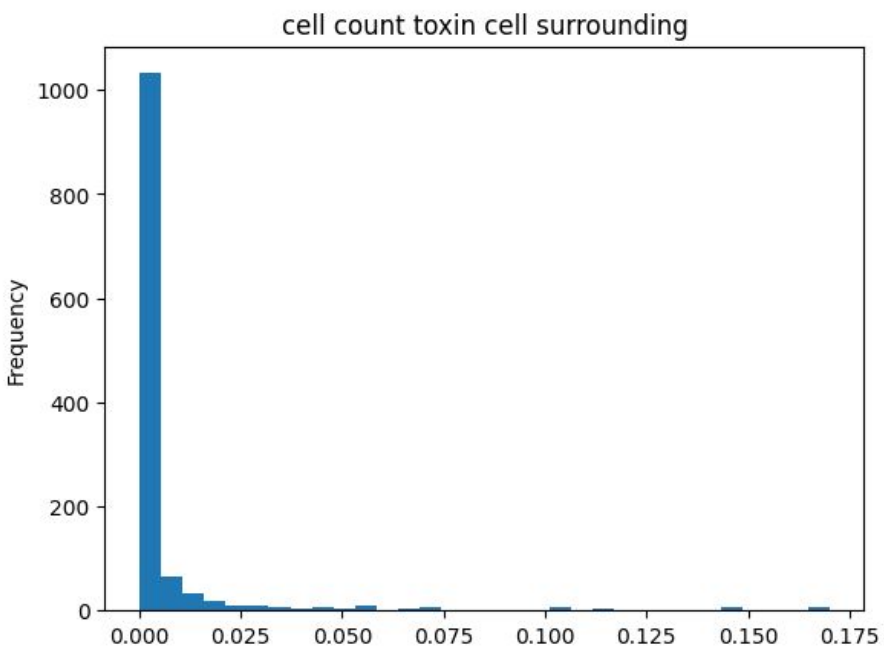


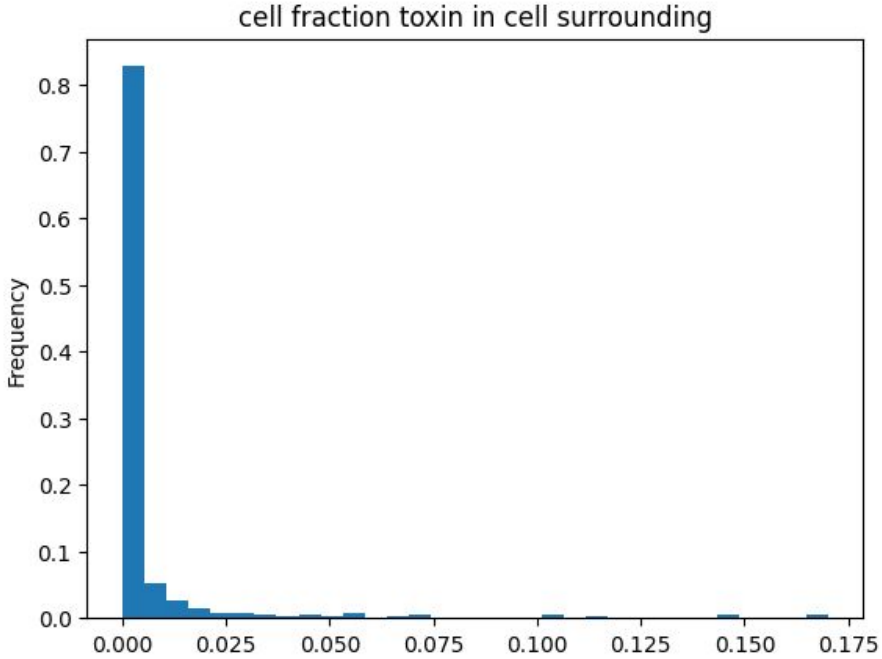


TimeStep pandas: pie

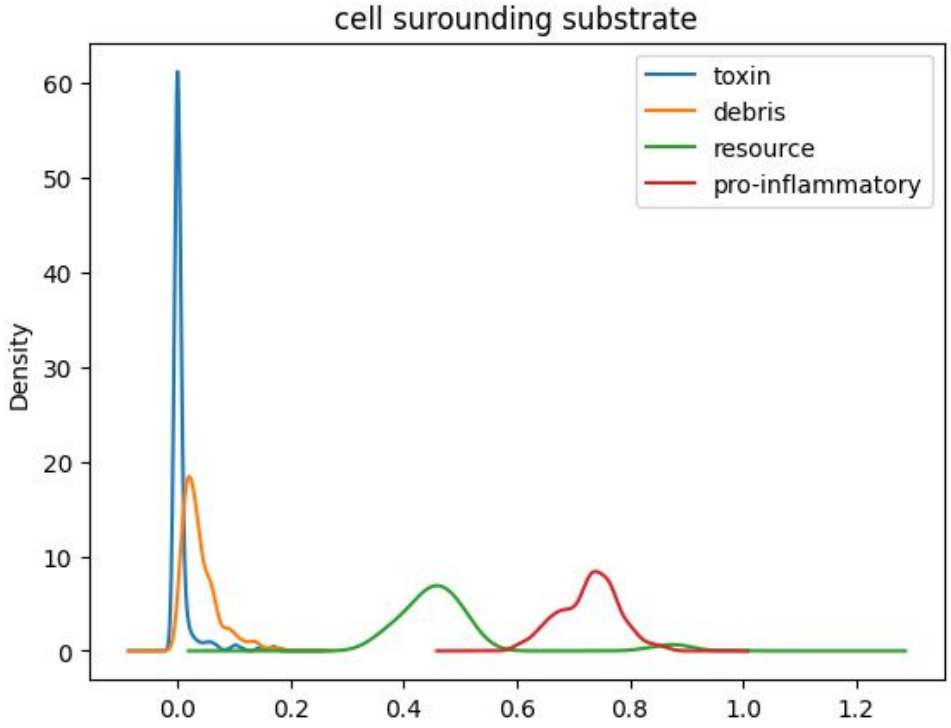


TimeStep pandas: histogram

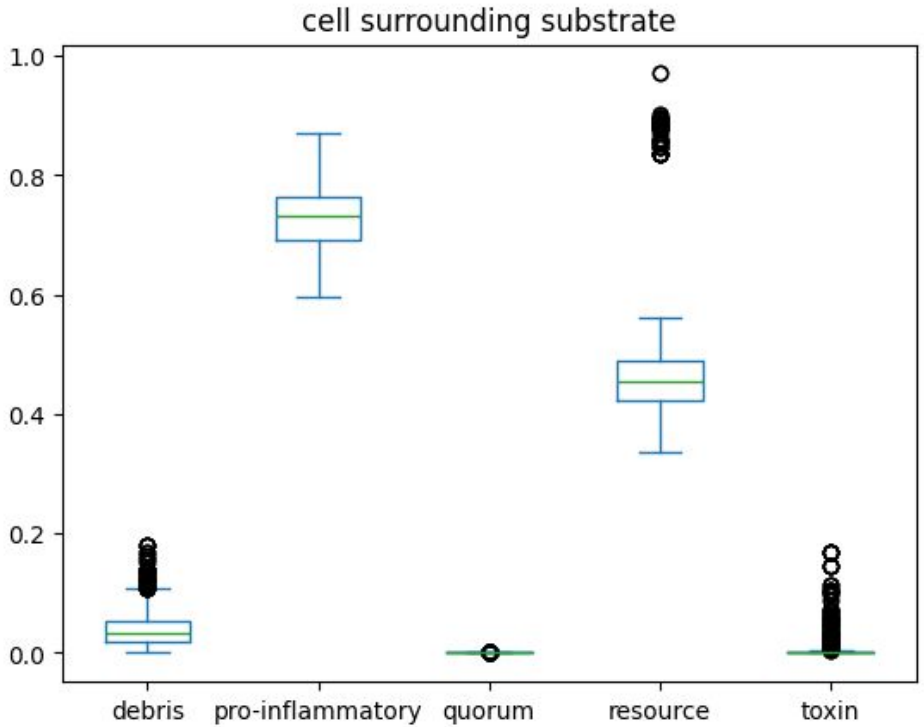




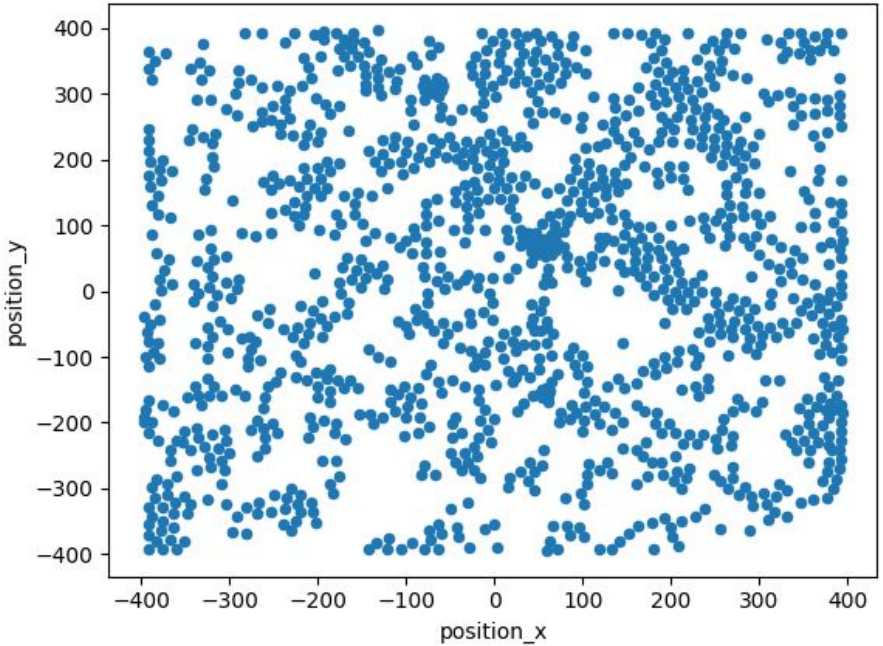
TimeStep pandas: kernel density estimation

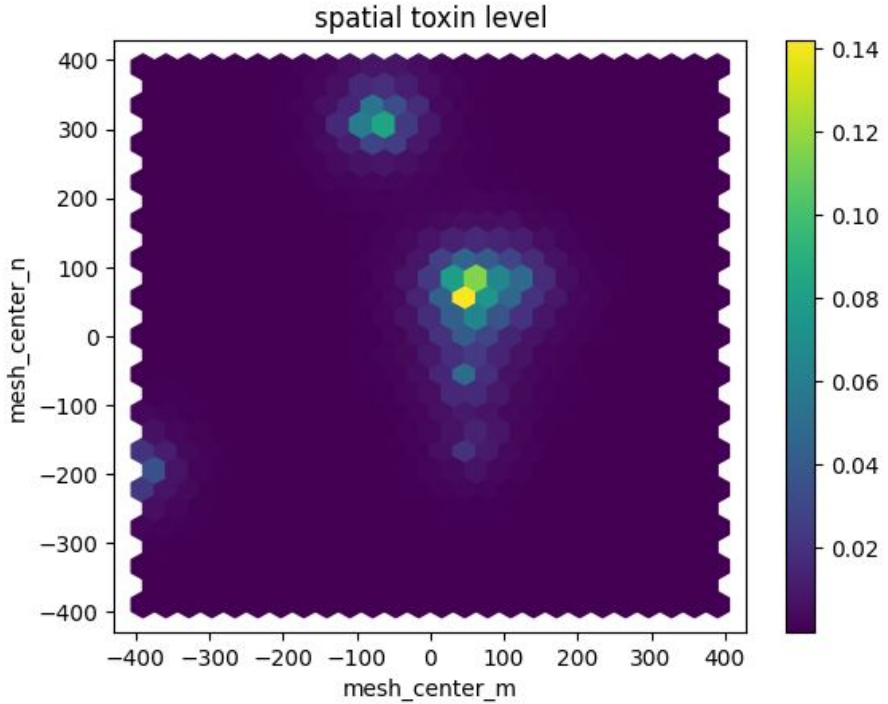


TimeStep pandas: box

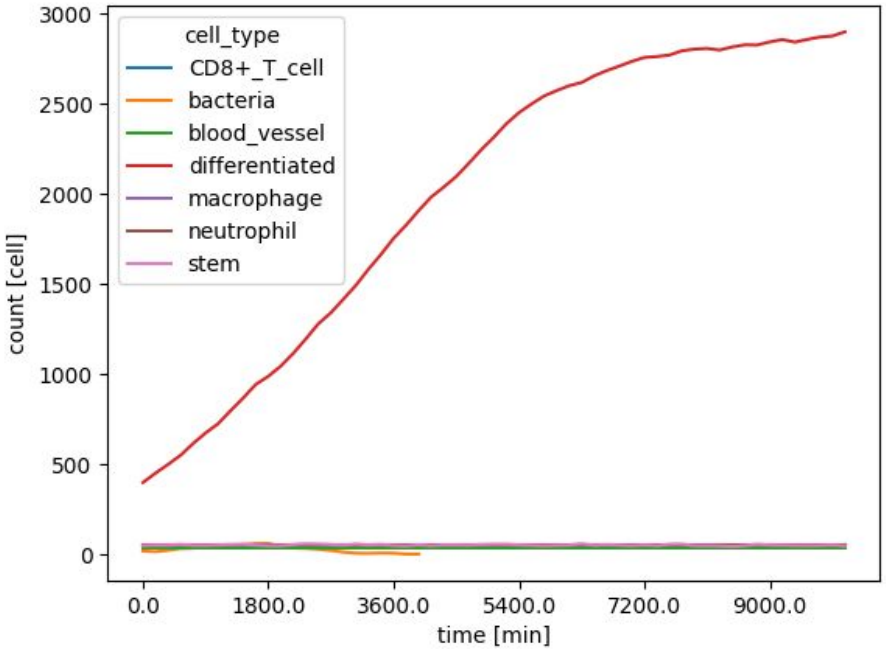


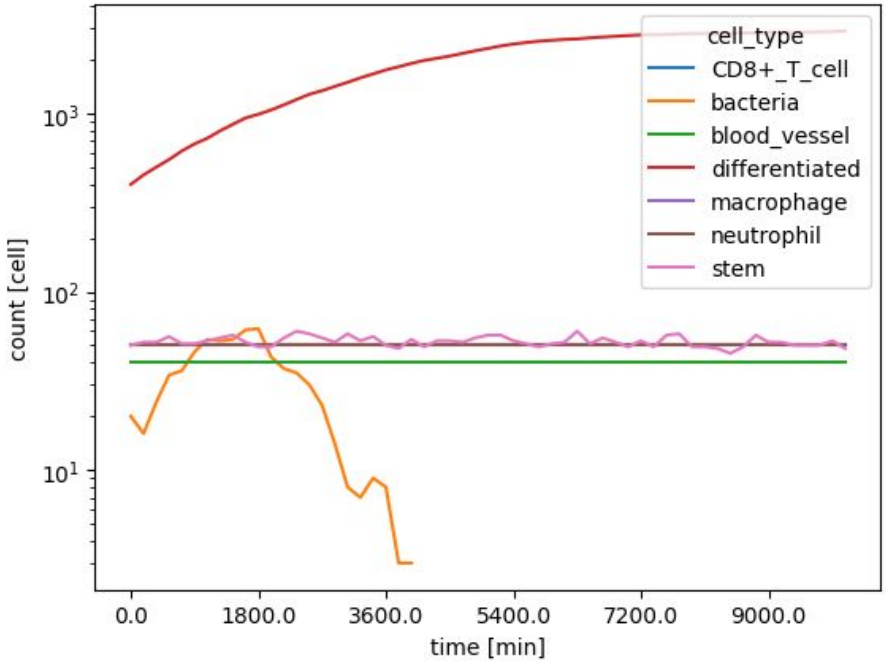
TimeStep pandas: scatter & hexbin



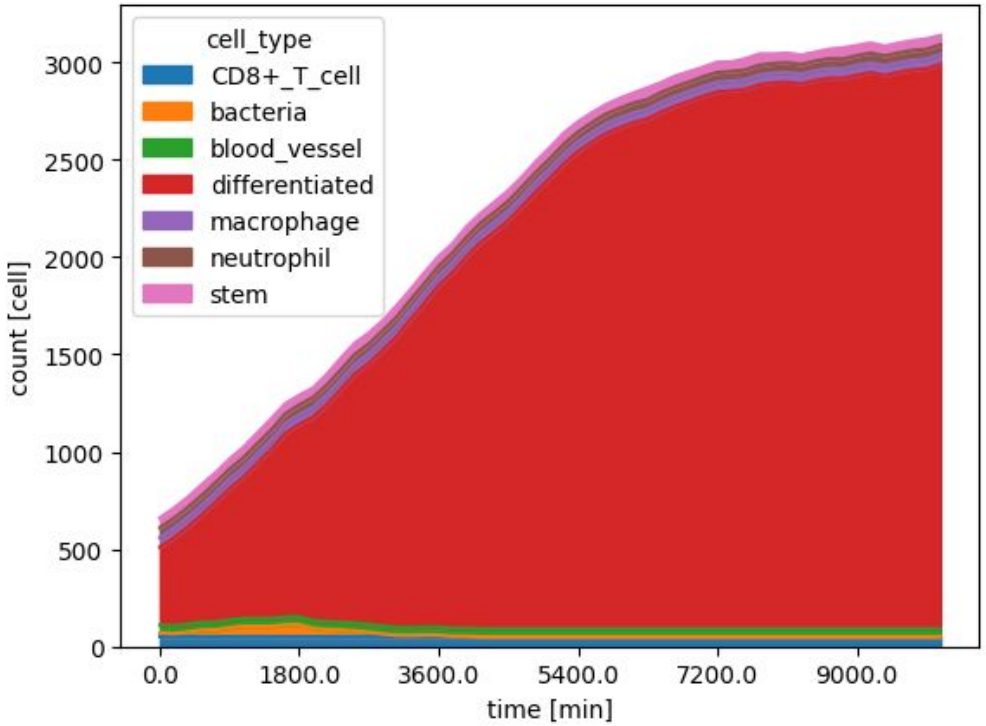


TimeSeries pandas: line



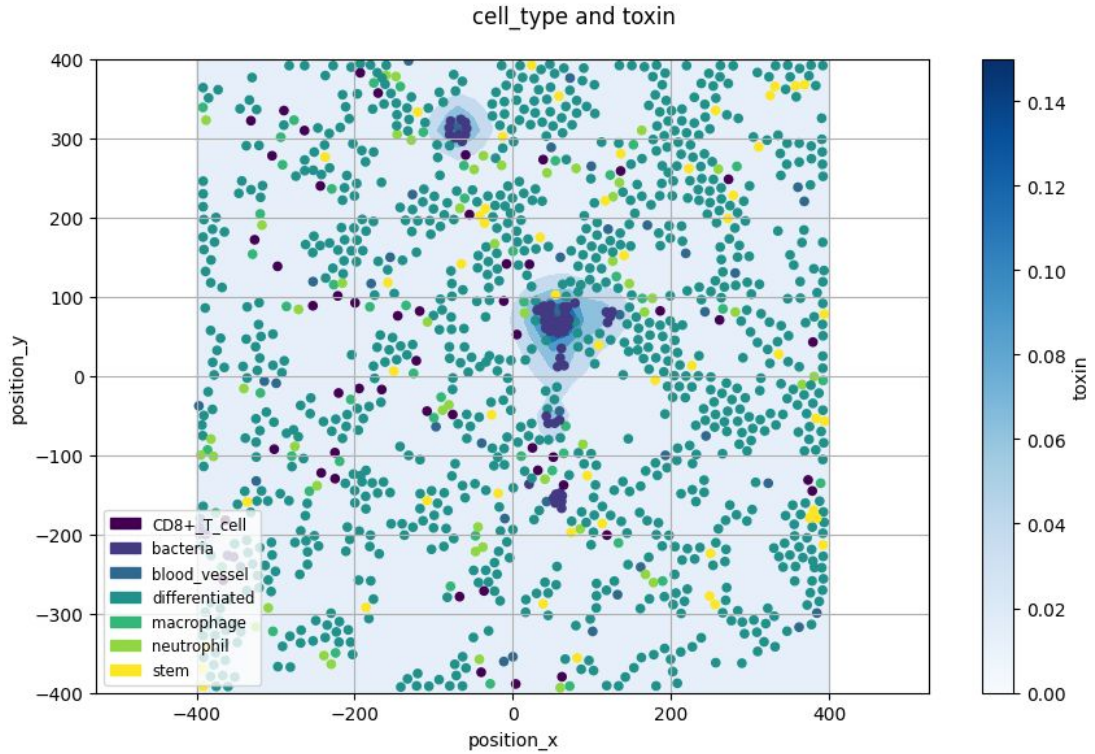


TimeSeris pandas: area



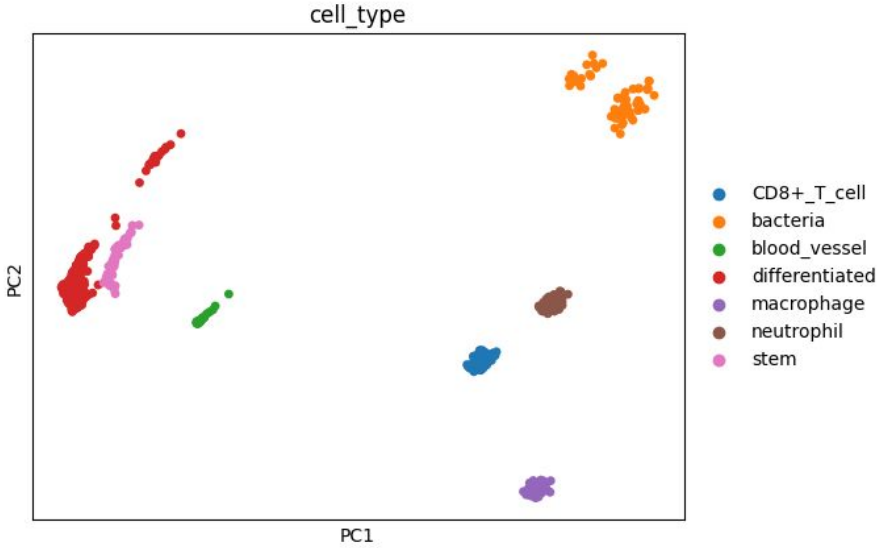
matplotlib

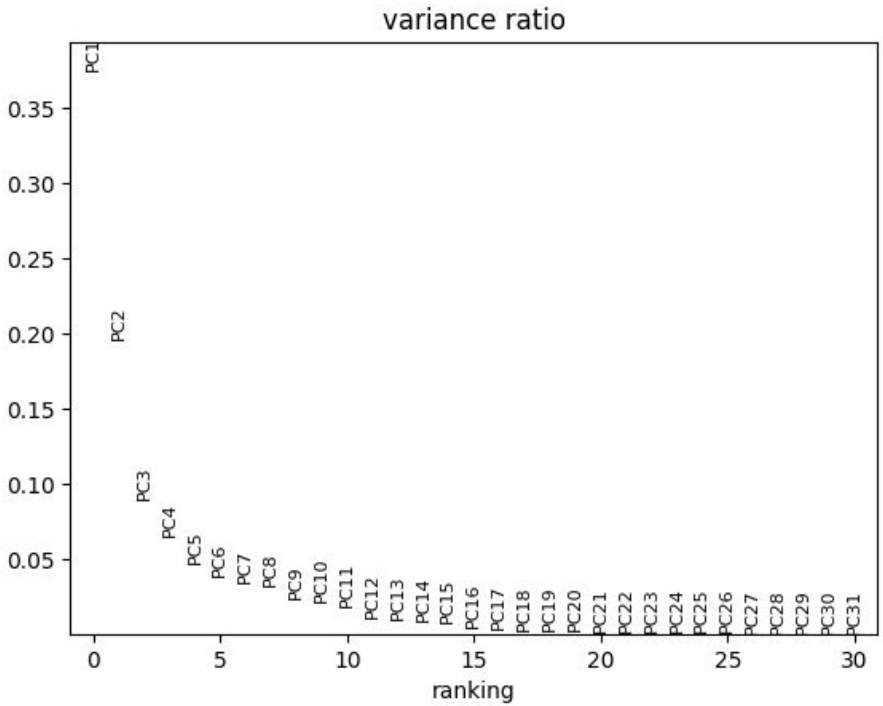
matplotlib embedding



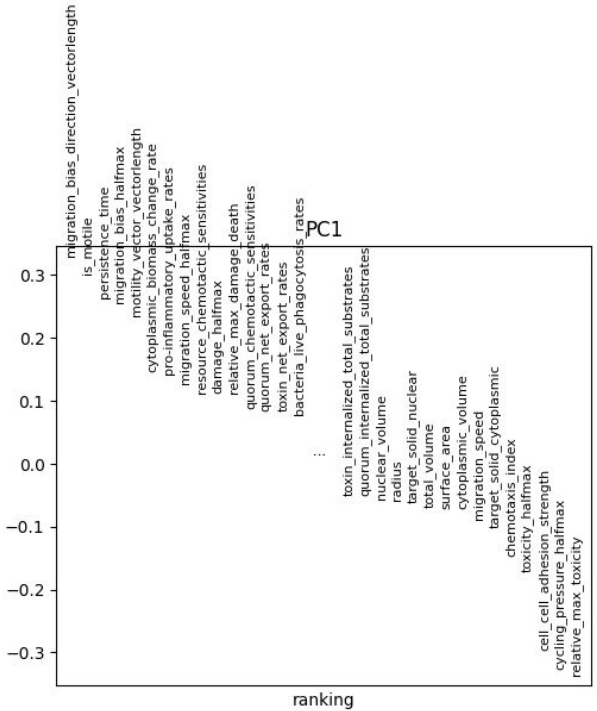
scanpy

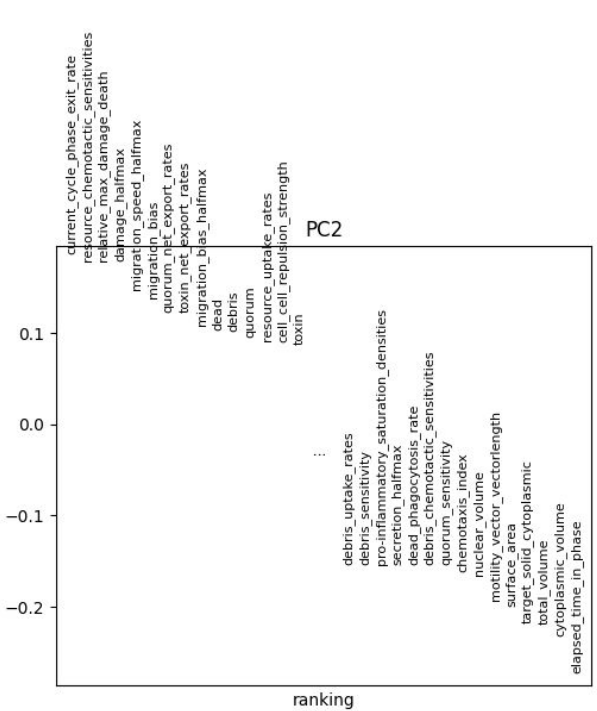
scanpy: pca & pca_variance_ratio

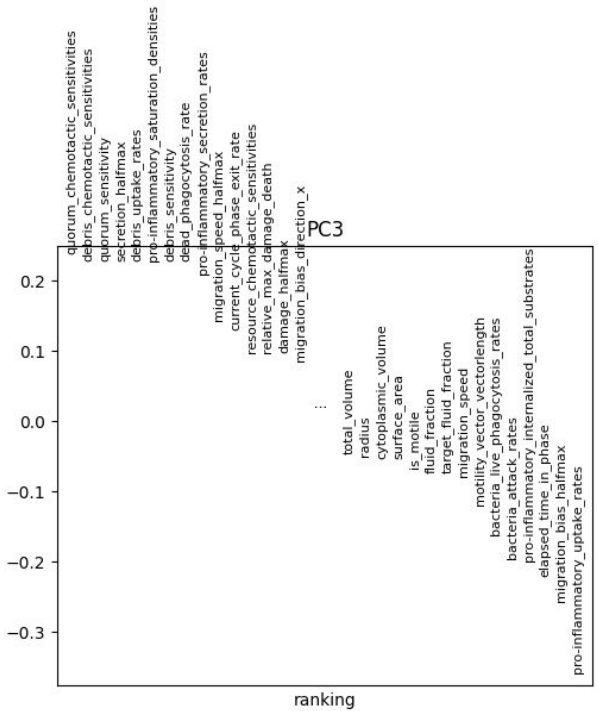




scanpy: pca_loadings

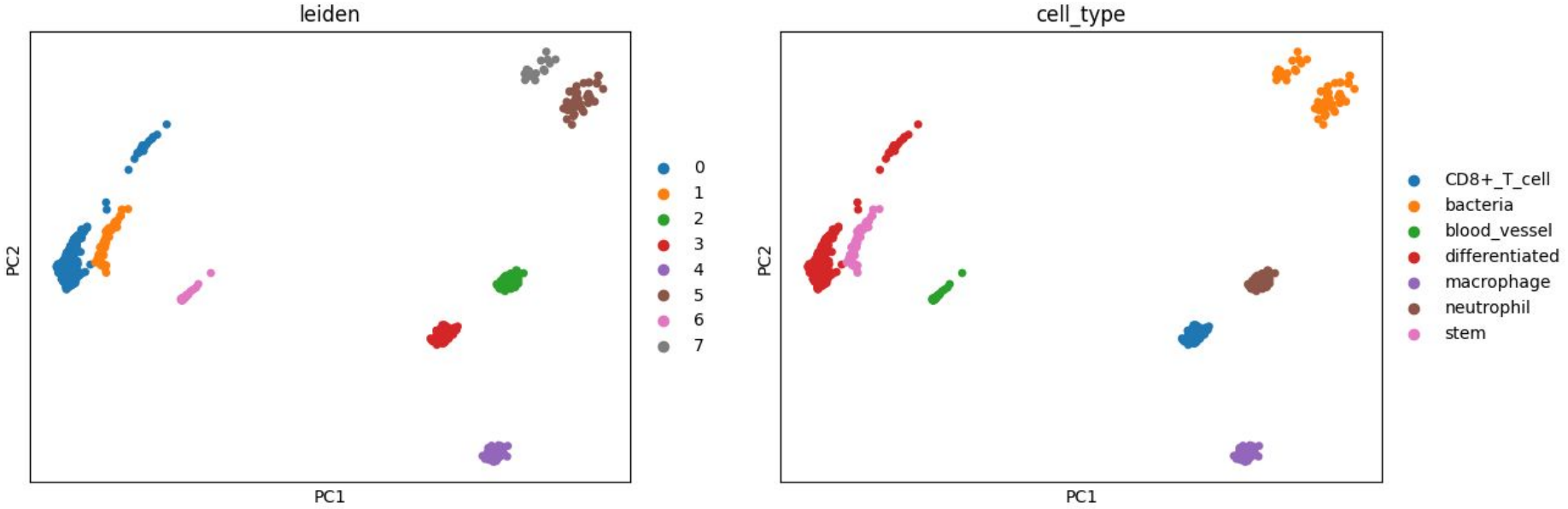




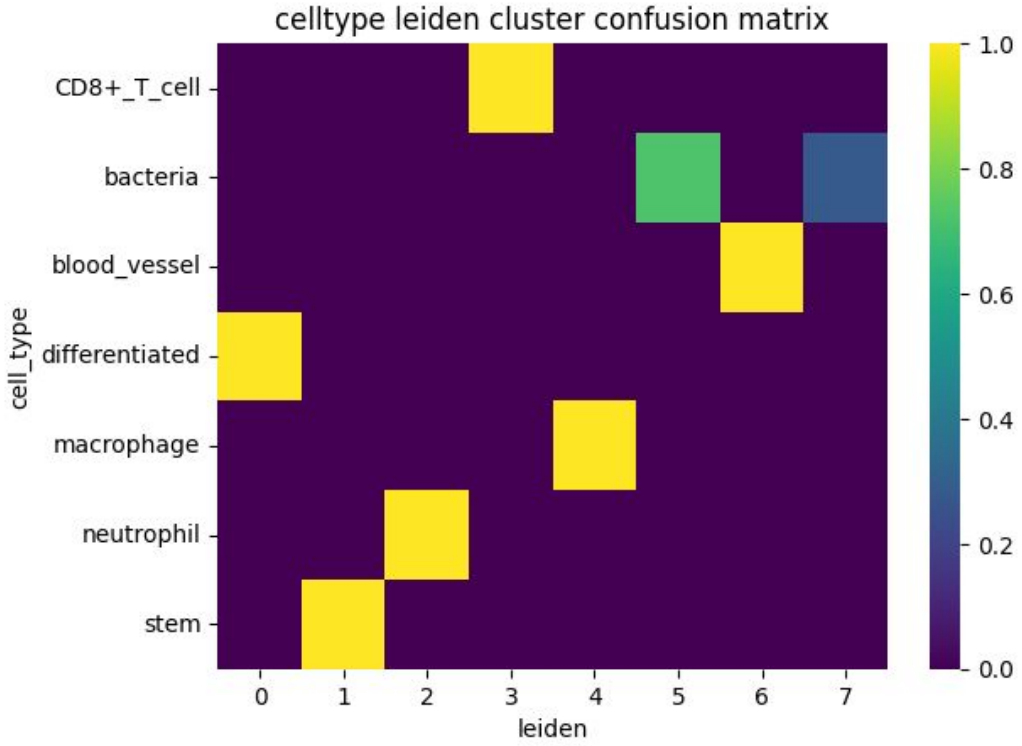


scanpy: leiden nearest neigbour clustering

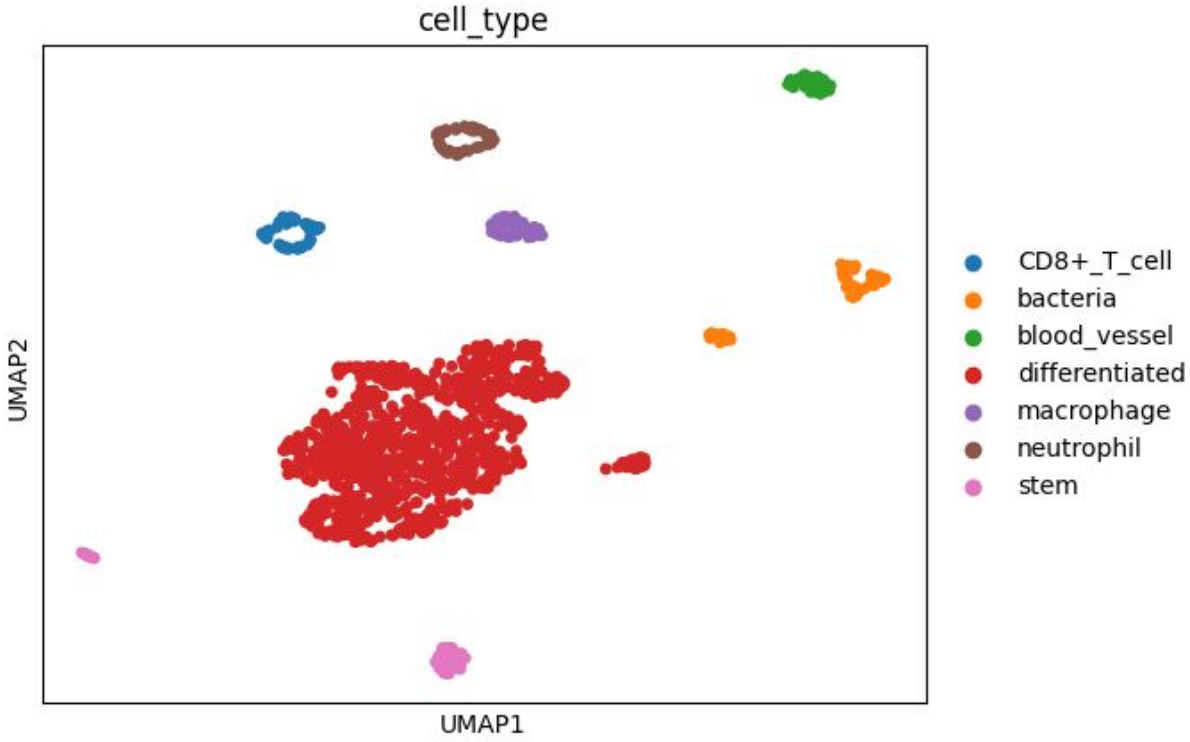
```
sc.pp.neighbors(ann, n_neighbors=15)  # compute the neighborhood graph.
sc.tl.leiden(ann, resolution=0.01)  # cluster the neighborhood graph.
```



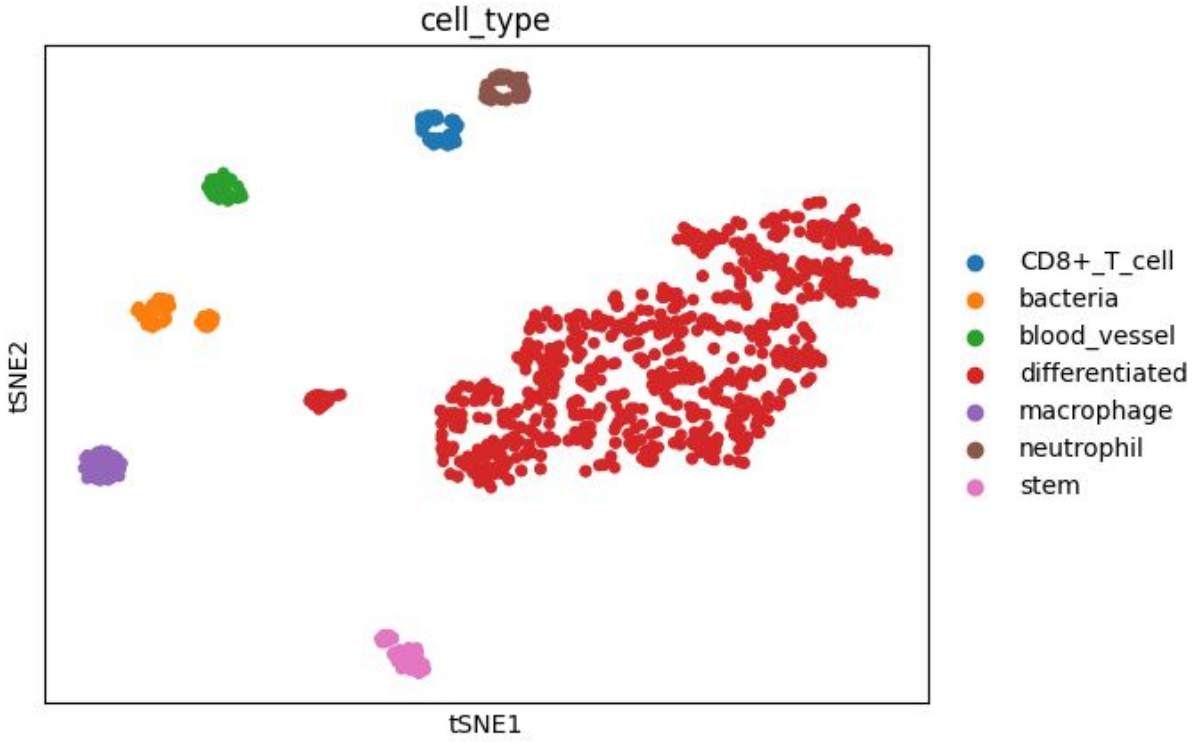
sns scanpy: confusion matrix



scanpy: umap


cell_type
UMAP2
UMAP1
CD8+_T_cell
bacteria
blood_vessel
differentiated
macrophage
neutrophil
stem

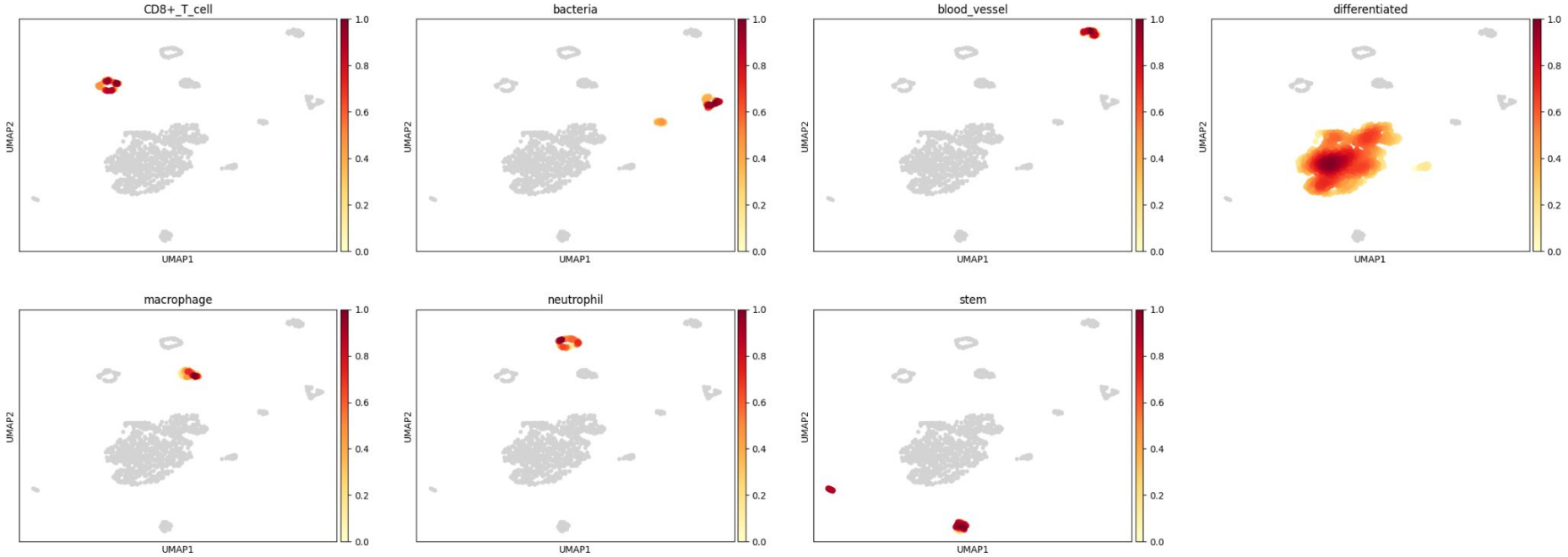
scanpy: tSNE


cell_type
tSNE2
tSNE1
CD8+_T_cell
bacteria
blood_vessel
differentiated
macrophage
neutrophil
stem

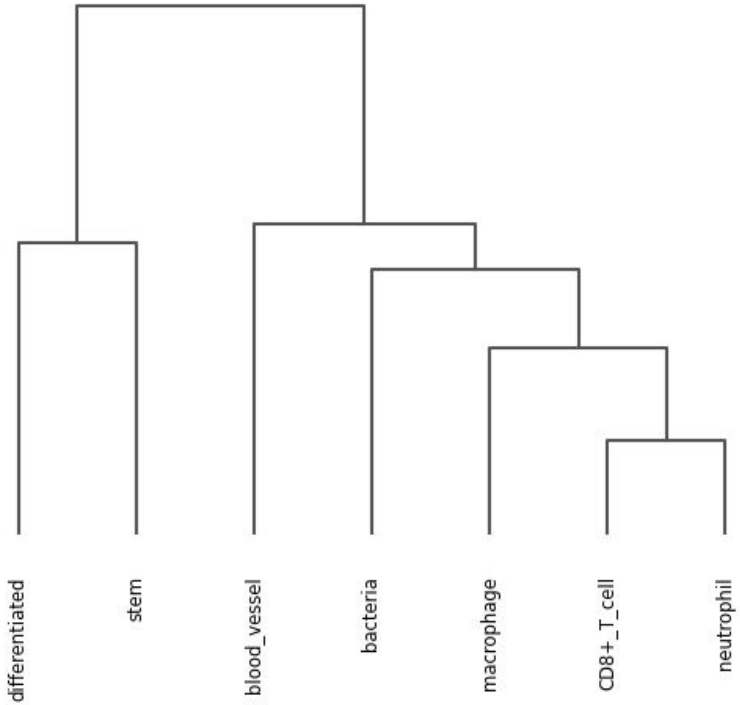
scanpy: other dimensional reduction

- fa: ForceAtlas2 force-directed graph.
- fr: Fruchterman Reingold.
- grid_fr: Grid Fruchterman Reingold.
- kk: Kamadi Kawai.
- lgl: Large Graph Layout.
- drl: Distributed Recursive Layout.
- rt: Reingold Tilford tree layout.
- rt_circular: Reingold Tilford circular layout.

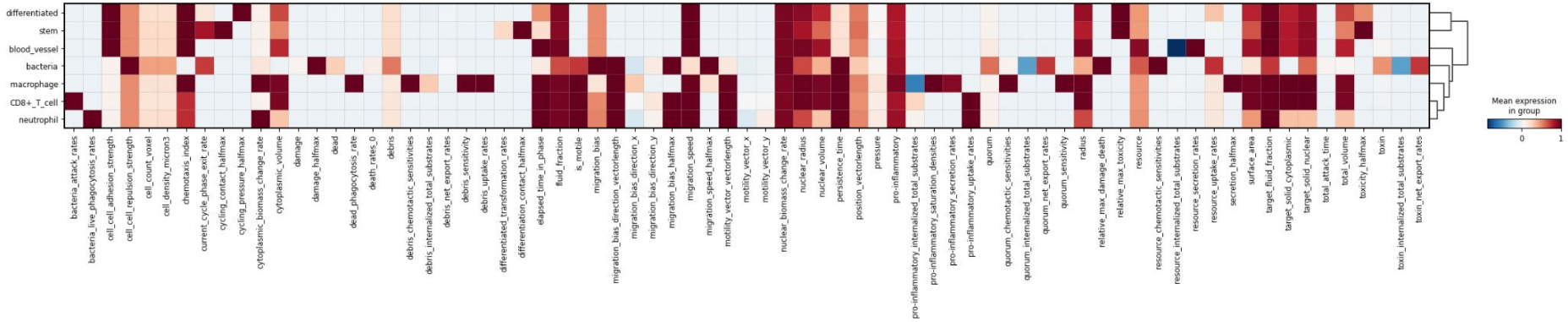
TimeStep scanpy: embedding_density



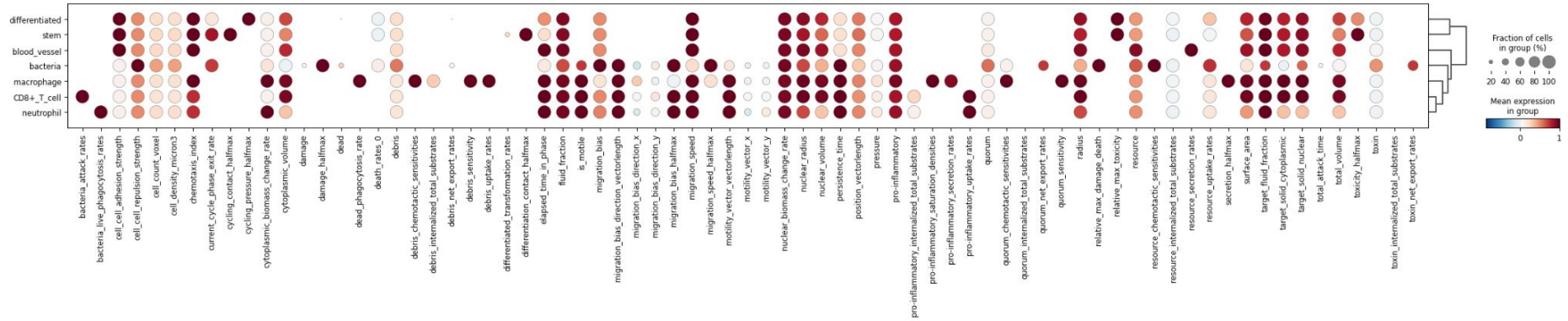
scanpy: dendrogram



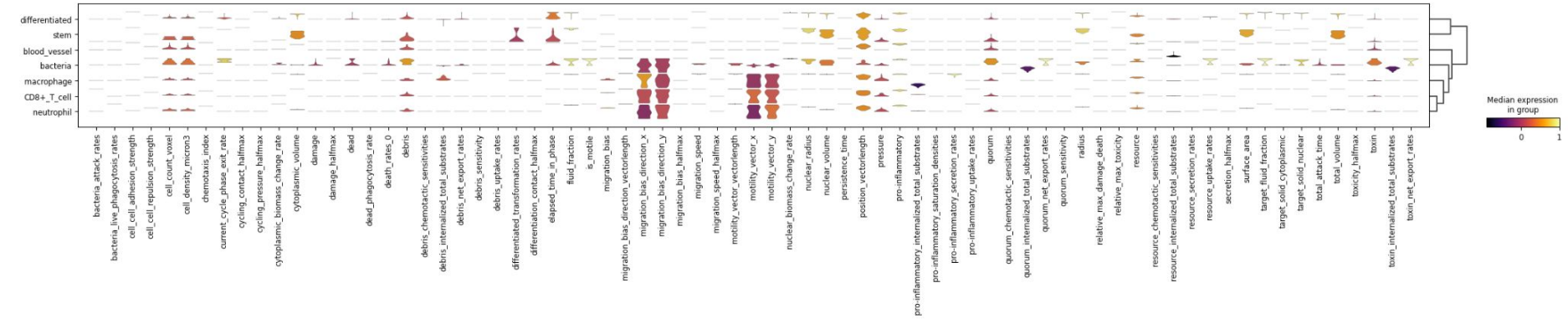
scanpy: matrixplot



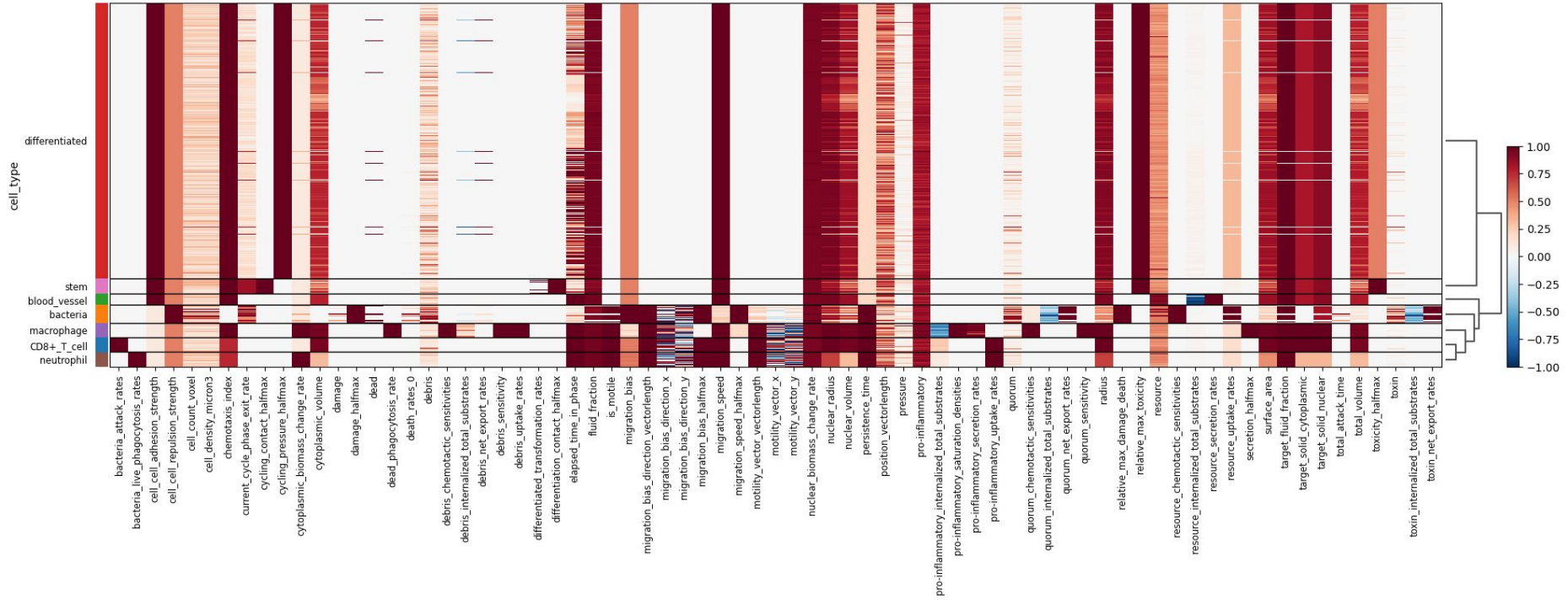
scanpy: dotplot



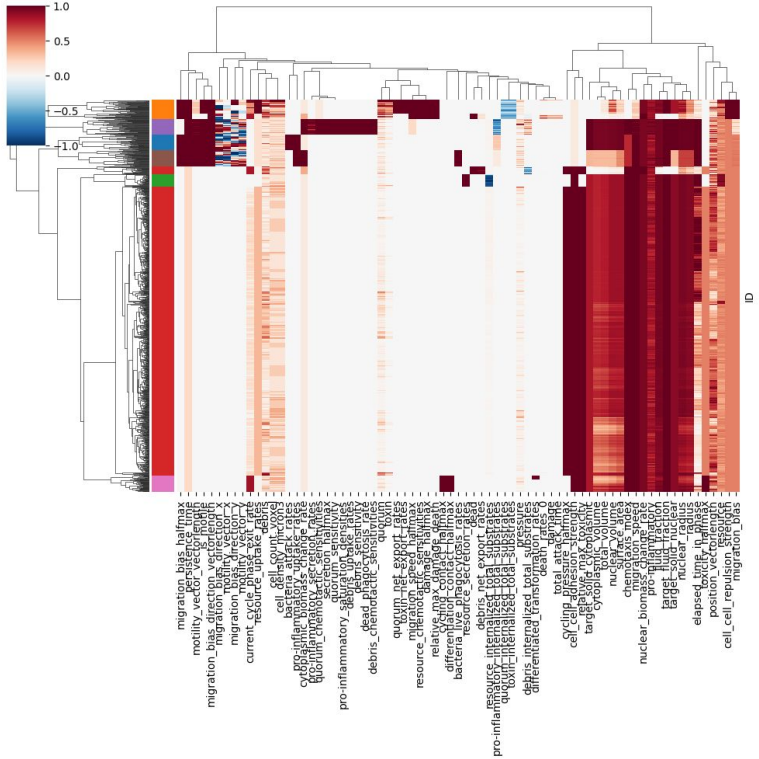
scanpy: stacked_violin



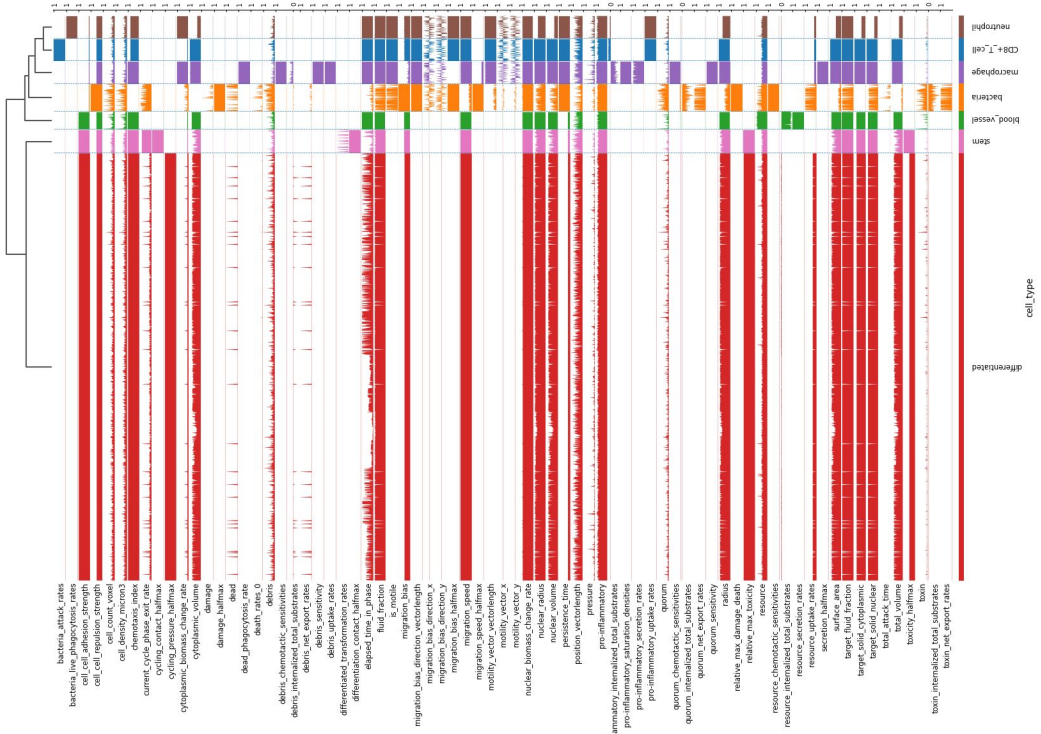
scanpy: heatmap



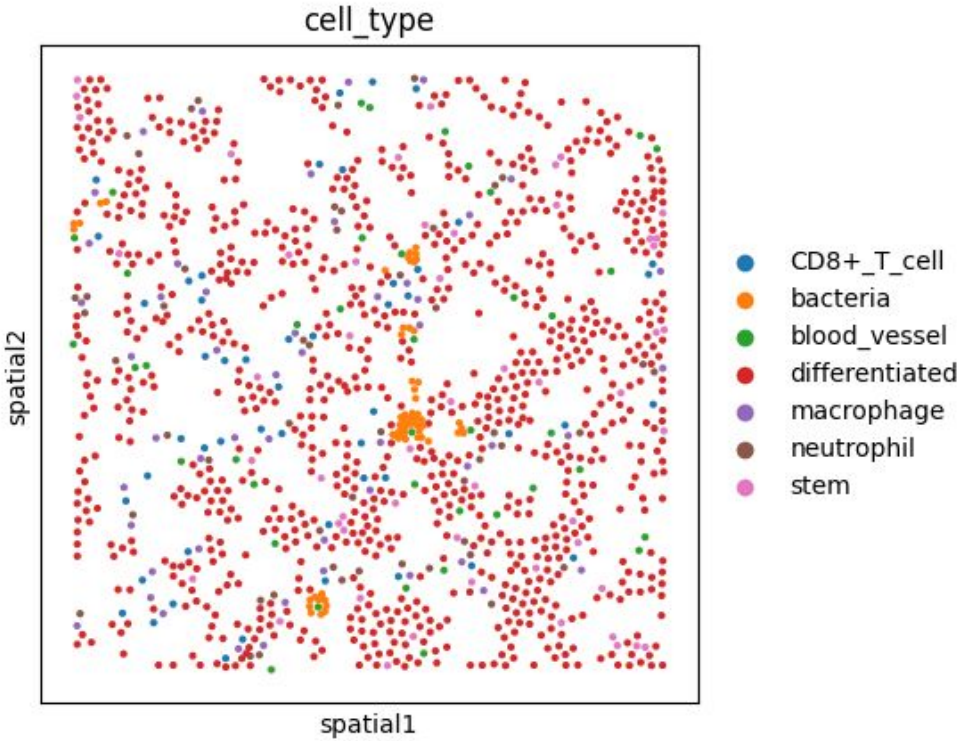
scanpy: clustermap



scanpy: trackplot



scanpy: spatial

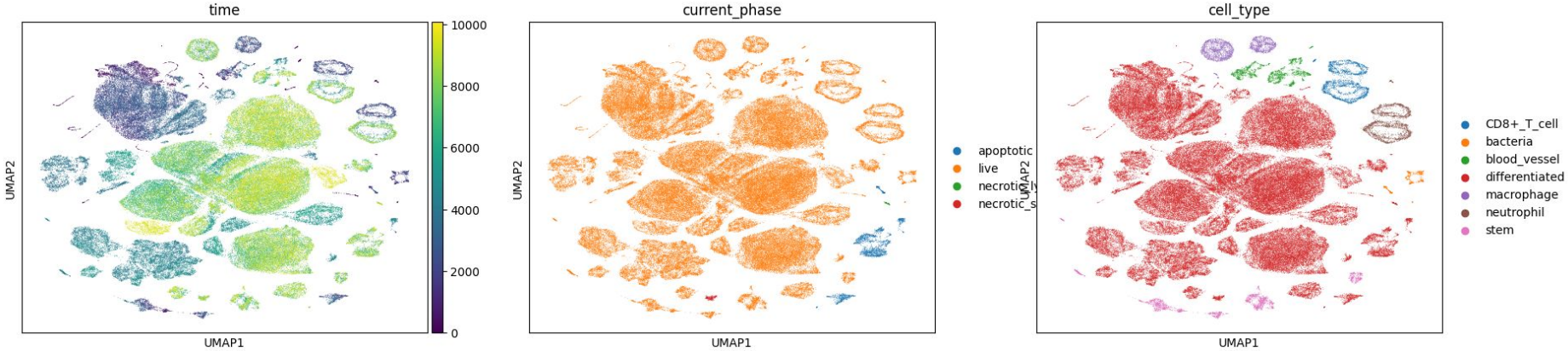


scanpy: global autocorrelation statistic Moran's I and Geary's C

	bacteria_attack_rates	bacteria_live_phagocytosis_rates	cell_cell_adhesion_strength	cell_cell_repulsion_strength	cell_count_voxel	cell_density_micron3	chemotaxis_index
gc	0.000000	0.000000	0.000000	0.000000	0.295582	0.295582	0.00000
mi	0.941978	0.938326	0.959807	0.959389	0.617114	0.617114	0.96043

2 rows × 73 columns

anndata & scanpy & timeseries

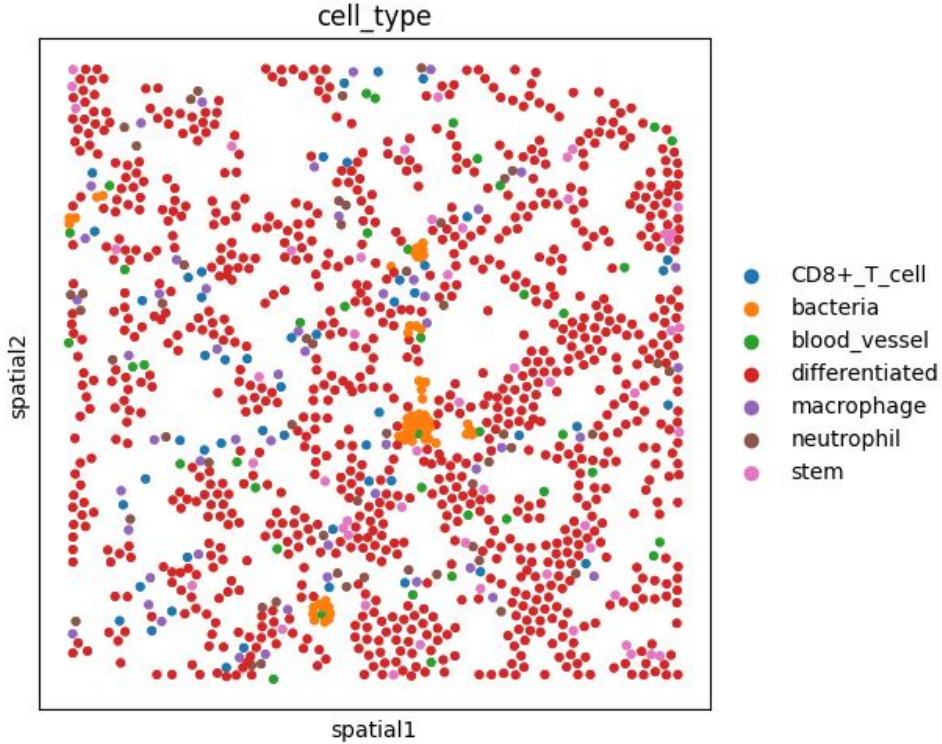


scanpy: “irrelevant” functions

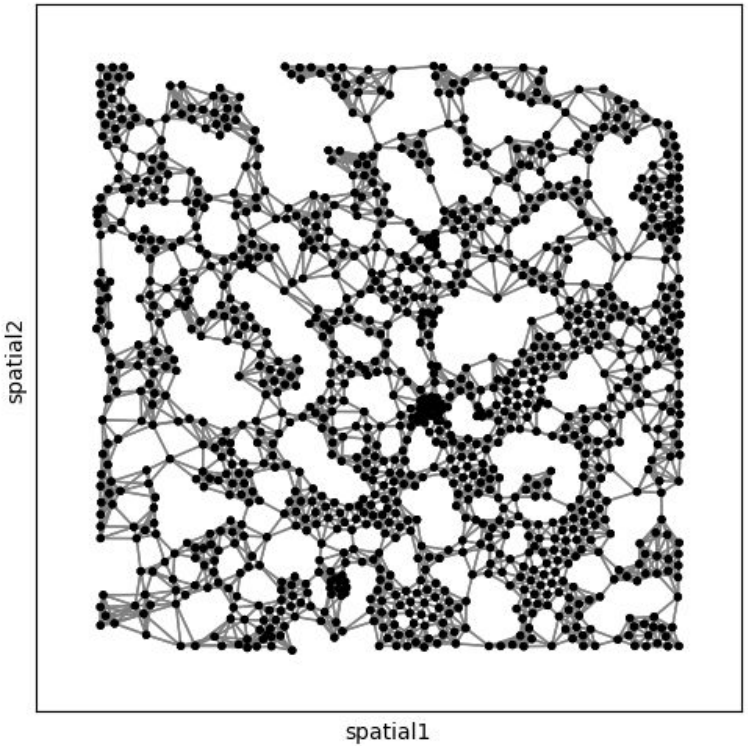
- pp.calculate_qc_metric # scRNAseq related
- pp.filter_cells # scRNAseq related
- pp.filter_genes # scRNAseq related
- pp.highly_variable_genes # scRNAseq related
- pp.log1p # scRNAseq related
- pp.normalize_total # scRNAseq related
- pp.regress_out # scRNAseq related
- pp.scale # get_anndata takes care of this.
- pp.subsample # maybe useful.
- pp.downsample_counts # scRNAseq related
- pp.combat # batch effect.
- tl.diffmap # we have time series data, we don’t need to infer.
- tl.dpt # we have time series data, we don’t need to infer.
- tl.ingest # map labels and embedding from reference to new data.
- tl.rank_gene_groups # scRNAseq related
- tl.filter_rank_genes_groups # scRNAseq related
- tl.mark_gene_overlap # scRNAseq related
- tl.score_gene # scRNAseq related
- tl.score_gene_cell_cycle # scRNAseq related
- tl.sim # simulate dynamic gene expression data

squidpy

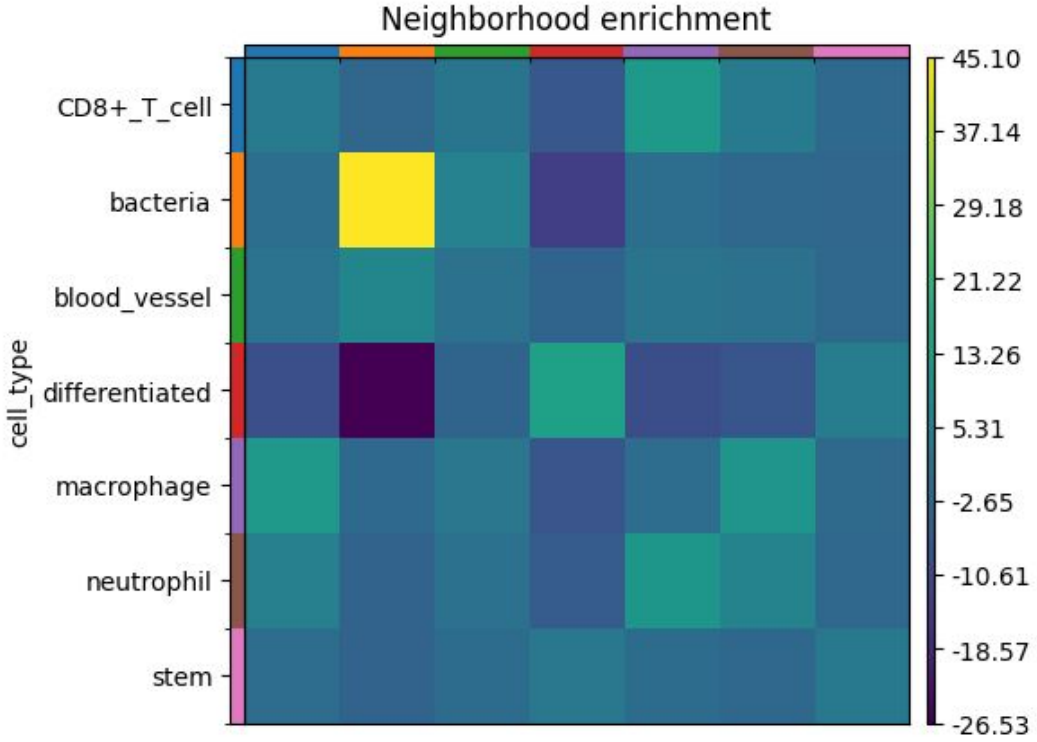
squidpy: spatial_scatter



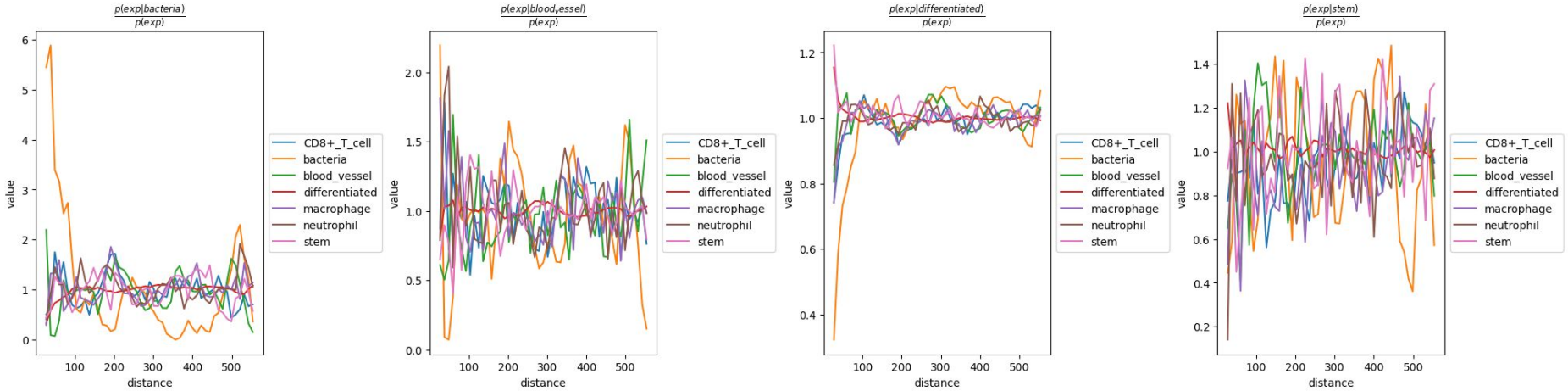
squidpy: spatial_neighbours



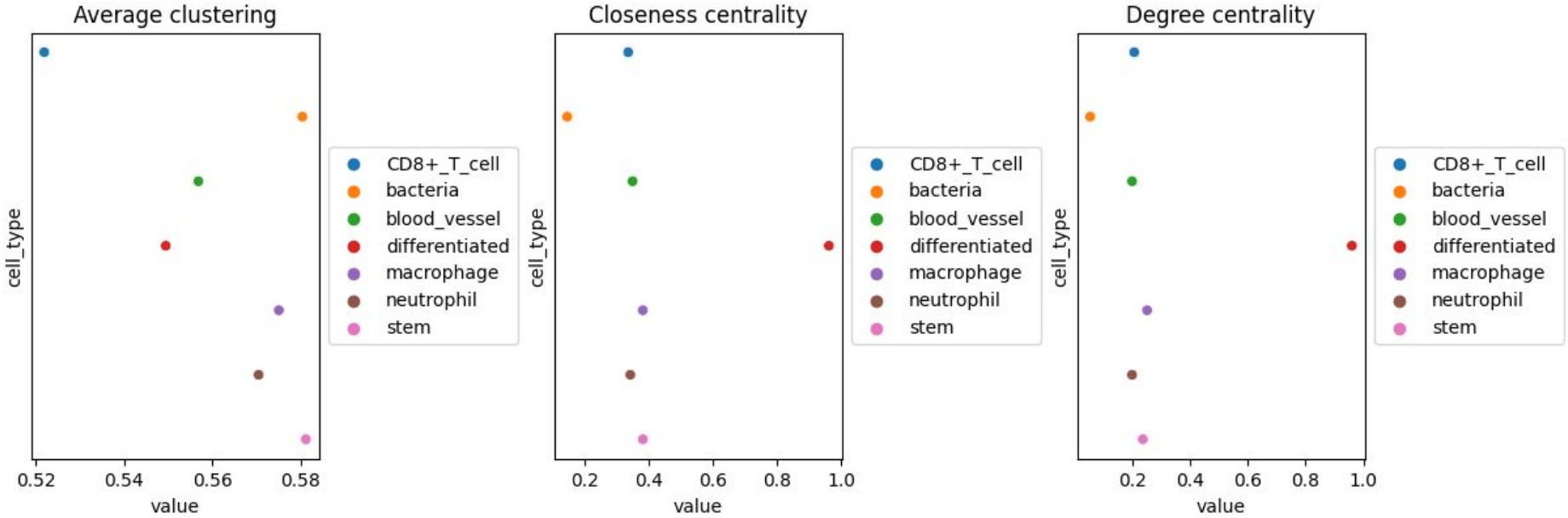
squidpy: nhood_enrichment



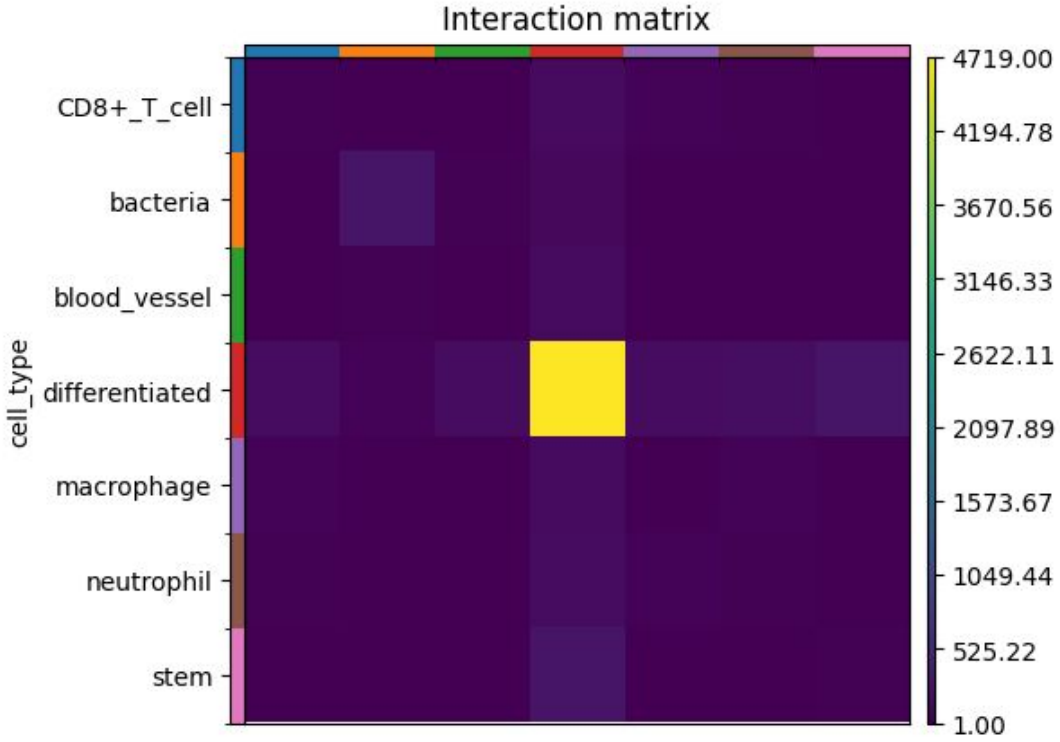
squidpy: co_occurrence



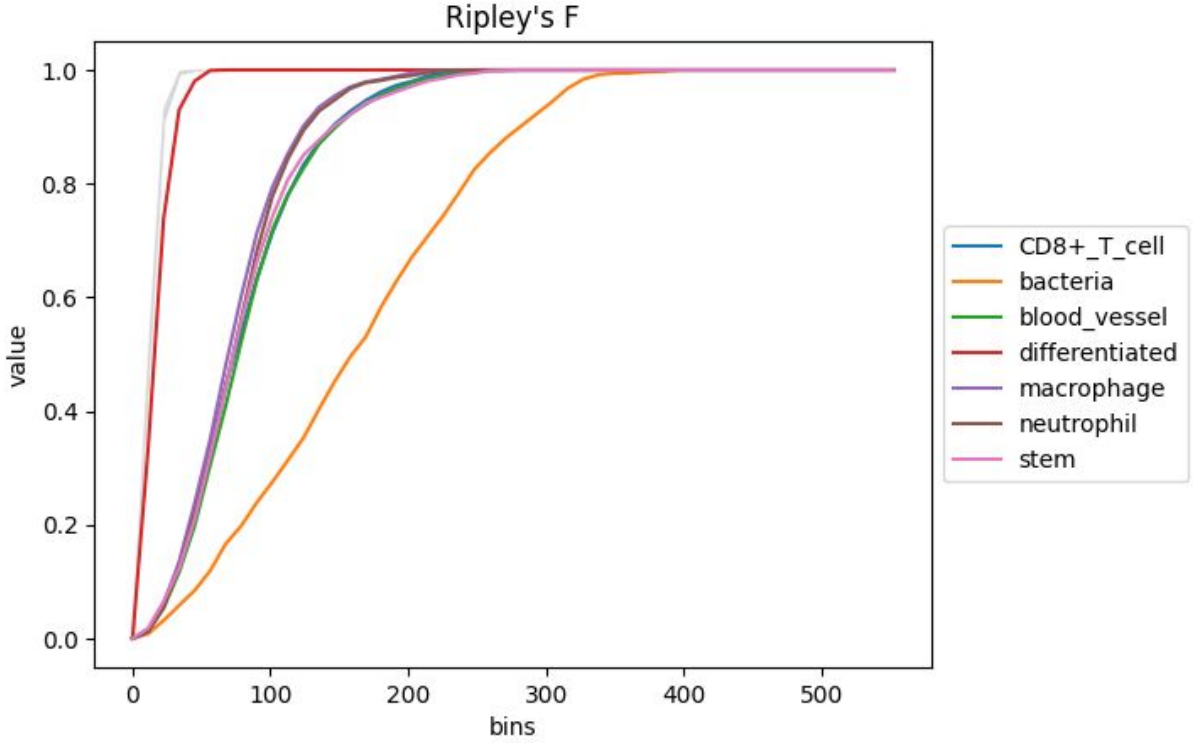
squidpy: centrality_scores



squidpy: interaction_matrix



squidpy: Ripley's statistics for point processes

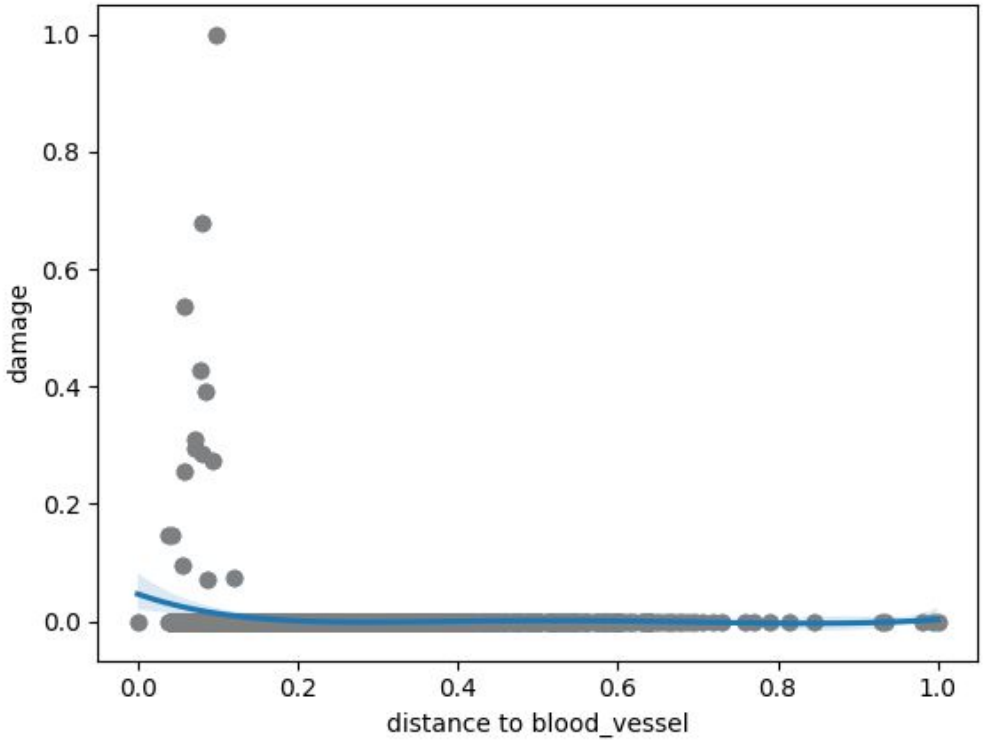


squidpy: global autocorrelation statistic Moran's I and Geary's C

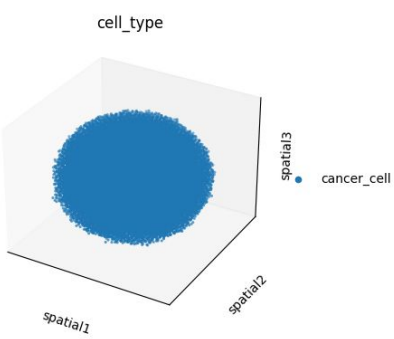
	I	pval_norm	var_norm	pval_norm_fdr_bh
position_vectorlength	0.992993	0.0	0.000273	0.0
quorum	0.934202	0.0	0.000273	
debris	0.927604	0.0	0.000273	
pro-inflammatory	0.870561	0.0	0.000273	
toxin	0.853246	0.0	0.000273	
damage_halfmax	0.603295	0.0	0.000273	
cell_cell_repulsion_strength	0.603295	0.0	0.000273	
relative_max_damage_death	0.603295	0.0	0.000273	
resource_chemotactic_sensitivities	0.603295	0.0	0.000273	
migration_speed	0.595514	0.0	0.000273	

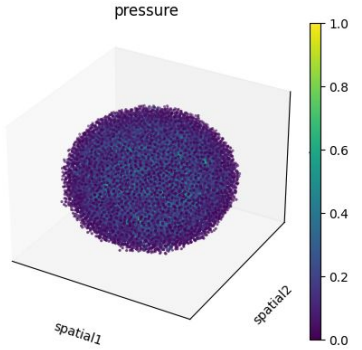
	C	pval_norm	var_norm	pval_norm_fdr_bh
position_vectorlength	0.009540	0.0	0.000273	0.0
quorum	0.030820	0.0	0.000273	0.0
debris	0.062550	0.0	0.000273	0.0
toxin	0.080504	0.0	0.000273	0.0
pro-inflammatory	0.128708	0.0	0.000273	0.0
cell_cell_repulsion_strength	0.340886	0.0	0.000273	0.0
relative_max_damage_death	0.340886	0.0	0.000273	0.0
resource_chemotactic_sensitivities	0.340886	0.0	0.000273	0.0
damage_halfmax	0.340886	0.0	0.000273	0.0
migration_speed	0.346057	0.0	0.000273	0.0

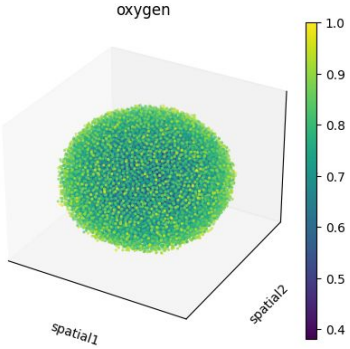
squidpy: var_by_distance

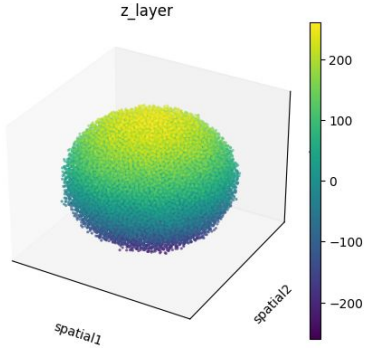


anndata & squidpy & 3D

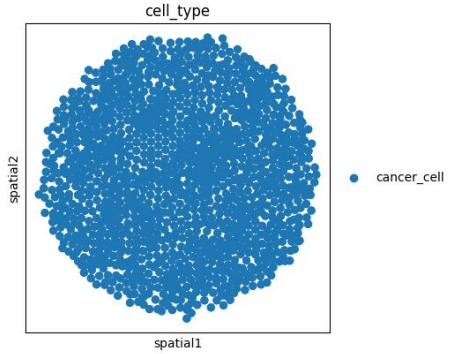


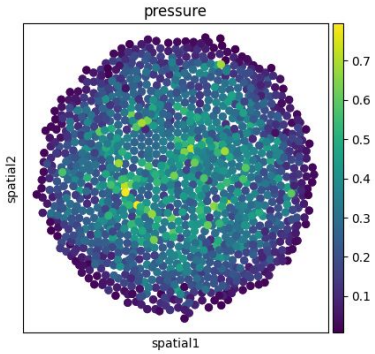


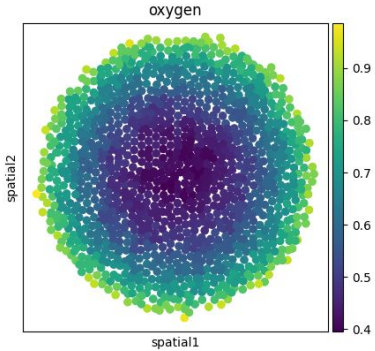


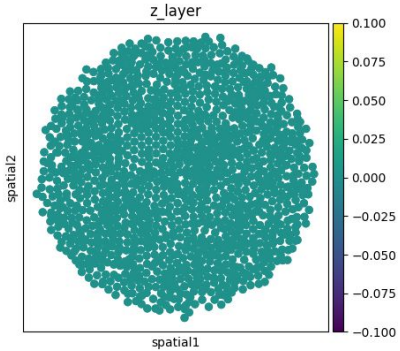


anndata & squidpy & 3D









squidpy: “irrelevant” functions

- gr.ligrec # ligand receptor related
- gr.sepal # to identify spatially variable genes, but works only on square and hex matrices.
- im.process # h&e and microscopy image related
- im.segment # h&e and microscopy image related
- im.calculate_image_features # h&e and microscopy image related
- pl.spatial_segment # h&e and microscopy image related
- sq.pl.extract # make a temporary anndata object for plotting

- deep learning.
- scvi-tools: single-cell variational inference tools.
- probabilistic models for single-cell omics data.
- publication: https://doi.org/10.1038/s41587-021-01206-w
- manual: https://docs.scvi-tools.org/en/stable/index.html
- pytorch: https://pytorch.org/
- pytorch lighnting: https://lightning.ai/
- pyro: https://pyro.ai/

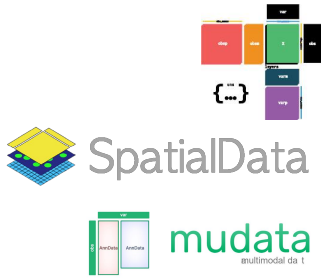
more from scverse

homepage

- https://scverse.org/

data analysis

- **muon**: multimodal omics analysis.
- **scirpy**: T cell receptor (TCR) or B cell receptor (BCR) repertoires analysisfrom scRNA-seq data.
- scverse **ecosystem**: https://scverse.org/packages/#ecosystem



data formats

- **anndata**: https://anndata.readthedocs.io/en/latest/
- **spatialdata**: https://spatialdata.scverse.org/en/latest/
- **mudata**: https://mudata.readthedocs.io/en/latest/