# scRNAseq
# and
# Optimal Transport

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# Gene trajectory inference for single-cell data by optimal transport metrics

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Check for updates

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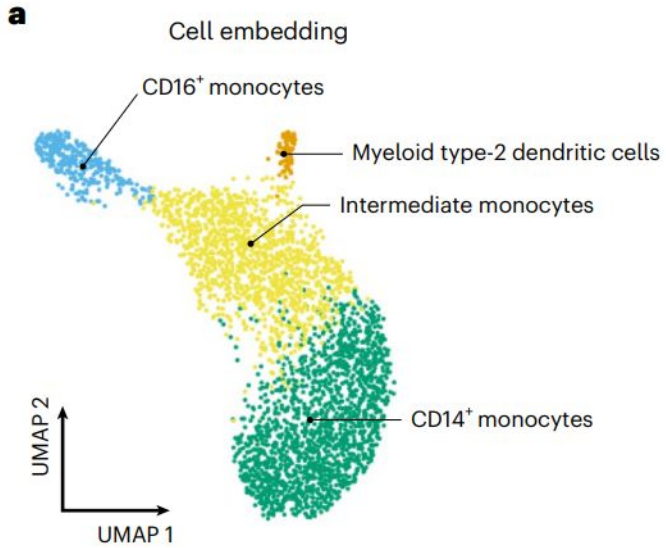
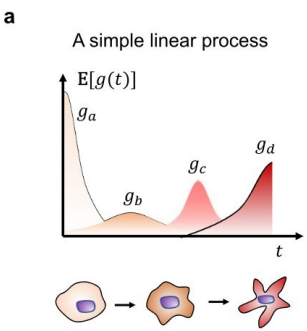
# Why Should I Care?

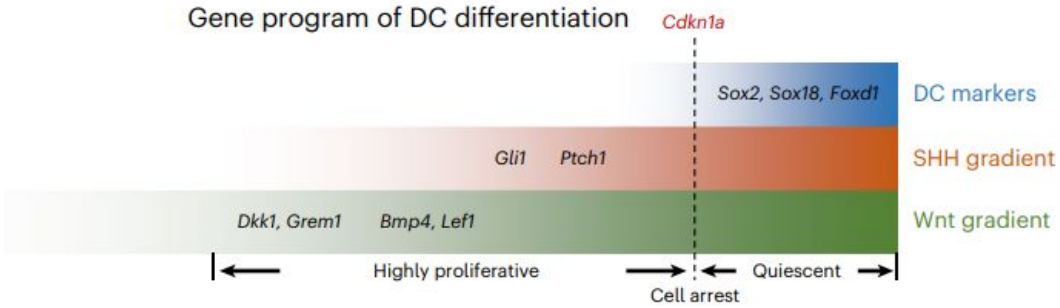
- Practical Use-Case of OT
- Can be Generalised to Other Data Types
- Interplay between Dynamical Systems and Data Analysis

- (Case Study in Examining Shapes of Data)

# Uncovering the “Idea” in a dataset.

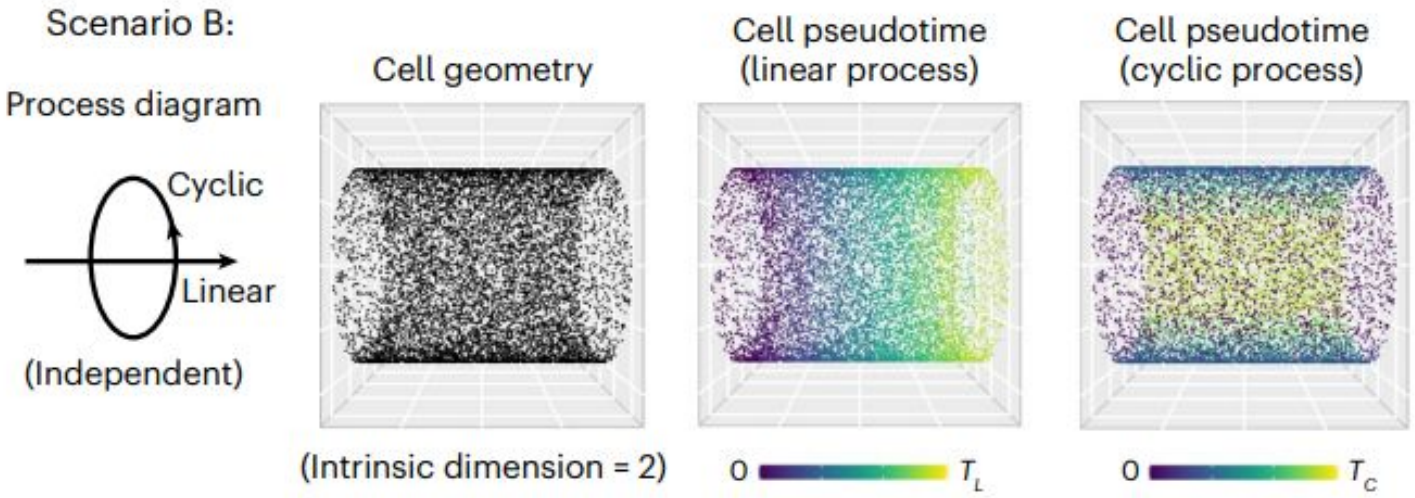


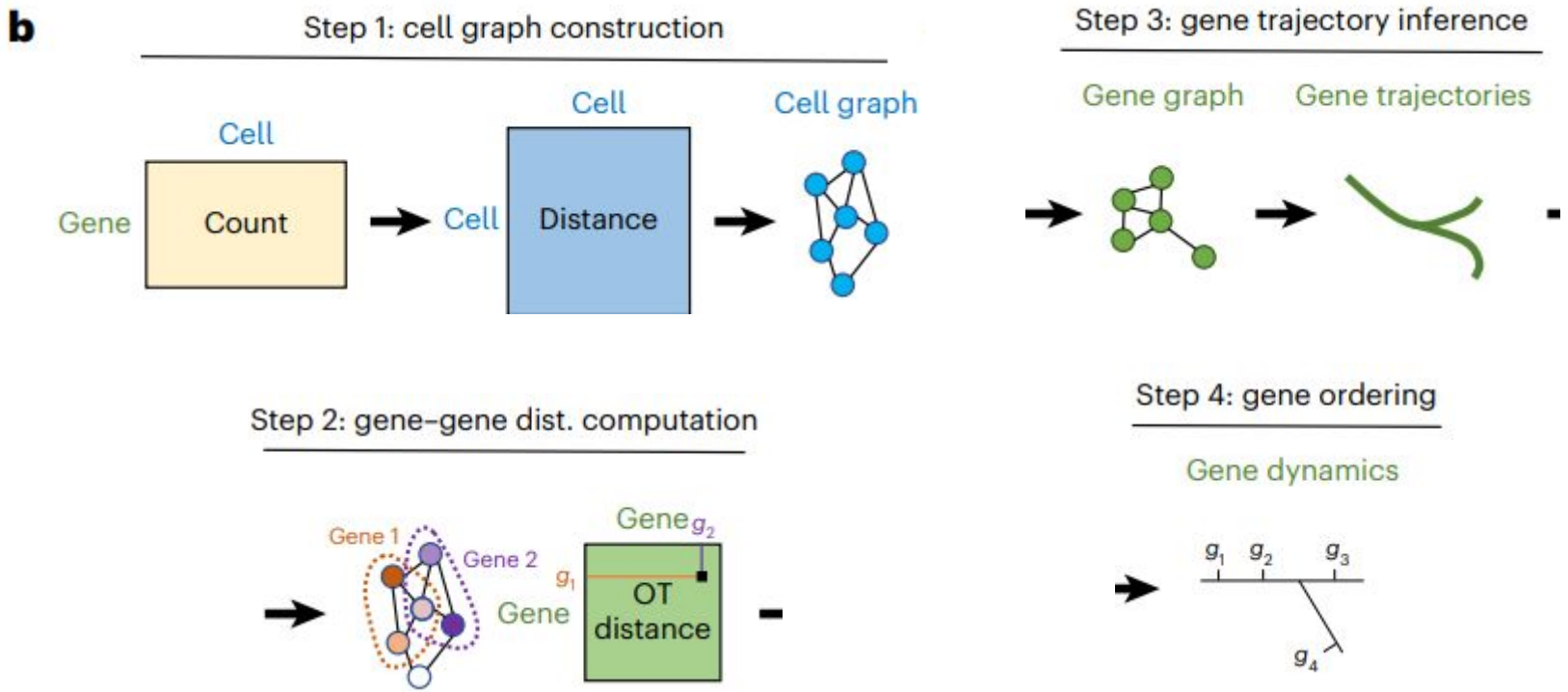

What can modelling a dataset actually *tell us* about the world
(as opposed to simulating it)

# The Geometry of Dynamical Processes

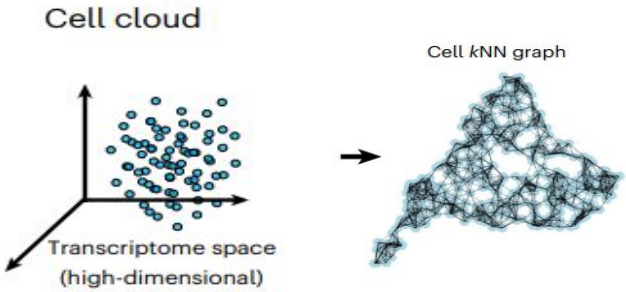



Datasets are shaped by the dynamics that generate them.
How can data science reconstruct those dynamics?

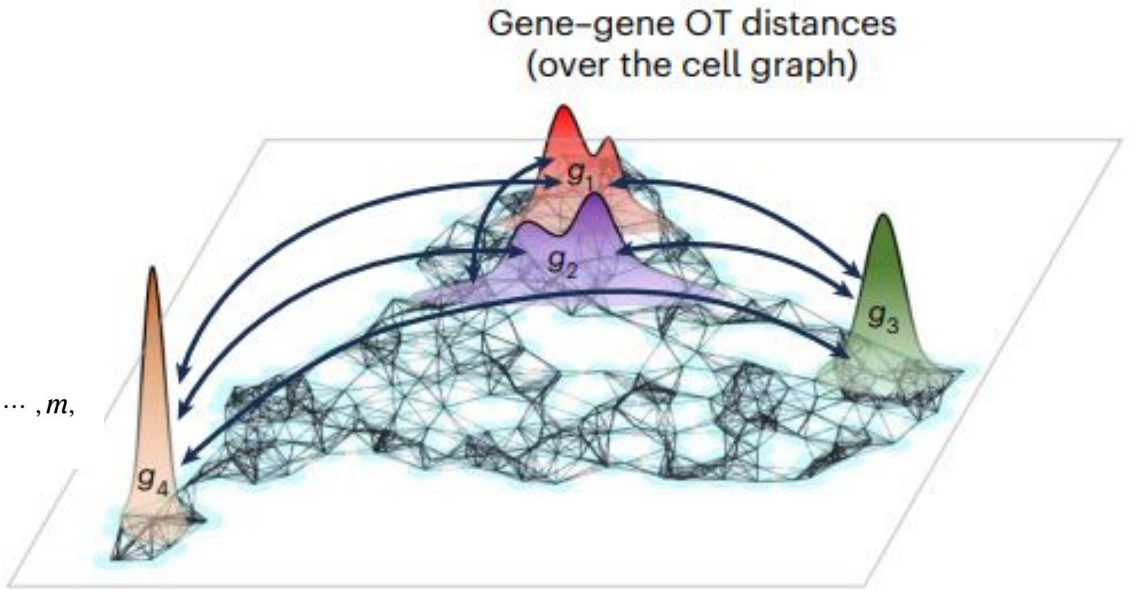
# Overview


b
Step 1: cell graph construction
Cell
Cell
Cell graph
Gene
Count
Cell
Distance
Step 3: gene trajectory inference
Gene graph
Gene trajectories
Step 2: gene–gene dist. computation
Gene 1
Gene 2
Gene $g_2$
$g_1$
Gene
OT distance
Step 4: gene ordering
Gene dynamics
$g_1$ $g_2$ $g_3$
$g_4$

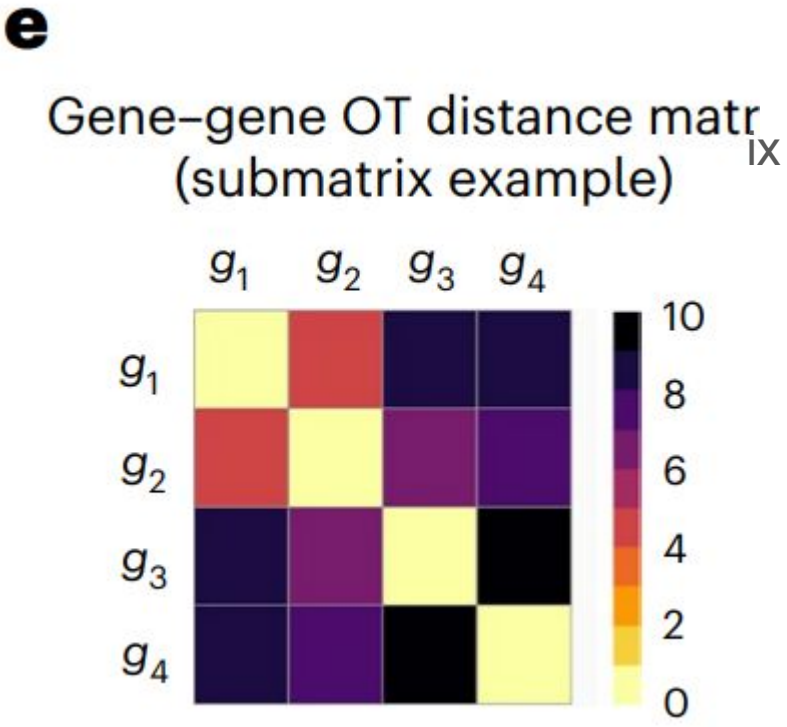
# Summarising Features with OT

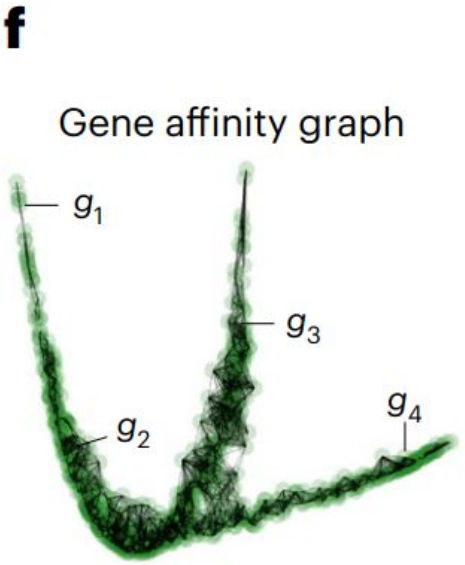



$$a(u,v) = \frac{1}{2}\left(\exp\left\{-\frac{d_{\mathrm{E}}^2(u,v)}{\sigma(u)^2}\right\} + \exp\left\{-\frac{d_{\mathrm{E}}^2(u,v)}{\sigma(v)^2}\right\}\right), \quad u,v = 1,\cdots,m,$$



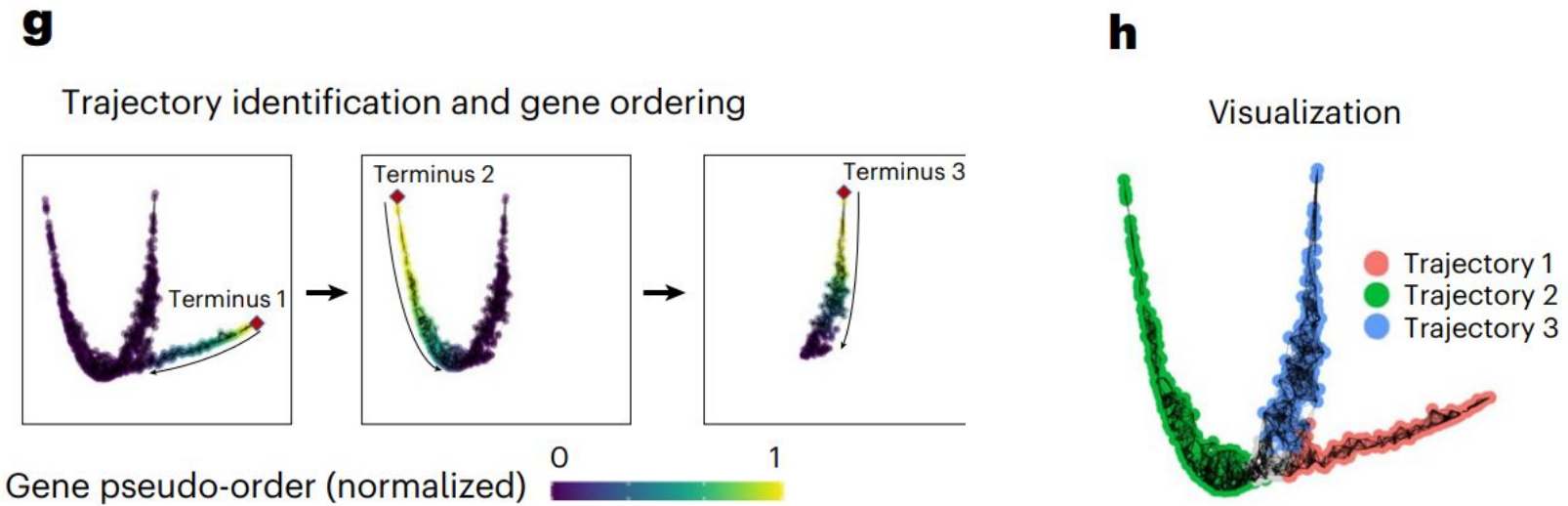
# Summarising Features with OT



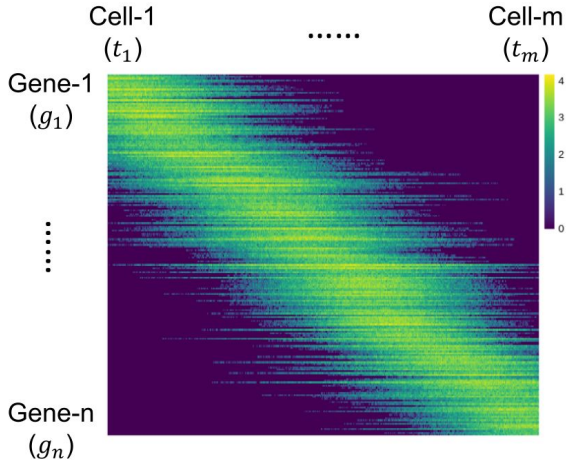

$$A_{i,j} = \frac{1}{2}\left(\exp\left\{-\frac{\delta^{(p)}(\rho_i,\rho_j)^2}{(\sigma_i)^2}\right\} + \exp\left\{-\frac{\delta^{(p)}(\rho_i,\rho_j)^2}{(\sigma_j)^2}\right\}\right)$$

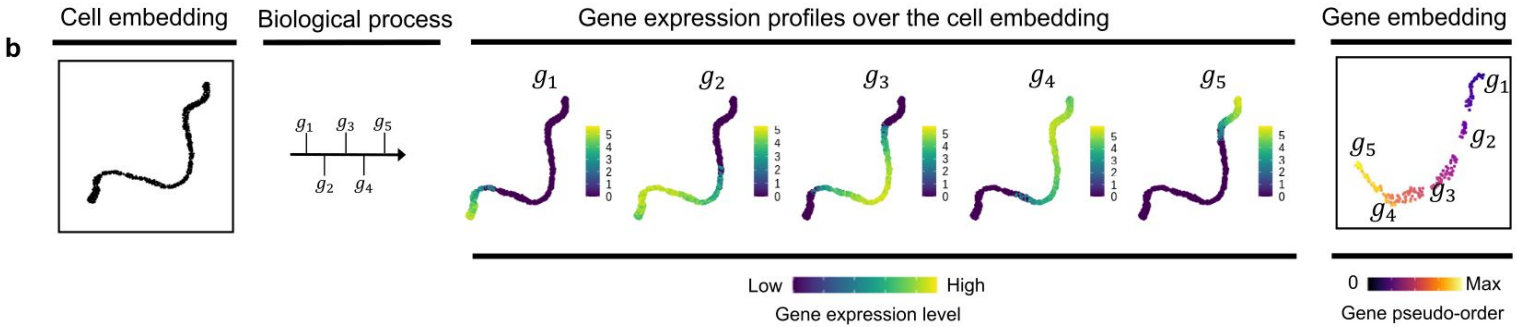
# Identifying Gene Programs From OT Geometry



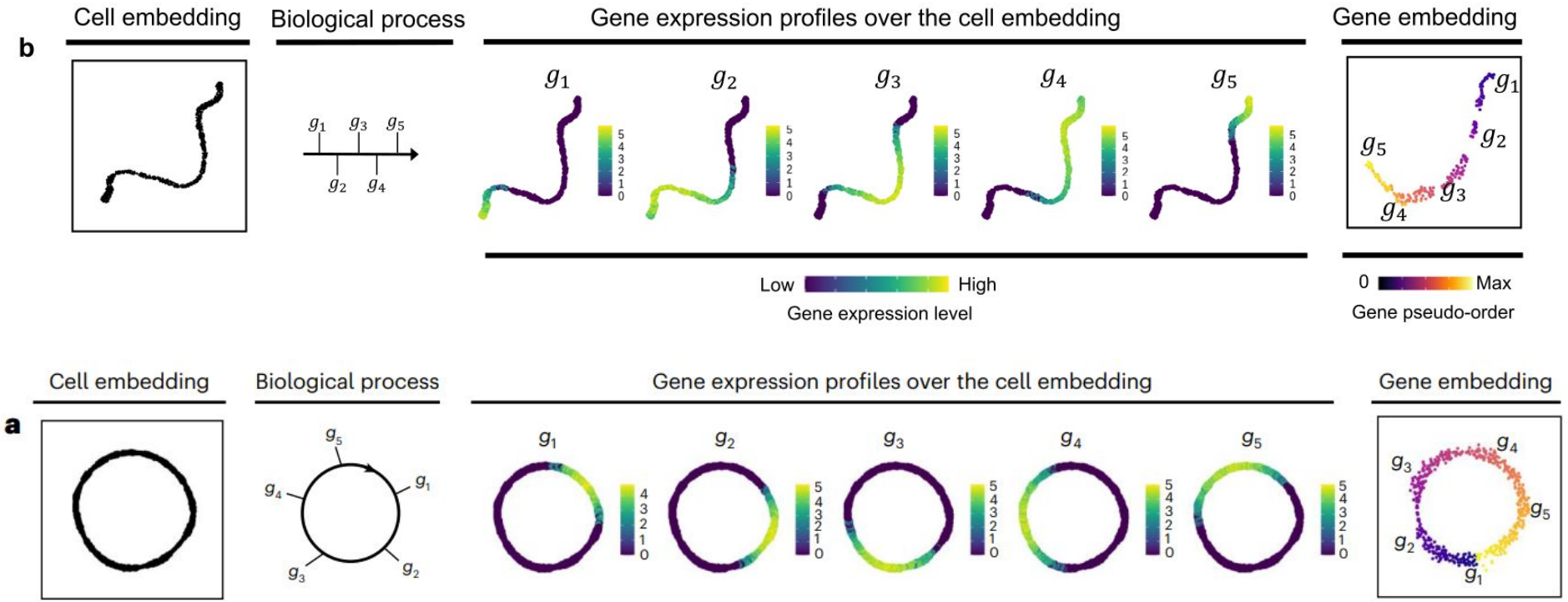

Termini were identified by maximal distance from origin in spectral embedding

# A Simplified Differentiation Dataset



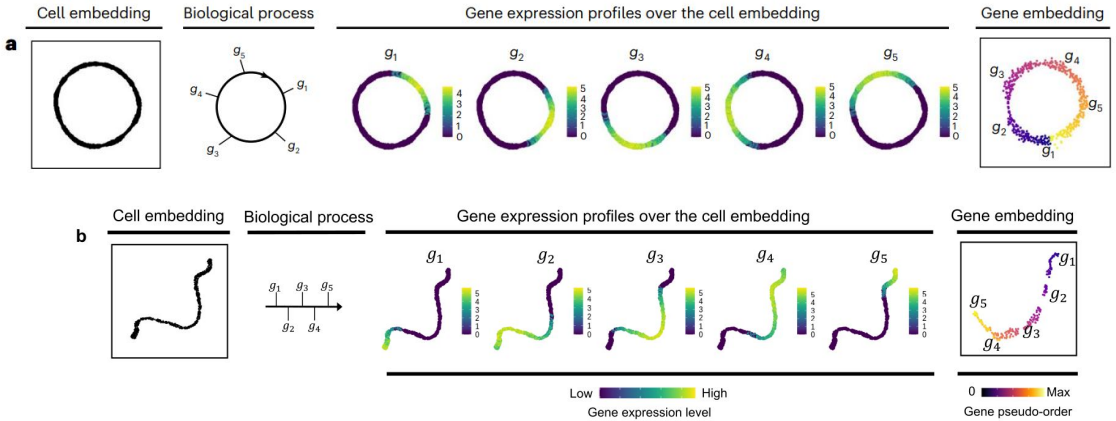



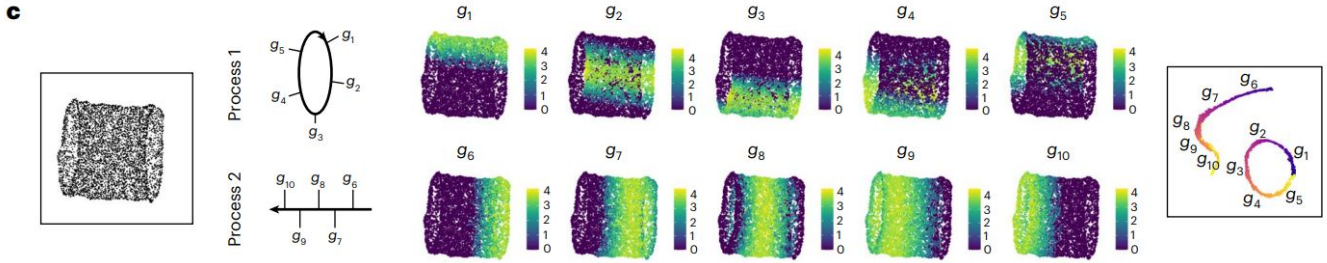
# Gene OT Networks for Simple Datasets



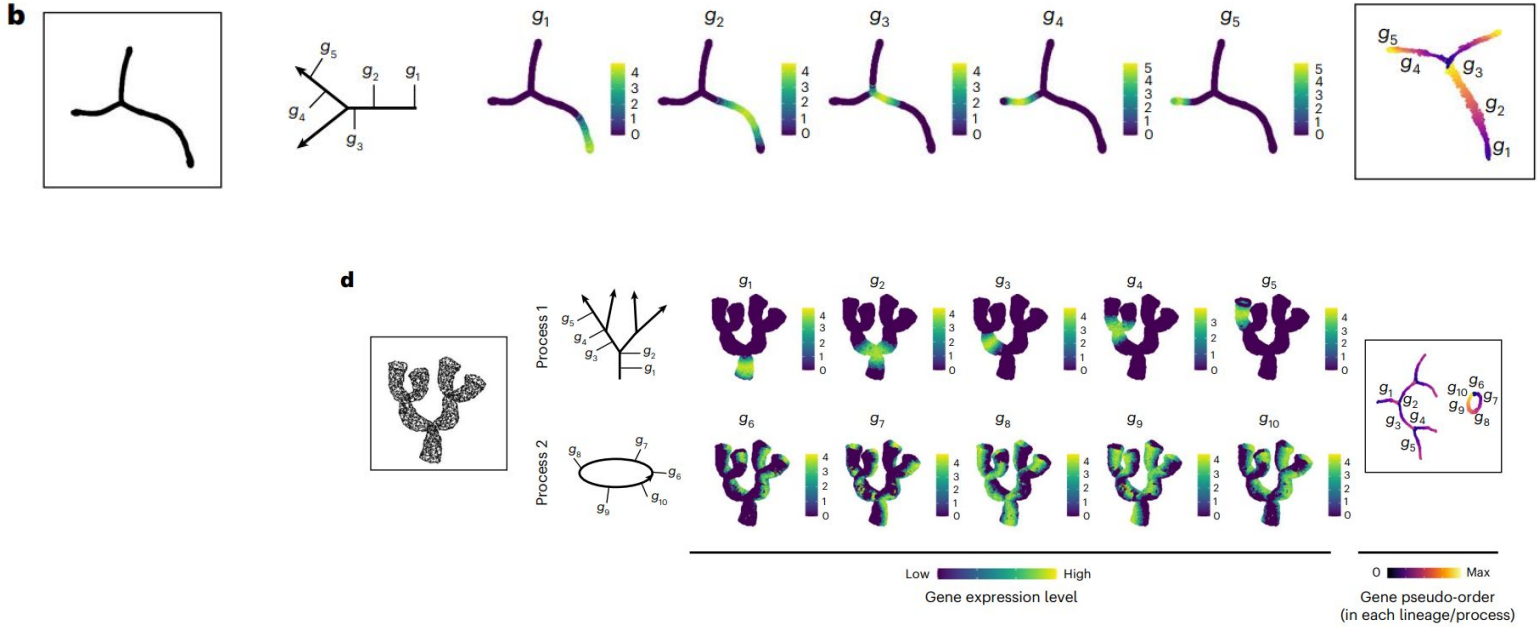
# Analysing Multiple Processes

The gene OT network has different components/communities relating to different processes.

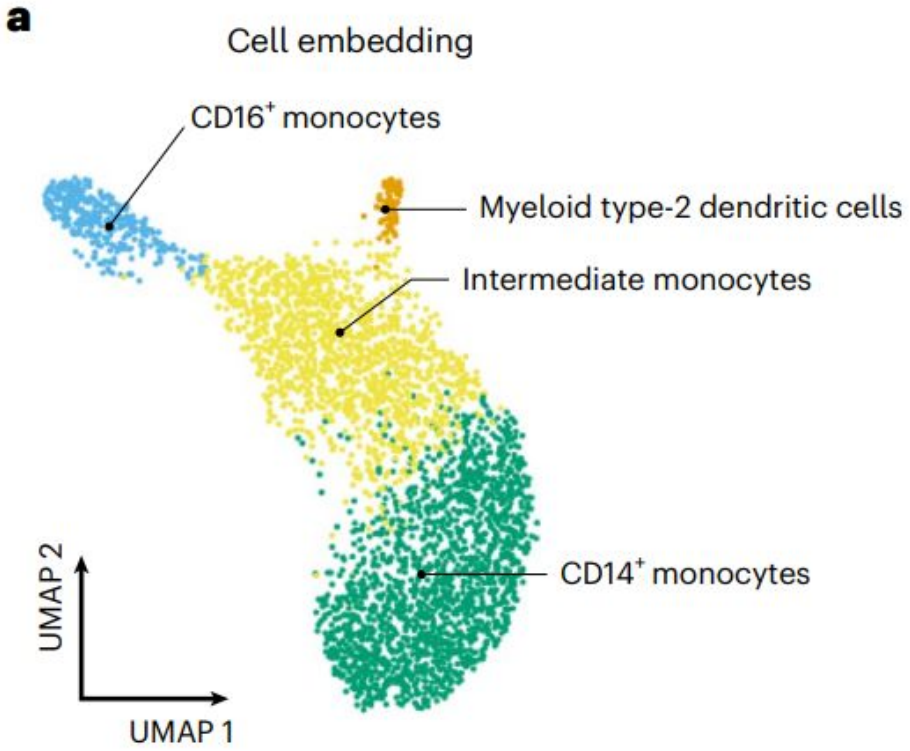


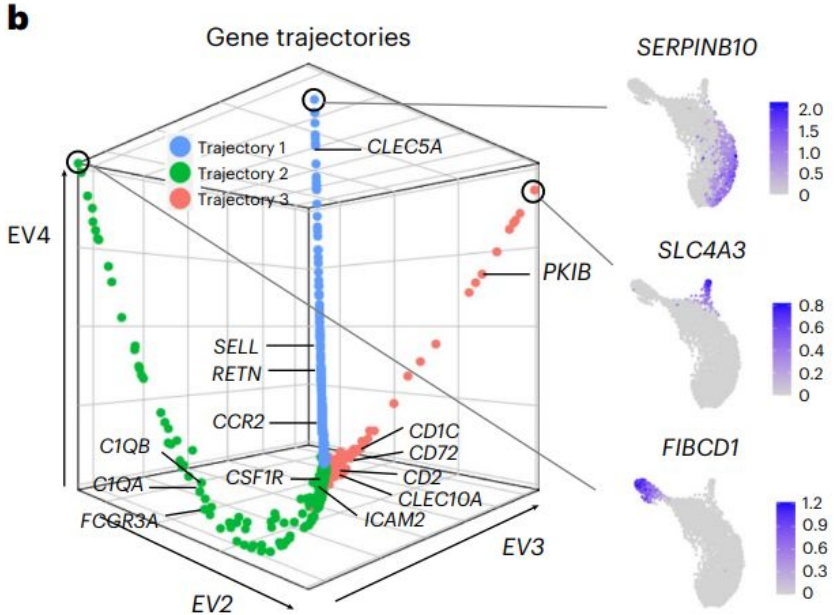



# Same Principle, Branched Differentiation



# Identifying Gene Programs From OT Geometry



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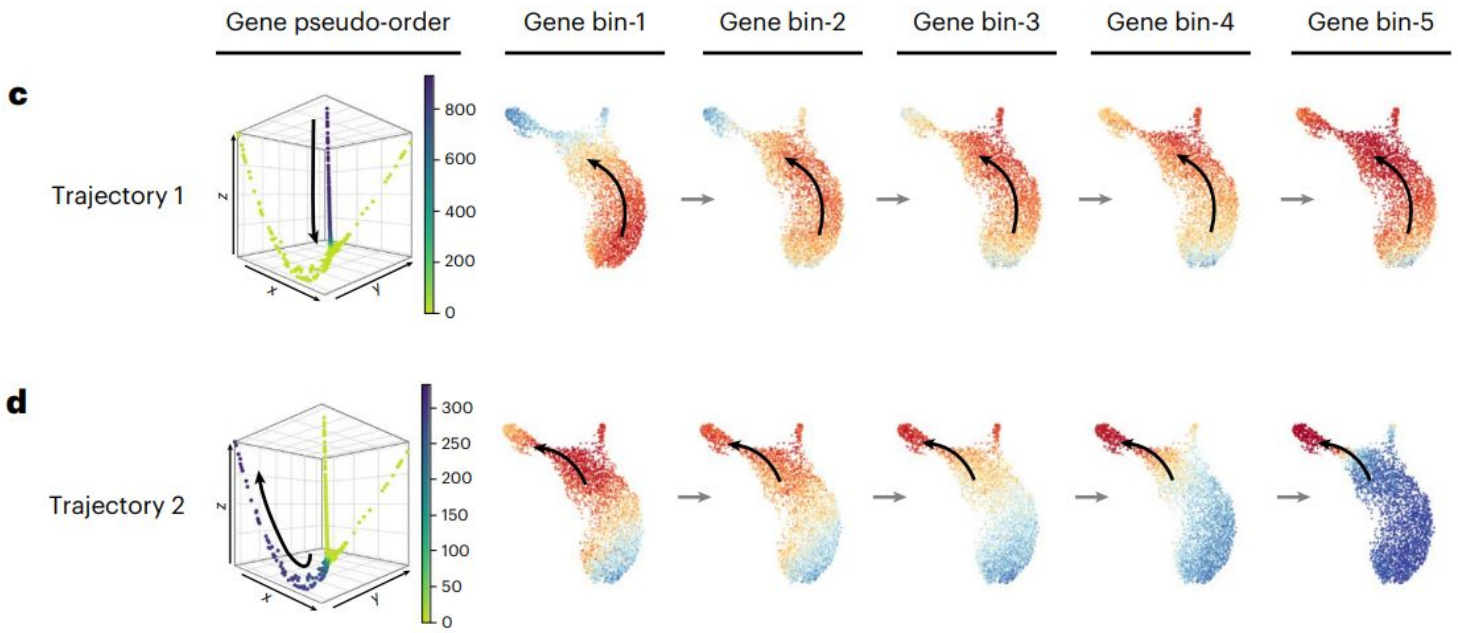
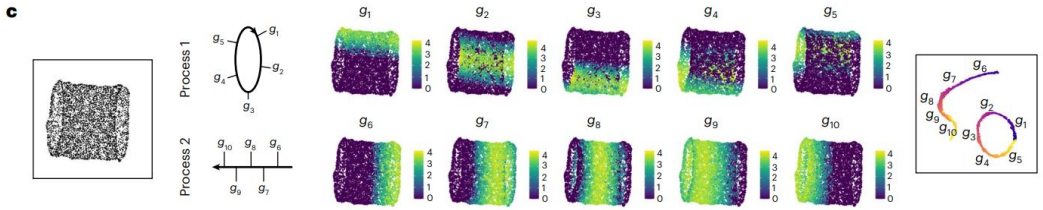
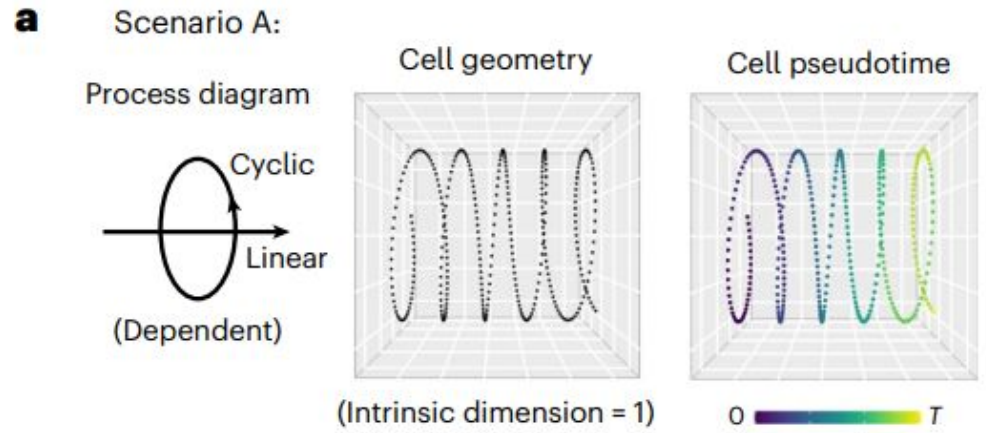



Visualise the Gene Trajectories on UMAP

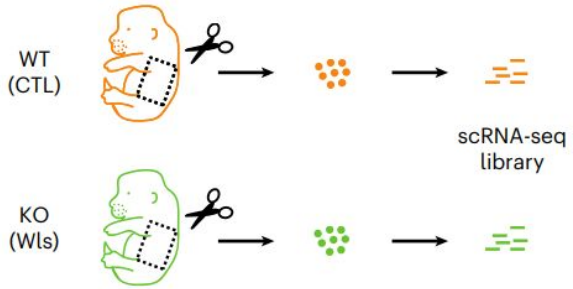
# A Problem with the Method

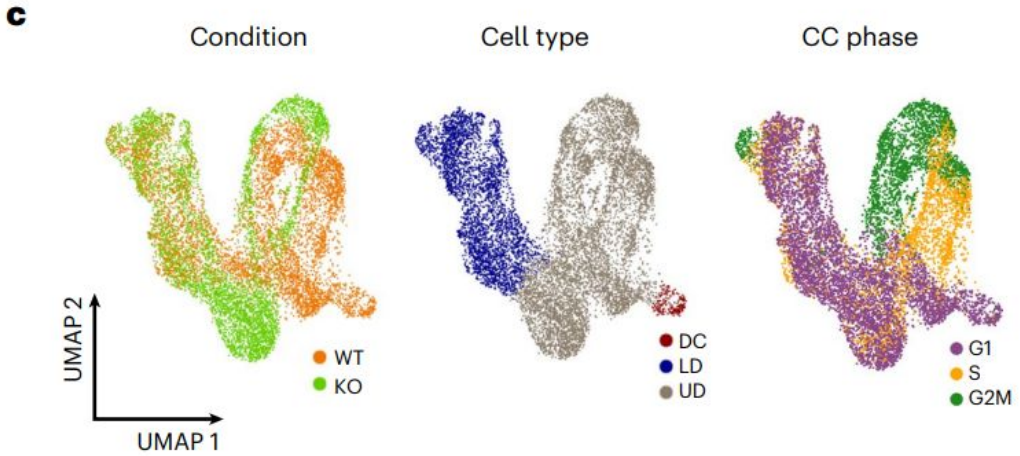



But What if…



# Differentiation of Dermal Condensates



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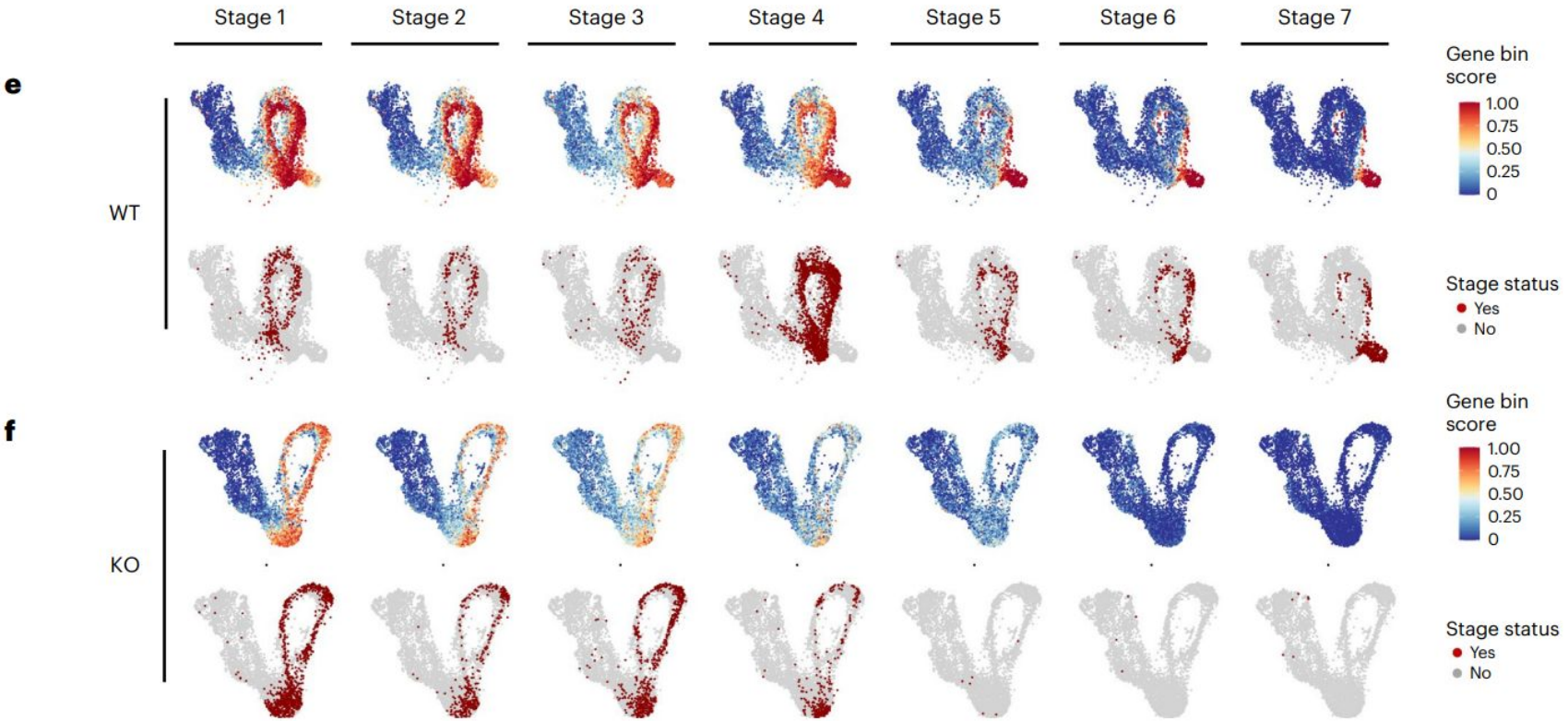
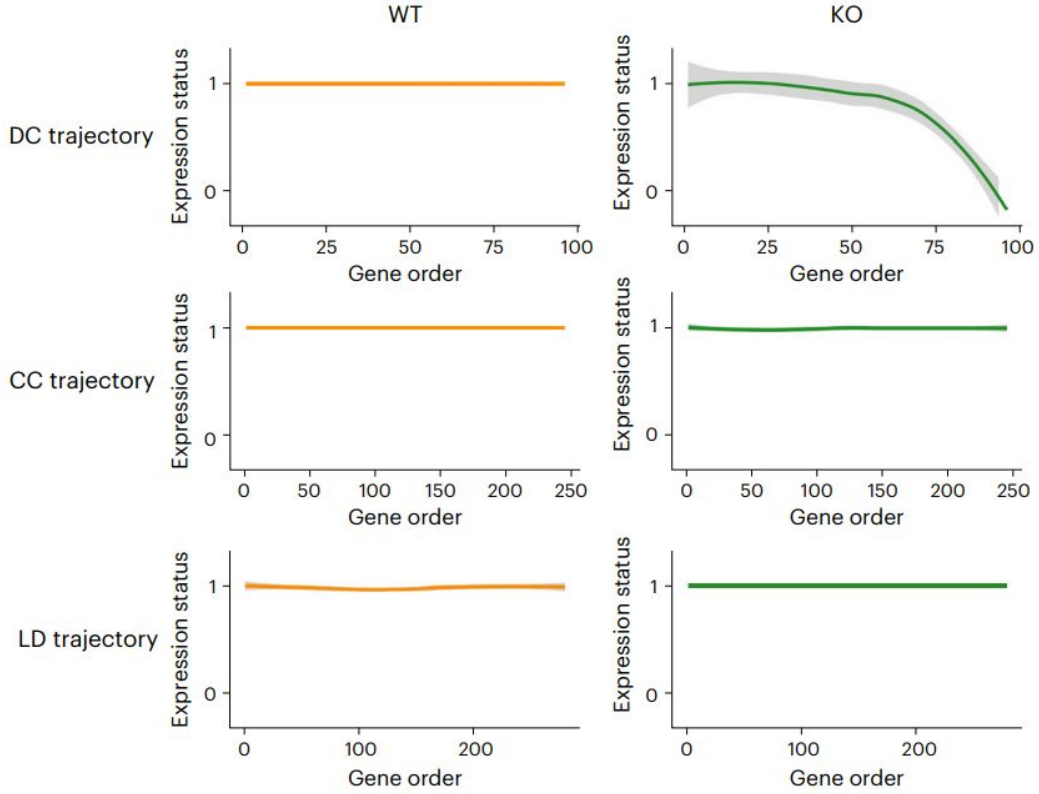
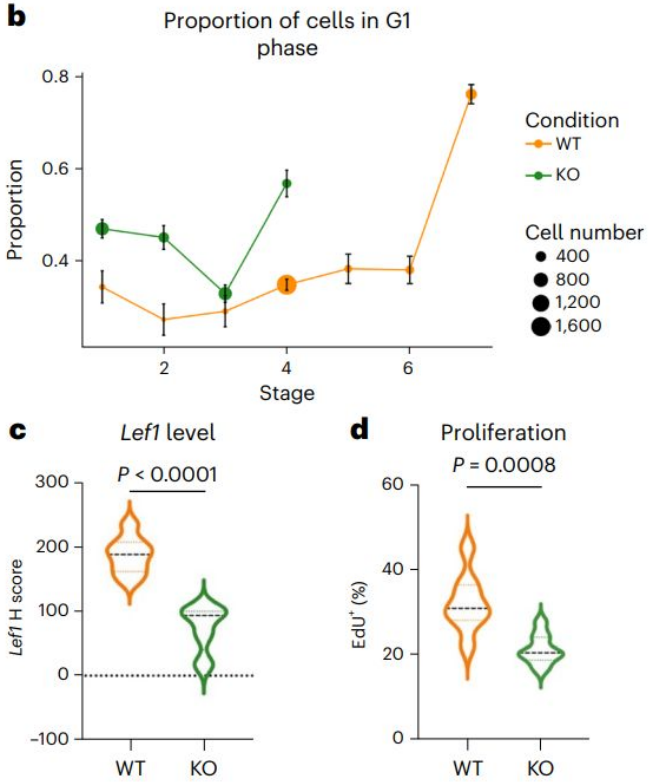


# Using Gene Trajectories to Decipher Mechanisms



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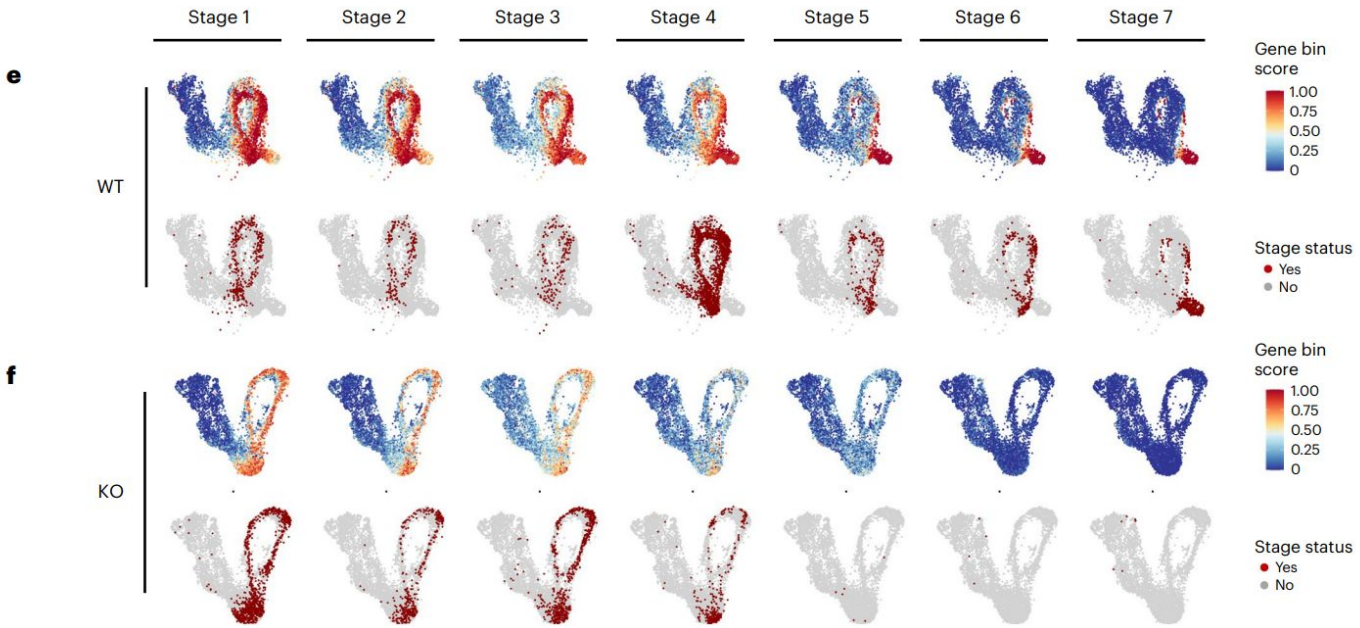
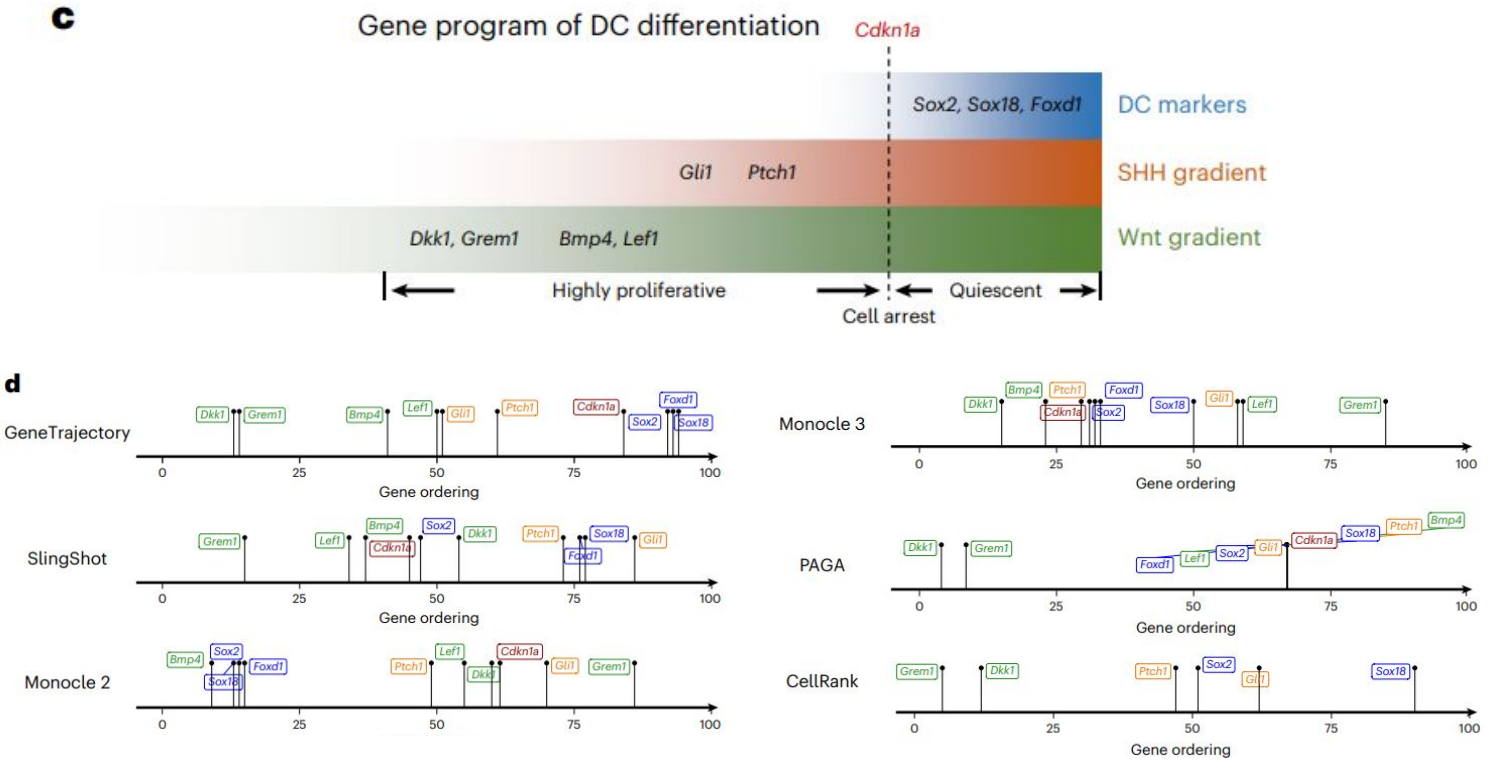


# Comparison to Other Methods



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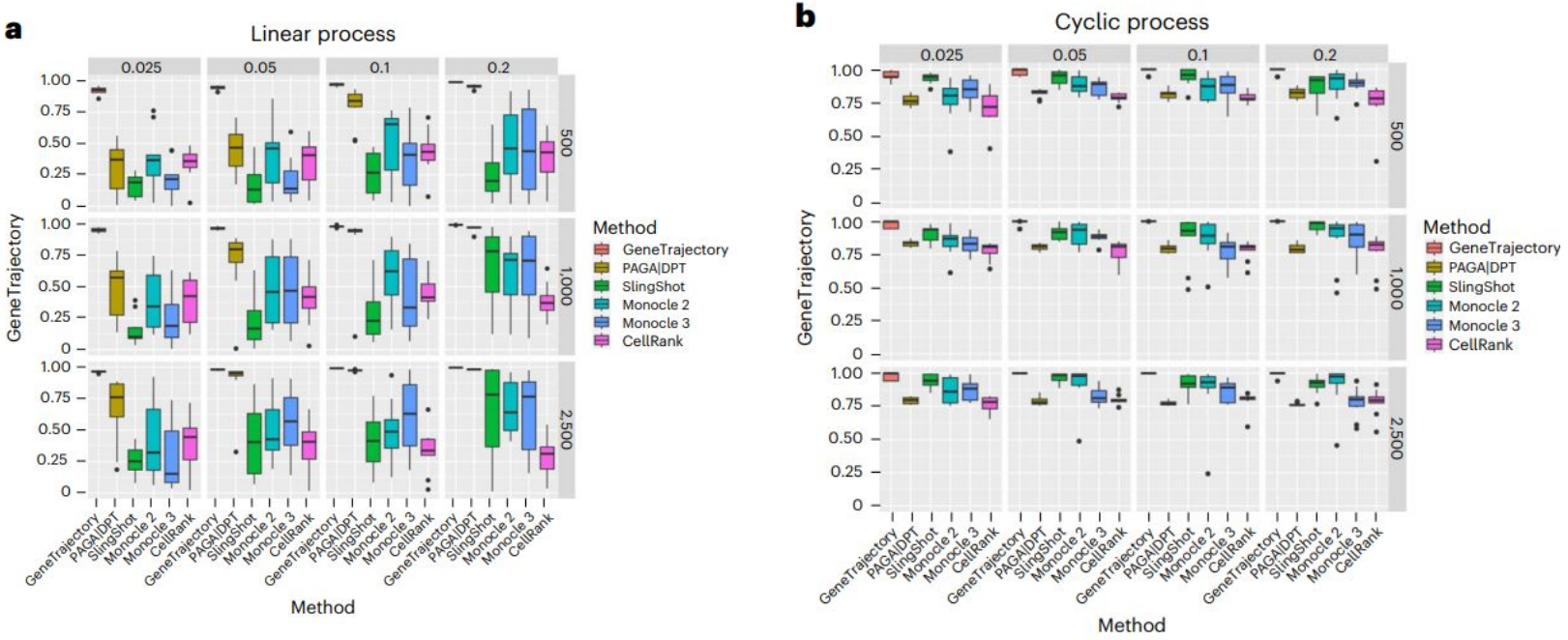
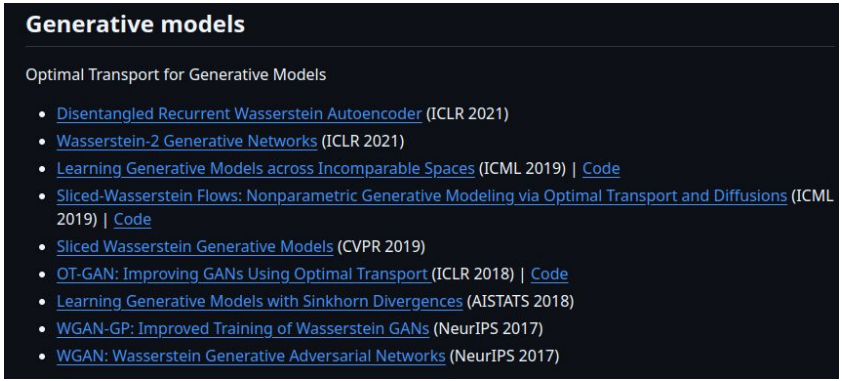



How good was the recovery of the order in which genes were expressed?

# What’s Next?

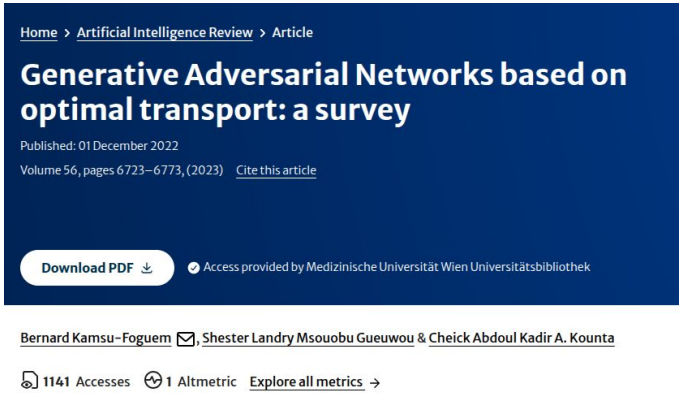


**Generative models**

Optimal Transport for Generative Models

- Disentangled Recurrent Wasserstein Autoencoder (ICLR 2021)
- Wasserstein-2 Generative Networks (ICLR 2021)
- Learning Generative Models across Incomparable Spaces (ICML 2019) | Code
- Sliced-Wasserstein Flows: Nonparametric Generative Modeling via Optimal Transport and Diffusions (ICML 2019) | Code
- Sliced Wasserstein Generative Models (CVPR 2019)
- OT-GAN: Improving GANs Using Optimal Transport (ICLR 2018) | Code
- Learning Generative Models with Sinkhorn Divergences (AISTATS 2018)
- WGAN-GP: Improved Training of Wasserstein GANs (NeurIPS 2017)
- WGAN: Wasserstein Generative Adversarial Networks (NeurIPS 2017)

https://github.com/kilianFatras/awesome-optimal-transport?tab=readme-ov-file#generative-models



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**Generative Adversarial Networks based on optimal transport: a survey**

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