Uncovering Developmental Lineages from Single-cell Data with Contrastive Poincaré Maps

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Abstract

Single-cell RNA-sequencing (scRNA-seq) enables the study of hierarchical and branching patterns in organismic development at high resolution. Analyzing such data requires visualization and analysis tools that faithfully represent the deep, tree-like structures formed by developmental lineages. Popular Euclidean embedding methods, such as UMAP and t-SNE, as well as domain-specific approaches like PHATE, distort hierarchical relationships in low dimensions, leading to a decrease in performance with growing tree depth. Hyperbolic geometry, which can represent trees with high accuracy in low dimensions, provides a natural remedy. However, existing hyperbolic methods, such as Poincaré Maps (PM), lose accuracy in deeper trees and require extensive feature engineering and memory. We present Contrastive Poincaré Maps (CPM), a self-supervised hyperbolic encoder that leverages contrastive learning in hyperbolic space to efficiently learn robust low-dimensional representations from scRNA-seq data. On synthetic trees with up to 5 generations and 34,000 individuals, CPM cuts distortion by $> 99\%$ and requires 13-fold less memory relative to PM. We further demonstrate CPM's utility on three biological case studies. CPM uncovers accurate hierarchies across 9 developmental stages in the mouse gastrulation dataset comprising 116,312 cells, disentangles global multi-lineage hierarchies in the chicken cardiogenesis dataset while preserving intra-lineage developmental trends, and enables sampling-density-invariant hierarchical analysis in the mouse hematopoiesis dataset. By leveraging hyperbolic geometry in combination with contrastive learning, CPM delivers a scalable framework that preserves hierarchical dependencies in developmental lineages, accelerates exploratory data analysis and opens new avenues for biological insights into developmental processes using scRNA-seq data.

A preliminary version of a part of this work was presented at the ICLR Workshop on Machine Learning for Genomics Explorations (Bhasker et al., 2024).

1 Introduction

Advances in high-throughput single-cell RNA sequencing (scRNA-seq) has transformed our ability to study dynamic biological processes by profiling gene expression at single-cell resolution (Macosko et al., 2015; Tang et al., 2009). It has been particularly powerful for dissecting lineage specific information and differentiation processes during development(Treutlein et al., 2014; Trapnell et al., 2014; Paul et al., 2015; Nestorowa et al., 2016; La Manno et al., 2018a; Pijuan-Sala et al., 2019). However, the resulting datasets capture thousands of genes across tens to hundreds of thousands of cells, making them inherently complex and high-dimensional. To make sense of this complexity, computational tools are needed to extract biologically meaningful patterns, such as the branching of cells into distinct lineages or transitions between cell states. Dimensionality reduction methods like UMAP (McInnes et al., 2018), t-SNE (Van der Maaten and Hinton, 2008), and MDS (Kruskal and Wish, 1978) are widely used to visualize cellular relationships in low-dimensional spaces. Additionally, specialized algorithms for single-cell data, including PHATE (Moon et al., 2019), diffusion maps (Nadler et al., 2005), Monocle (Trapnell et al., 2014), and PAGA (Wolf et al., 2019), enable reconstructing developmental trajectories, estimate pseudotime, and infer gene expression dynamics, critical for insights into cell fate decisions and uncovering the regulatory programs that drive tissue development and cellular diversity.

A common feature of both general-purpose and single-cell-specific computational tools is their reliance on Euclidean embeddings to represent high-dimensional gene expression data in two or three dimensions for visualization and analysis. However, Euclidean space is inherently limited in its ability to faithfully capture hierarchical or tree-like relationships, such as those underlying cell differentiation and lineage branching during development (Nickel and Kiela, 2017). These limitations can lead to distortions in representing developmental trajectories, particularly when complex bifurcations or nested lineage hierarchies are present. On the other hand, hyperbolic spaces, which are negatively curved geometric manifolds, offer a powerful alternative, as they are mathematically well-suited for embedding hierarchical structures with high fidelity even in low dimensions (Nickel and Kiela, 2017; Sala et al., 2018).

Building on the insight that hyperbolic geometry is well-suited for representing hierarchical structures, Klimovskaia et al. (2020) introduced Poincaré Maps (PM), a method designed to embed single-cell data into hyperbolic space. This approach extends a broader line of research on hyperbolic graph embeddings (Nickel and Kiela, 2017; Chamberlain et al., 2017; Chami et al., 2019) and their advantages in downstream machine learning tasks (Ganea et al., 2018; Weber et al., 2020). Poincaré Maps have demonstrated the ability to learn biologically meaningful representations across several single-cell datasets (Klimovskaia et al., 2020).

However, the method has several practical limitations. Although PM can effectively represent data structured as shallow hierarchies, their performance degrades with increasing tree depth, making them less suitable for modeling complex developmental trajectories (Bhasker et al., 2024). Additionally, the method relies on manual feature engineering to achieve good performance, entails a memory-intensive training process, and lacks support for efficient updates as new data becomes available. These factors limit its scalability and usability in large-scale single-cell studies.

In this work, we present Contrastive Poincaré maps (CPM), a scalable contrastive learning-based approach for efficiently representing high-dimensional single-cell data in a low-dimensional hyperbolic space while preserving the inherent hierarchical structures in the data. Our method

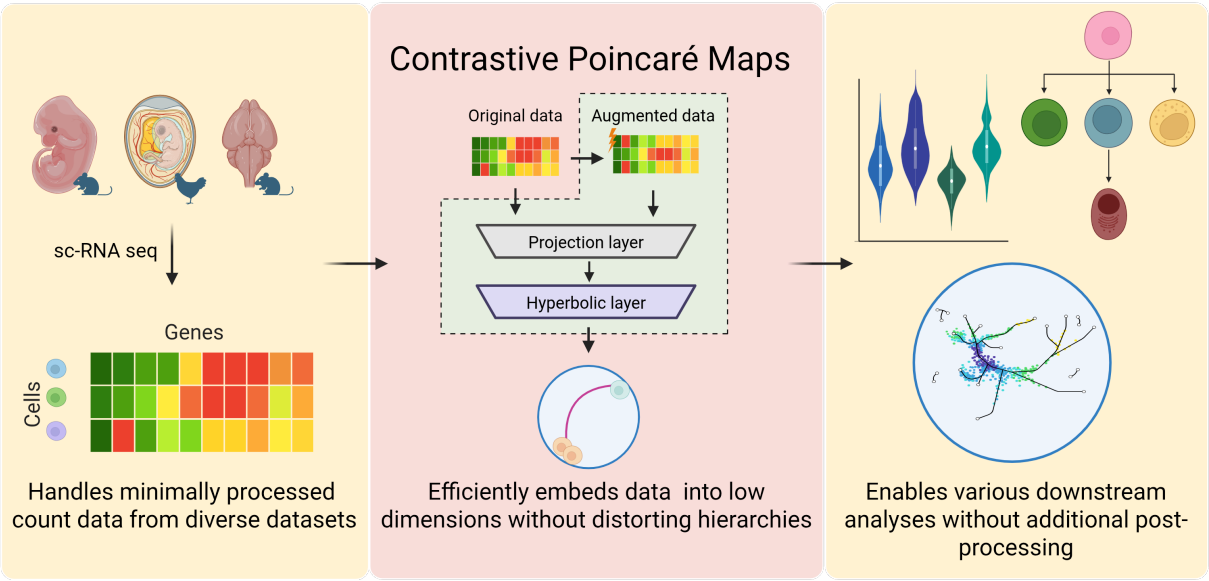

Figure 1: **Contrastive Poincaré Maps** is an efficient, low-distortion embedding method that handles minimally processed transcriptomic data from a wide range of specimens and supports multiple downstream analyses without further post-processing, delivering especially strong performance in lineage detection applications. Figure was created in BioRender. Bhasker, N. (2025) https://BioRender.com/t83d482

builds on PM (Klimovskaia et al., 2020), as well as contrastive approaches for representing tabular data (Bahri et al., 2022). We validate our method using synthetic data and three published scRNA-seq datasets. On synthetic trees with up to 5 generations and 34,000 individuals, CPM cuts distortion by $> 99\%$ and requires 13-fold less memory relative to PM. CPM uncovers accurate hierarchies across 9 developmental stages in the mouse gastrulation dataset comprising 116,312 cells, disentangles global multi-lineage hierarchies in the chicken cardiogenesis dataset while preserving intra-lineage developmental trends, and enables sampling-density-invariant hierarchical analysis in the mouse hematopoiesis dataset.

2 Results

We present Contrastive Poincaré maps (CPM), a contrastive learning-based approach to represent high-dimensional single cell data in a low-dimensional hyperbolic space (see Fig. 1). Our method builds on prior work on shallow hyperbolic embedding methods for single cell data analysis (Klimovskaia et al., 2020), as well as contrastive approaches for representing tabular data (Bahri et al., 2022). Contrastive learning facilitates improved data representation by effectively managing complexity in higher dimensions (Chen et al., 2020), demonstrating proven feature representation capabilities (Grill et al., 2020), robustness to noise (Ghosh and Lan, 2021), and generalization across various downstream tasks (Oord et al., 2018; Radford et al., 2021).

2.1 Setup

CPM processes the gene expression matrix in batches, applying an augmentation strategy that randomly replaces gene expression values with those from random cells in the dataset. This kind of augmentation strategy contributes to the learning of robust representations across diverse cells. We subsequently project both views of the data into a latent space. The function of the projection block is twofold, acting as both a dimensionality reduction and noise reduction method, which can be adapted and trained end-to-end, unlike conventional methods such as Principal Component Analysis (PCA). The latent representations of the data are then embedded into hyperbolic space using hyperbolic graph neural networks (Chami et al., 2019). We choose a two-dimensional representation space, the Poincaré disk, with curvature $\kappa = -1$. The choice of a two-dimensional representation space is motivated by ease of visualization and interpretability of the resulting embeddings; varying or learning the curvature as opposed to using a fixed value has been shown to have little effect (see, e.g., (Chami et al., 2019)), motivating our choice of $\kappa = -1$. We use the classical InfoNCE contrastive loss for training our model. The distance between both views of the data is calculated in hyperbolic space. The embeddings are learned by reducing the distance between similar cells and increasing the distance between dissimilar cells.

As is standard in deep learning approaches, we tuned crucial hyperparameters, especially the number of layers, batch size, and learning rate. Experimentation on synthetic data showed that the performance of the model is robust to significant variation in these hyperparameters (see Supplementary Fig. 11). We observed that the number of projection layers and the rate of perturbation used to construct augmentations in a batch has to be carefully balanced to control the distortion of our embeddings (see Fig. 11).

Our case studies explore early organogenesis in mouse gastrulation (Pijuan-Sala et al., 2019), developmental trajectories in mice hematopoiesis (Paul et al., 2015), and multi-lineage developmental trajectories in chicken cardiogenesis (Mantri et al., 2021).

We compare our model to widely used dimensionality reduction, visualization and lineage detection methods such as t-SNE (Maaten and Hinton, 2008), UMAP (McInnes et al., 2018) and PHATE (Moon et al., 2019) respectively. We also compare against Poincaré Maps (PM), which has outperformed the aforementioned approaches on both synthetic and real world tree-like data. We use Q-scores (Lee and Verleysen, 2010) and worst-case distortion for evaluation (see sec. 4.7), which are standard metrics in the manifold embedding literature. Q-scores offer an unsupervised, scale-free, rank-invariant criterion for assessing embeddings. By operating on neighbor ranks rather than raw pairwise distances, they remain unaffected by global scaling, making them a robust baseline metric for evaluating the fidelity of any dimensionality-reduction method. Worst-case distortion provides a provable upper bound on the weakest links in the embedding, making downstream tasks like lineage detection more trustworthy.

2.2 Synthetic Data

In our initial set of experiments, we generated a diverse collection of synthetic datasets varying in size and structural complexity, following methods described in Moon et al. (2019). For illustrative purposes, we selected three representative examples: (i) **Synthetic data 1** – a deep binary tree with 15 hierarchical levels, where each node branches into two children; (ii) **Synthetic data 2** – an imbalanced binary tree with 10 levels, in which each node also has

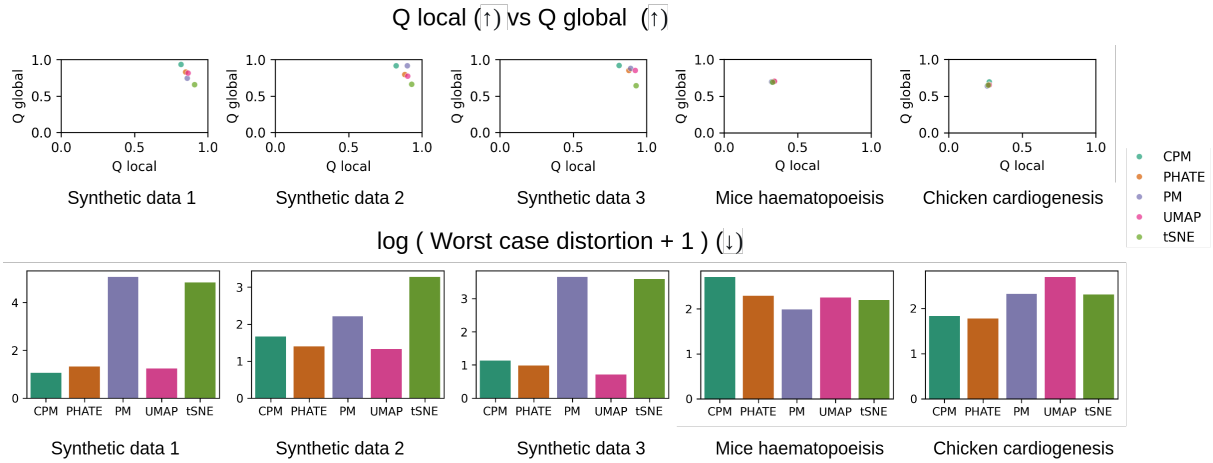

Figure 2: **Quantitative evaluation**. Contrastive Poincaré Maps achieves competitive representation accuracy across diverse real and synthetic datasets, requiring minimal hyperparameter tuning and no additional PCA-based dimensionality reduction. Synthetic data 1 and Synthetic data 2 represent deep (15 and 10 hierarchical levels, respectively), heterogeneous, balanced binary trees, while Synthetic data 3 is a deep, heterogeneous, imbalanced binary tree. Real datasets encompass shallow hierarchies (mice haematopoiesis and mouse brain) and a shallow, multi-lineage topology (chicken cardiogenesis).

two children, but branches are sampled randomly to introduce structural irregularity; and (iii) **Synthetic data 3** – a balanced binary tree with 10 levels, each node branching into two children, with no randomness in structure. To enhance heterogeneity within the trees, one branch at each depth level was constrained to contain one third of the total samples for that level.

CPM achieves high global accuracy across all datasets with low distortion, outperforming the hyperbolic PM baseline (Fig.2). On synthetic trees with up to 5 generations and 34,000 individuals, CPM cuts distortion by $> 99\%$ and requires 13-fold less memory relative to PM. Compared to other Euclidean state-of-the-art methods, CPM achieves comparable performance with minimal hyperparameter tuning (Supplementary Fig. 11), despite not relying on additional pre-processing steps such as Principal Component Analysis (PCA) or batch effect correction with Scanorama (Hie et al., 2024). For a fair comparison with CPM, Supplementary Fig 10 shows the performance of all the methods without any additional pre-processing steps. We further see that CPM provides significant time and memory benefits compared to PM (see Fig. 3). Notably, in terms of memory, CPM is competitive with the shallow methods, which are untrained and hence have a much smaller parameter budget.

Visualizations for the individual datasets are provided in Supplementary Figures 12, 13, 14. There is no continuous progression between hierarchical levels in Poincaré maps, as demonstrated in CPM. All hierarchical levels beyond the root appear to be pushed toward the horizon, resulting in an unnatural representation that fails to preserve the inherent hierarchical structure (see Supplementary Fig. 12). On closer inspection, we also see an unnatural intersection between branches on some of the visualizations produced by PHATE, t-SNE and UMAP (see Supplementary Figures 12, 13, 14).

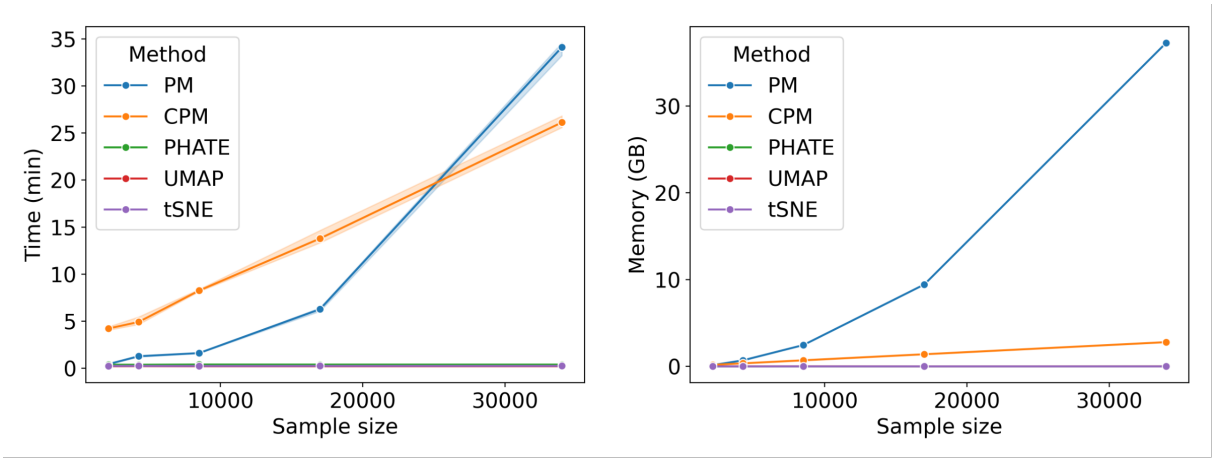

Figure 3: **Space and time complexity analysis**. Time and memory requirements for each embedding approach are assessed across varying sample sizes using synthetic data. Contrastive Poincaré Maps (CPM) demonstrates substantial efficiency improvements in both computational time and memory usage compared to data-driven counterparts requiring explicit training steps.

2.3 Case study 1: Mouse gastrulation and early organogenesis

We analyze data from Pijuan-Sala et al. (2019), encompassing 116,312 cells from mouse embryos at nine developmental stages between embryonic days 6.5 and 8.5. This dataset captures the transcriptional dynamics during the critical phases of gastrulation and early organ formation. The dataset was normalized to 10000 counts per cell, Log1p transformed and filtered to contain 2000 highly variable genes. The first important observation is that state-of-the-art approaches, except CPM, fail to produce an embedding for the complete dataset (containing 100,000 cells), due to their reliance on pairwise distances for the computation of embeddings, which scales quadratically in the number of cells and runs out of memory on a fairly sophisticated infrastructure (cluster equipped with 112 CPUs with 1TB of RAM). Since our method processes data in batches during training, it efficiently generates embeddings within a reasonable time (approx. 2-3 hours). Unfortunately, the metrics that we use in our work also rely on pairwise distances for their computation and fail to produce results for the complete dataset. However, the performance of all the methods on a subsample of the dataset is illustrated in Supplementary Fig 18.

In line with the findings of (Pijuan-Sala et al., 2019), we observe (based on Figs. 4, 5, 6): (i) a decline in the frequency of pluripotent epiblast cells over time, (ii) the appearance of mesodermal and definitive endodermal cells as early as E6.75, (iii) the origin of gut endoderm from visceral as well as definitive endoderm cells, (iv) the formation of red blood cells in two consecutive waves — the first at E7.5 and the second at E8.25, and (v) high expression of Kdr gene in the endothelial region (see Supplementary Fig 25).

A simple phylogenetic tree, as seen in Fig. 4, reveals the presence of mature visceral endoderm cells as early as E6.5. This could be explained by the fact that the authors sampled extra-embryonic structures alongside the gastrulating embryo to investigate the convergence of primitive streak-derived definitive endoderm with visceral endoderm-derived cells at the molecular level. The original study (Pijuan-Sala et al., 2019) performed analyses such as flow cytometry,

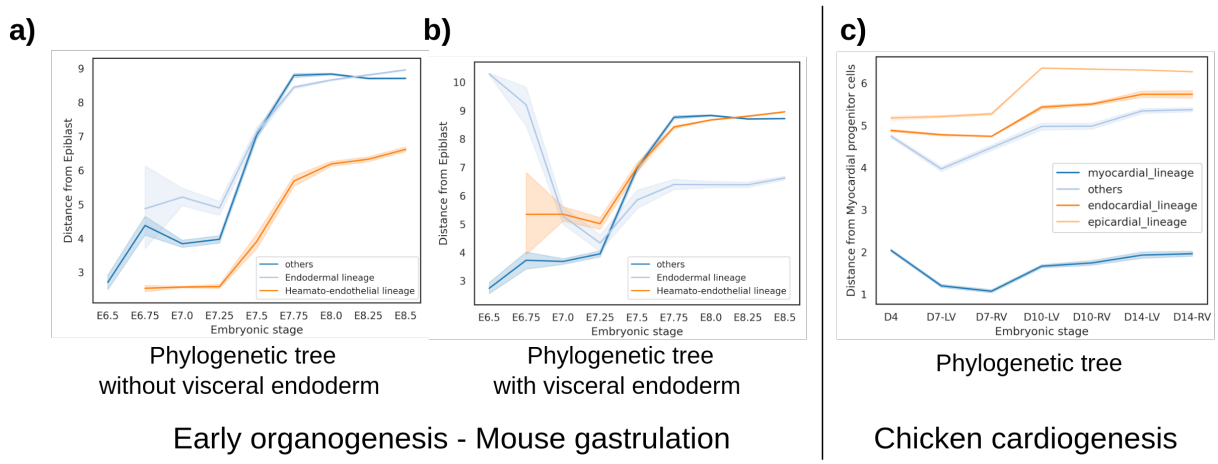

Figure 4: **Application to organogenesis**. Illustration of how distances within Contrastive Poincaré Maps reflect developmental progression across lineages in mouse gastrulation and chicken cardiogenesis datasets. (a, b) Differentiation across embryonic stages in the endodermal and haemato-endothelial lineages from the mouse gastrulation dataset: (a) Endodermal lineage excluding visceral endoderm; (b) Endodermal lineage including visceral endoderm, supported by evidence for the presence of visceral endoderm as early as embryonic stage E6.5. (c) Differentiation across developmental stages in myocardial, epicardial, and endocardial lineages from the chicken cardiogenesis dataset.

in addition to scRNA-seq, to arrive at these findings. In contrast, CPM facilitated the observation of these findings with a single embedding method with minimal hyperparameter tuning.

One of the main conclusions of Pijuan-Sala et al. (2019) was that densely sampled large-scale single-cell profiling has the potential to help advance the understanding of embryonic development. Thanks to its scalability, CPM enables such large-scale analyses, whereas other embedding methods are prohibitively memory-intensive in this regime.

2.4 Case study 2: Mice hematopoiesis

We analyze dataset from Paul et al. (2015), comprising scRNA-seq profiles of approximately 2,730 mouse bone marrow-derived myeloid progenitor cells, including common myeloid progenitors (CMP), granulocyte-monocyte progenitors (GMP), and megakaryocyte–erythroid progenitor (MEP). It captures transcriptional heterogeneity across these cell types, revealing lineage-specific gene expression patterns. This dataset is widely used to study hematopoietic differentiation, transcriptional priming, and to benchmark single-cell analysis methods. The processed dataset was obtained from (Klimovskaia et al., 2020).

Paul et al. (2015) use scRNA-seq to reveal that GMPs are transcriptionally heterogeneous and already primed for distinct myeloid fates (neutrophils, monocytes, and basophils), challenging the classical stepwise model of hematopoiesis. The transcription factor Cebpa is identified as a key regulator in this early lineage commitment. Regarding basophil origin, the authors present strong evidence for a basophil-neutrophil-monocyte progenitor (BNMP) within the GMP pool, supporting a model of gradual, transcriptionally guided differentiation.

However, subsequent analyses using Partition-based Graph Abstraction (PAGA) (Wolf et al.,

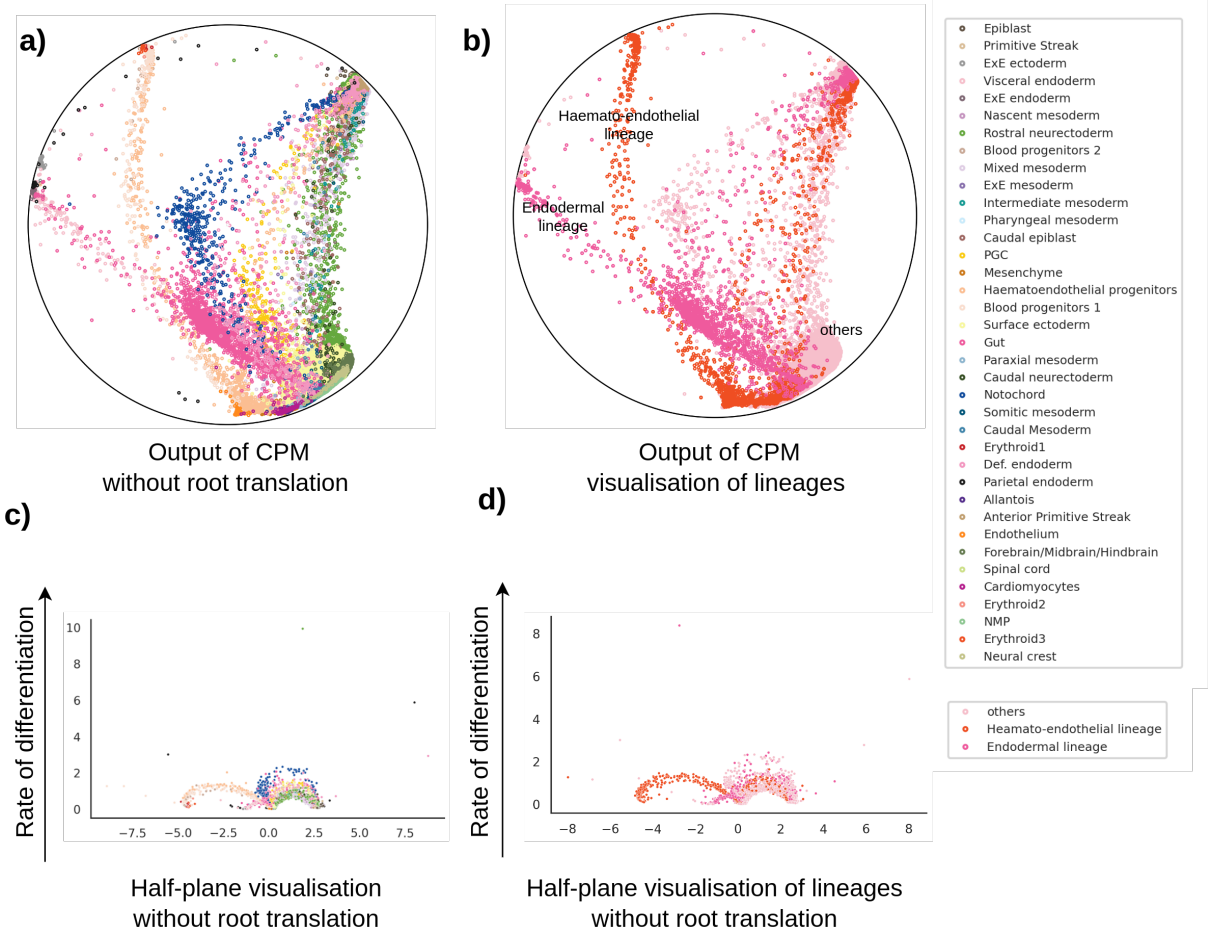

Figure 5: **Analysis of early organogenesis during mouse gastrulation.** (a, b) Visualization of the embedding learned by Contrastive Poincaré Maps for the mouse gastrulation dataset, comprising 116,312 cells across nine developmental stages. Contrastive Poincaré Maps accurately preserves the global hierarchy of lineages (b) as well as the relationships among individual cells (a). (c, d) Visualization of the embedding following transformation into the Poincaré half-plane, enabling inference of differentiation origins and rates.

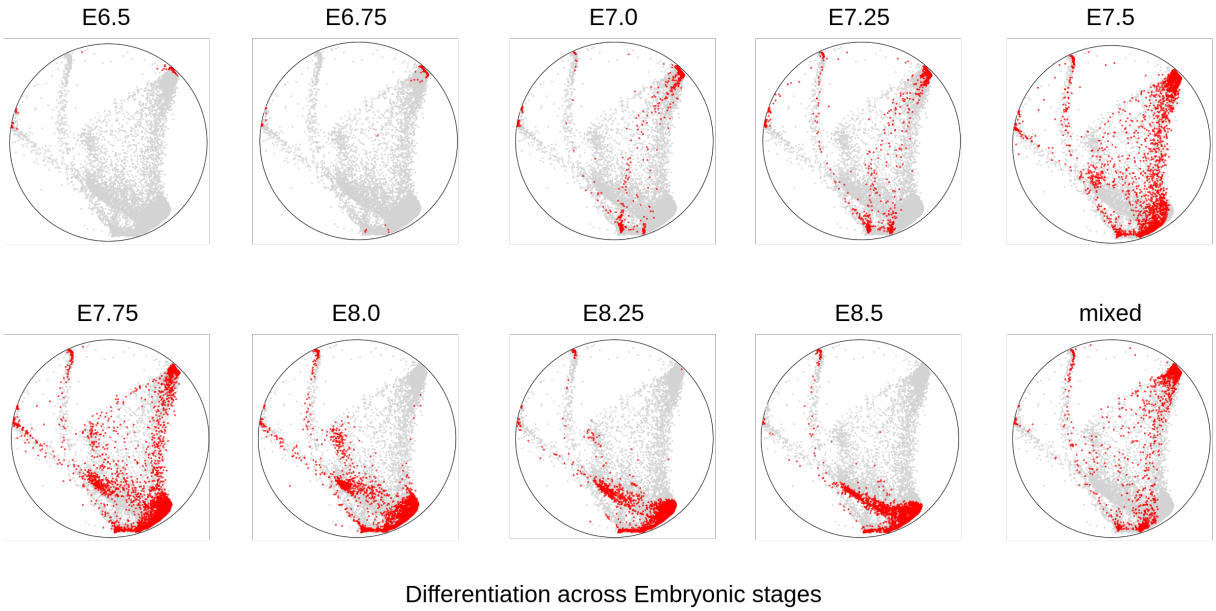

Figure 6: **Early organogenesis during mouse gastrulation** Time-lapse visualization of cell differentiation across nine developmental stages overlaid on the embedding produced by Contrastive Poincaré Maps. The embedding provides evidence for the early emergence of endothelial lineage cells and highlights two distinct waves in the formation of red blood cells.

2019) suggest that basophil lineage trajectories are dataset-dependent and may reflect multiple origins. While Paul et al. (2015) data support the BNMP model, other datasets such as Nestorowa et al. (2016) suggest erythroid-megakaryocyte-basophil progenitor model, and the more densely sampled Dahlin et al. (2018) dataset provides evidence for both possibilities. This indicates that basophil development may not follow a singular, fixed path, but rather may involve context-dependent or plastic differentiation routes.

On applying Poincaré maps to the dataset from Paul et al. (2015), Klimovskaia et al. (2020) observed that their method effectively captured the hierarchical relationships among various myeloid progenitor populations. Notably, Poincaré maps positioned the 16Neu cluster downstream of the 15Mo cluster, suggesting a potential sequential relationship between these cell types. This contrasts with the canonical hematopoietic hierarchy, where neutrophils and monocytes are typically considered to arise independently from a common progenitor. The authors attribute this discrepancy to possible mislabeling in the original dataset.

Fig. 7 illustrates the canonical cell ordering derived from the embeddings generated from CPM, PM and PHATE. For each method, we plot the median distance of cells from the root against their angular separation. Among the methods, only CPM successfully distinguishes MEP from GMP, thereby supporting the BNMP model. This is consistent with both the dataset characteristics and previous findings using PAGA. Furthermore, in contrast to PM and PHATE, CPM positions dendritic cells proximal to eosinophils and downstream of the lymphoid lineage, rather than near erythroid cells. This arrangement aligns with established hierarchies (Fig. 7 a)).

We also visualize the trajectory between the 1Ery and 14Mo cell types by interpolating be-

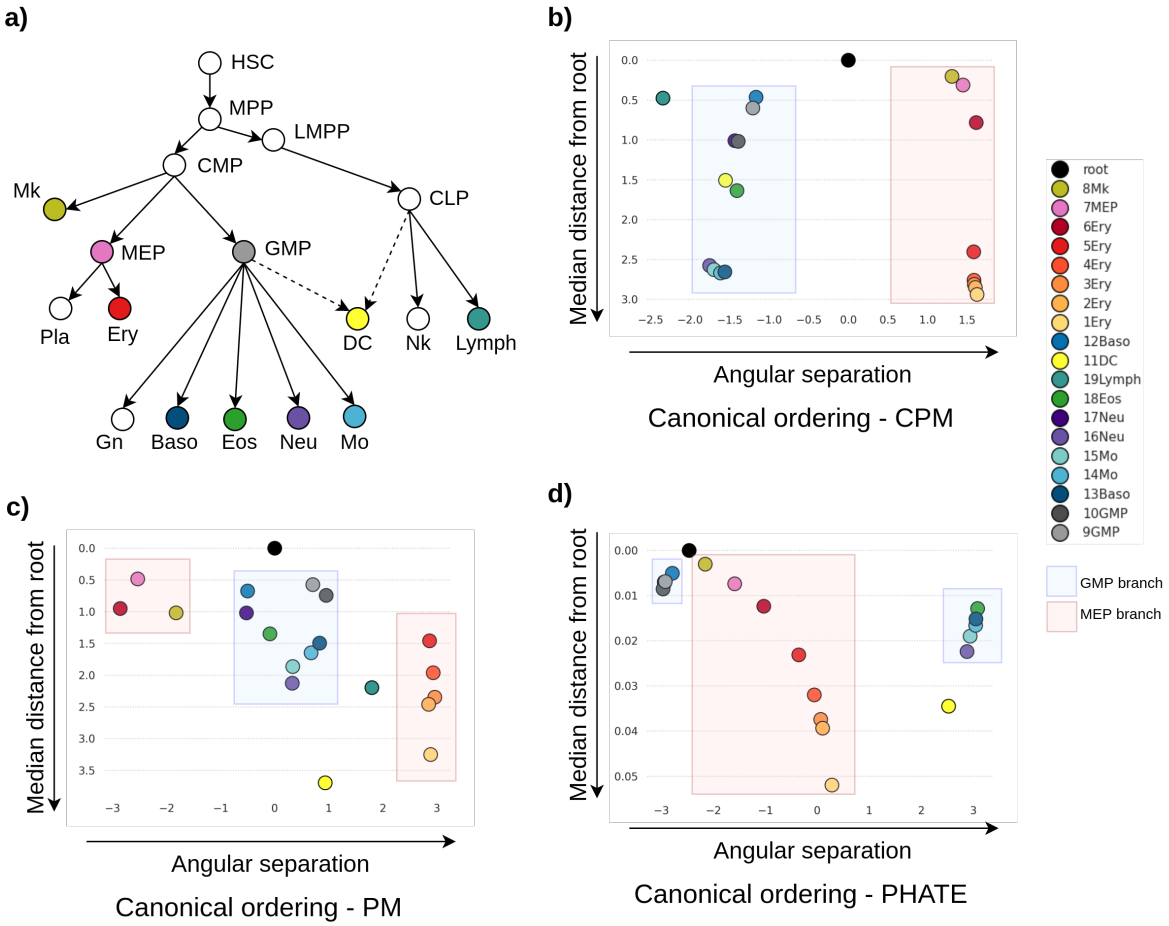

Figure 7: **Canonical ordering of cell types** Distances and angular relationships in the Contrastive Poncaré Maps embedding more faithfully preserve the canonical haematopoietic hierarchy than Poincaré Maps or PHATE, with particularly accurate reconstruction of the myeloid branch comprising basophils, neutrophils, monocytes, and eosinophils. (a) Reference haematopoietic lineage tree. (b–d) Cell type ordering based on pairwise distances and angles in Contrastive Poincaré Maps, Poincaré Maps, and PHATE embeddings, respectively.

tween between points along these branches. For CPM and PM, interpolation is performed along geodesics (see Appendix A.4.2). In CPM embedding, the trajectory passes through intermediate Ery and Mk cell types, consistent with known biological progression (Fig. 8). In contrast, this pattern is not observed in PM or PHATE embeddings. These results indicate that CPM not only accurately represents the individual cell types, but also captures the underlying structure of the dataset by preserving meaningful transitional relationships in the embedding space. Visualizations of embeddings and gene expressions for certain genes of interest are provided in Supplementary Figures 16, 26.

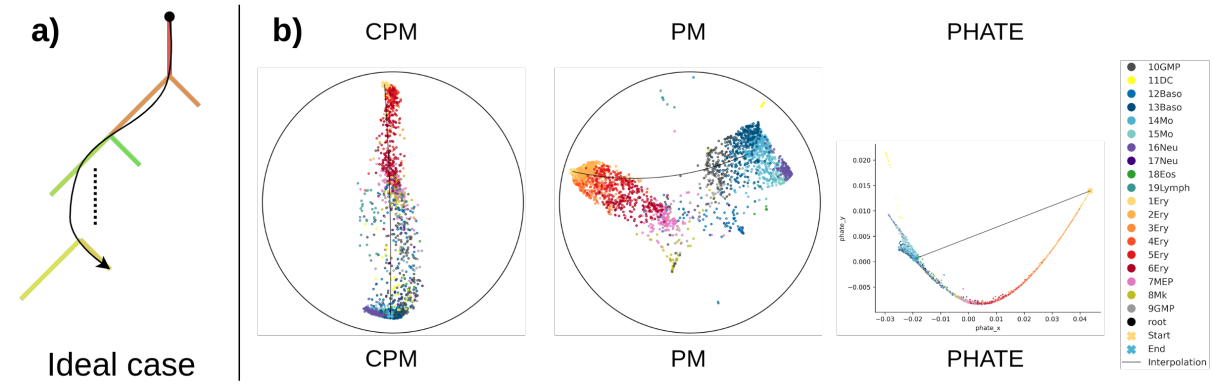

Figure 8: **Interpolation between hierarchical levels.** (a) In hierarchical structures, the path between two nodes should ideally traverse intermediate points that reflect the underlying organization. (b) For the mouse haematopoiesis dataset, only Contrastive Poincaré Maps embedding yields a trajectory that passes through the intermediate Ery and Mk cell types when interpolating between 1Ery and 14Mo.

2.5 Case study 3: Chicken cardiogenesis

We analyze scRNA-seq data from Mantri et al. (2021), which includes transcriptomic profiles from 22,315 individual cells collected across four embryonic stages (days 4, 7, 10, and 14). This dataset contains gene expression profiles from cells spanning multiple lineages and provides a high-resolution view of how cellular differentiation and morphogenetic processes are coordinated during heart development, offering key insights into cardiac lineage specification. The dataset was processed following the approach described in Mantri et al. (2021), with the exception that CPM operated on the full dataset containing 18,797 genes prior to Scanorama integration and the selection of the top 2000 highly variable genes.

State-of-the-art methods achieved optimal performance primarily when additional pre-processing steps, such as Scanorama integration, were applied to correct for batch effects in the dataset. In contrast, our approach distinctly clustered the myocardial, endocardial, and epicardial lineages without requiring such corrections, while simultaneously preserving the intrinsic global hierarchical structure of the data. Notably, our method also clearly separates hematopoiesis related cell populations, including erythrocytes, macrophages, and dendritic cells (see Fig. 9a).

To further analyze lineage organization using the CPM method, we embedded each lineage independently (see Fig.9c). These embeddings reveal well preserved intra-lineage hierarchies and effectively capture the differentiation continuum from immature to mature cell states across

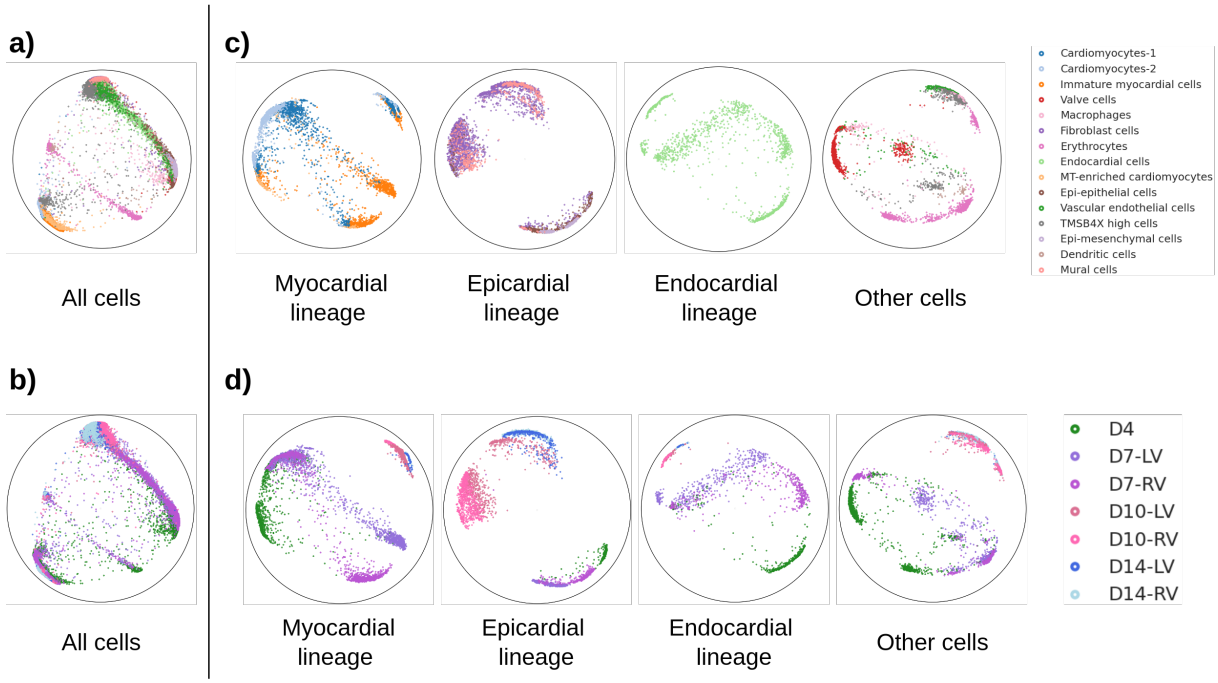

Figure 9: **Chicken cardiogenesis** (a,b) Embedding learned by Contrastive Poincaré Maps for the chicken cardiogenesis dataset, comprising 22,315 cells from multiple lineages across four developmental stages. Contrastive Poincaré Maps preserves the global hierarchical structure of the data. (c,d) Lineage-specific embeddings, highlighting well-preserved intra-lineage hierarchies that capture differentiation trajectories from immature to mature cell types over developmental time.

developmental stages (see Fig.9d). The gene expression for certain genes of interest and the visualizations of embeddings for state-of-the-art methods are shown in Supplementary Figures 17, 23.

3 Discussion

Robust computational methods are essential for scRNA-seq analysis due to the inherent sparsity, noise, and high dimensionality of single-cell data. Without appropriate models, biological signal is easily confounded by technical variation and dropout effects. As datasets grow in size and complexity, conventional tools lack the scalability and resolution required for accurate cell-type classification, trajectory inference, and gene regulatory analysis. Thus, rigorous computational frameworks are critical to extract meaningful insights and ensure reproducibility across single-cell studies.

Contrastive Poincaré Maps (CPM) is a novel contrastive learning method for learning hyperbolic representation of single-cell data. Hyperbolic representation offers distinct advantages over traditional Euclidean embeddings, particularly for modeling hierarchical structure. Biological systems frequently exhibit nested organization, such as developmental lineages or differentiation trajectories, that Euclidean space struggles to represent without distortion. Hyperbolic geometry, with its exponential volume growth, is inherently suited to capturing such hierarchies with high fidelity. This enables more accurate preservation of both global and local relationships among cells

Building on these geometric advantages, our method demonstrates several key strengths across synthetic and real scRNA-seq datasets. It achieves competitive representation accuracy without requiring standard pre-processing steps such as PCA, batch correction, or data subsampling, thereby reducing potential sources of bias and information loss. Unlike methods that rely on aggressive dimensionality reduction or batch correction (e.g., Scanorama), our approach maintains fidelity to the underlying transcriptomic structure while remaining computationally efficient. It scales to datasets exceeding 100,000 cells (Pijuan-Sala et al., 2019) with minimal memory and runtime overhead, enabling robust performance even in large, heterogeneous populations.

Notably, the method captures differentiation trends and complex trajectories, including multi-lineage hierarchies, directly from the embedding. This robustness also extends to single-nucleus RNA sequencing data and fine-grained resolution of developmental processes, such as embryonic stage-specific lineage branching during mouse brain development (Supplementary section F). Furthermore, the embedding remains stable across a range of hyperparameter settings, and its geometry enables biologically meaningful interpolation between cell hierarchies, reflecting continuous transitions inherent to cellular differentiation.

While the current framework effectively models hierarchical and continuous structure in scRNA-seq data, several avenues remain open for exploration. A particularly promising direction lies in improving interpretability: unlike widely used visualization tools such as UMAP or t-SNE, whose Euclidean embeddings often suffer from high representation error and distortion of global structure, hyperbolic embeddings preserve both local and global geometry. This preservation opens the door to quantitative interpretability of the latent space, such as assessing biological variation along geodesic paths, offering a principled means to link embedding structure with gene expression dynamics. Future extensions to multimodal data, including spatial transcriptomics and chromatin accessibility, may further enhance the resolution and biological insight afforded

by hyperbolic representations.

4 Methods

Let $\mathcal{X} = \{x_i\}_{i=1}^n$ be the given scRNA-seq dataset with n cells and d features per cell, i.e., $x_i \in \mathbb{R}^d$. In this work, we focus on representing data in hyperbolic space by learning a mapping, $\phi : \mathcal{X} \to \mathbb{P}^2$ between data space $\mathcal{X}$ and hyperbolic representation space $\mathbb{P}^2$, which maps a data point $x_i \in \mathcal{X}$ to $\phi(x_i) \in \mathbb{P}^2$.

4.1 Hyperbolic Geometry

Hyperbolic spaces are smooth Riemannian manifolds with constant negative curvature. In this work, we adopt the Poincaré ball and Poincaré half-plane models of hyperbolic space, which are two of several known parametrizations. The *Poincaré ball model* defines a hyperbolic space within the Euclidean unit ball, i.e.,

$$\mathbb{P}^d = \{x \in \mathbb{R}^{d+1} : \|x\| < 1\} \tag{4.1}$$

$$d_{\mathbb{P}}(x, y) = \operatorname{acosh}\left(1 + 2\frac{\|x - y\|^2}{(1 - \|x\|^2)(1 - \|y\|^2)}\right) , \tag{4.2}$$

where $\|\cdot\|$ denotes the usual Euclidean norm. The exponential map $\operatorname{Exp}_x : T_x\mathbb{P}^d \to \mathbb{P}^d$, an important geometric tool, which, e.g., characterises geodesics in the space, is given by

$$\operatorname{Exp}_x(v) = \cosh(\|v\|_M)x + \sinh(\|v\|_M)\frac{v}{\|v\|_M} ,$$

where $\|v\|_M = \sqrt{\langle v, v\rangle_M}$ is computed with respect to the Minkowski product $\langle u, v\rangle_M = -u_0v_0 + \sum_{i=1}^d u_iv_i$. Geodesics in the Poincare model can be computed via simple retractions of the form

$$\begin{aligned} \mathcal{R} : \mathbb{R}^{d+1} &\to T_x\mathbb{P}^d \\ x &\mapsto P(x + v) \end{aligned}$$

where P is an orthogonal projection onto $\mathbb{P}^d$, given by

$$P(v) = \begin{cases} \frac{v}{\|v\|}, \|v\| \leq q \\ v, \text{else} . \end{cases}$$

Throughout this work, we will focus on the two-dimensional setting, i.e., $\mathbb{P}^2$.

4.2 Synthetic data generation

We generated synthetic datasets using PHATE Moon et al. (2019), which relies on diffusion-limited aggregation. The ground truth hierarchies were binary trees, with each depth level branching into two subtrees. To introduce heterogeneity, one branch at every level was constrained to contain one-third of the total samples at that depth level. The total number of samples in the is given by n_l(root level) $+(d \times n_l)$, where n_l is the number of samples per level and d is the depth of the tree. We also generated an *imbalanced* tree with randomly sampled branches to simulate more realistic scenarios.

4.3 Data pre-processing

The synthetic data was standardized to have zero mean and unit variance. The mouse gastrulation dataset was normalized to 10000 counts per cell, Log1p transformed and filtered to contain 2000 highly variable genes. The processed mice hematopoiesis dataset was obtained from Klimovskaia et al. (2020). The chicken cardiogenesis dataset was processed following the approach described in Mantri et al. (2021), with the exception that CPM operated on the full dataset containing 18,797 genes prior to Scanorama integration and the selection of the top 2000 highly variable genes. While our method operates without the need for additional dimensionality reduction techniques, PCA was applied to the other baselines along with their respective pre-processing steps.

4.4 Model architecture and optimization

Contrastive Poincaré Maps (CPM) adopts sampling strategy of SCARF (Bahri et al., 2022). For each batch, a positive sample is obtained by constructing an additional corrupted view: a randomly chosen fraction of feature entities is substituted with values from other training examples. This kind of augmentation strategy contributes to the learning of robust representations across diverse cells. The encoder consists of a projection block and a hyperbolic block. The projection block is composed of linear layers with ReLU activation. The function of the projection block is twofold, acting as both a dimensionality reduction and noise reduction method, which can be adapted and trained end-to-end, unlike conventional methods such as Principal Component Analysis (PCA). The hyperbolic block comprises of hyperbolic linear layers with ReLU activation (Chami et al., 2019). We choose a two-dimensional representation space, the Poincaré disk, with curvature $\kappa = -1$. The choice of a two-dimensional representation space is motivated by ease of visualization and interpretability of the resulting embeddings; varying or learning the curvature as opposed to using a fixed value has been shown to have little effect (see, e.g., (Chami et al., 2019)), motivating our choice of $\kappa = -1$. A single forward pass of the model can be written as,

$$H = \sigma(W_e X^e + b_1),$$

where H is the latent representation learnt by the projection block, W_e are the parameters of the projection block, X^e is the input data, b_1 is the bias, and $\sigma(.)$ is the non-linear ReLU activation unit. The representations are subsequently projected to the Poincaré disk using the exponential map $Exp_o(.)$ and processed by the hyperbolic block, as seen in the following equation:

$$Z^h = \sigma^{\otimes}(W_h \otimes \mathrm{Exp}_o(H) \oplus \mathrm{Exp}_o(b_2)) \ .$$

Here, W_h and b_2 are the trainable parameters of the hyperbolic block and Z^h is the hyperbolic representation learnt by the model; $\sigma^{\otimes}(.) = Exp_o(\sigma(Log_o(.)))$, where $Log_o(.)$ is the logarithmic map (Chami et al., 2019).

Hyperbolic representations of both augmented views of the input are learnt by using encoder blocks with shared weights. Their similarity, referred to as *Poincaré similarity*, is computed from Poincaré distance (Eq. 4.1) as $1/(1 + d_{\mathbb{P}}(x, y))$. These similarities are incorporated into the classical InfoNCE contrastive loss for training. We use Riemannian Adam (Bécigneul and Ganea, 2023) for optimisation, using different learning rates for the projection and hyperbolic blocks.

4.5 Hyperparameter tuning

The most important hyperparameters include batch size, corruption rate for data augmentation, the number of projection and hyperbolic layers, dimensions of the latent representation and learning rates for the projection and hyperbolic blocks. The learning rate for the hyperbolic block is usually higher than the learning rate for the projection block. The selection of batch size is a trade-off between performance and speed. A batch size of 128 worked well for most of the datasets used in this study. The number of hyperbolic layers depends on the complexity and depth of the input hierarchies. We set the number of hyperbolic layers to 2 for the deepest synthetic tree used in this study. It is also crucial to strike a balance between the number of projection layers and number of cells to be considered for augmentation in a batch, as these control the distortion of our embeddings. A corruption rate of 0.2 and one projection layer achieved good performance on most of the datasets used in this study.

4.6 Complexity

The memory complexity of CPM is $\mathcal{O}(b^2)$, where b is the batch size used for training. The time complexity mainly consists of the calculation of the pairwise similarities for learning the embedding, which is $\mathcal{O}(b^2)$. The time complexity for the entire training process can be summarized as $\mathcal{O}(b^2ed)$, where e is the number of epochs and d is the dimension of feature space. For all the datasets used in this study, the training loss converged within 200 epochs. The training time ranged from a few minutes (< 15) for synthetic datasets, 33-35 minutes for chicken cardiogenesis dataset (22,315 cells and 18,798 genes) to 2-3 hours for mouse gastrulation dataset (>100,000 cells and 2000 genes). The total memory consumption was less than 20GB for all the datasets used in this study.

4.7 Quantitative evaluation metrics

Let $\phi : \mathcal{X} \to \mathcal{M}$ denote an embedding of a data set $\mathcal{X}$. In the case of Poincaré embeddings (standard and contrastive), $\mathcal{M} = \mathbb{P}^2$, i.e., the hyperbolic plane. For Euclidean embeddings, $\mathcal{M} = \mathbb{R}^d$, for small d.

Distortion. Consistent with conventions in the classical metric embedding literature, the representation error of ϕ can be quantified using *distortion*:

$$\frac{1}{c_M} d_{\mathcal{M}}(\phi(x), \phi(y)) \leq d_{\mathcal{X}}(x, y) \leq c_M(\phi) d_{\mathcal{M}}(\phi(x), \phi(y)) \quad \forall x, y \in \mathcal{X} \ .$$

If ϕ is an isometric embedding, then $c_M(\phi) = 1$.

Computational distortion scores. The parameter c_M can be difficult to compute in practice, as access to the map ϕ is required in closed form to evaluate $\phi(x)$ over the whole data space. Therefore, our analysis focuses on the following computational distortion scores (see, e.g., (Weber, 2020)).

1. **Worst-case distortion:** In certain applications, one may be interested in a worst-case

analysis, particularly when robustness guarantees are required across all pairs of points.

$$D_{\text{worst}}(\phi) = \max_{1 \le i < j \le |\mathcal{X}|} \left| \left(\frac{d_{\mathcal{M}}(x_i, x_j)}{d_{\mathcal{X}}(x_i, x_j)} \right)^2 - 1 \right| . \tag{4.3}$$

Here, $d_{\mathcal{M}}$ denotes the distance in the representation space (hyperbolic or Euclidean) and $d_{\mathcal{X}}$ the distance in the data space.

2. **k-MAP score:** The MAP score is a ranking loss, which measures the preservation of local proximity. We build the similarity graph of $\mathcal{X}$ and assess how well the relationship of a point $x \in \mathcal{X}$ with its k-hop neighbors is preserved under the hyperbolic embedding ϕ:

$$\text{MAP}(\phi) = \frac{1}{|\mathcal{X}|} \sum_{x \in \mathcal{X}} \frac{1}{\deg(x)} \sum_{i=1}^{|\mathcal{N}_k(x)|} \frac{|\mathcal{N}_1(x) \cap R_{x,i}|}{|R_{x,i}|} \in [0, 1] . \tag{4.4}$$

Here, $R_{x,i}$ denotes the smallest set of nearest neighbors required to retrieve the ith neighbor of $\phi(x)$ in $\mathcal{M}$.

If ϕ is an isometric embedding, then $\text{D}_{\text{worst}} = 0$ and $\text{MAP} = 1$.

Q-scores. Q-scores, introduced by Lee and Verleysen (2010), are widely used metrics in the manifold embedding literature. Let $Q = \{q_{kl}\}_{k,l \in [N]}$ be the *co-ranking matrix* defined as

$$\begin{aligned}
q_{kl} &:= |\{(k,l) : \ \mu_{ij} = k, \nu_{ij} = l\}| \\
\mu_{ij} &:= |\{k : \ d_{\mathcal{X}}(x_i, x_k) < d_{\mathcal{X}}(x_i, x_j) \text{ and } \{d_{\mathcal{X}}(x_i, x_k) = d_{\mathcal{X}}(x_i, x_j) \text{ if } 1 \le k < j \le N\}\}| \\
\nu_{ij} &:= |\, \{k : \ d_{\mathcal{M}}(x_i, x_k) < d_{\mathcal{M}}(\phi(x_i), \phi(x_j)) \\
&\qquad \text{and } \{d_{\mathcal{M}}(\phi(x_i), \phi(x_k)) = d_{\mathcal{M}}(\phi(x_i), \phi(x_j)) \text{ if } 1 \le k < j \le N\}\} \,|
\end{aligned}$$

Here, $|I|$, denotes the cardinality of a set I. The Q-curves are then given by

$$Q(\phi, K) := \frac{1}{KN} \sum_{(k,l) \in I_K} q_{kl} , \tag{4.5}$$

which are computed over blocks $I_K := \{1, \ldots, K\} \times \{1, \ldots, K\}$ of the co-ranking matrix, restricted to the upper half of I_K, due to symmetry. The local and global Q-scores of hyperbolic embedding ϕ are computed as

$$K_{\max} := \operatorname*{argmax}_K \left(Q(\phi, K) - \frac{K}{N-1} \right) \tag{4.6}$$

$$Q_{local}(\phi) := \frac{1}{K_{\max}} \sum_{K=1}^{K_{\max}} Q(\phi, K) \tag{4.7}$$

$$Q_{global}(\phi) := \frac{1}{N - K_{\max}} \sum_{K=K_{\max}}^{N-1} Q(\phi, K) . \tag{4.8}$$

The split of the Q-curve at $K_{\max}$ distinguishes the local from global regimes. Q_{local} and Q_{global} range from 0 (worst) to 1 (best).

4.8 Visualization

Contrastive Poincaré Maps are visualized using the 2D Poincaré disk layout (Klimovskaia et al., 2020). To obtain a magnified view, a linear rescaling of the co-ordinates can be applied. By default, the point with the smallest average distance to all others is placed at the origin. Alternatively, the embedding can be translated so that a chosen reference point is mapped to the origin, while maintaining all pairwise hyperbolic distances. Owing to the increased resolution near the origin in hyperbolic space, this translation method is particularly useful for inspecting hierarchical structure when a root is known, or for analyzing cell lineages in multi-lineage datasets. The translation of the entire embedding x to place r at the origin is defined as:

$$\tau_\phi(r, x) = \frac{(1 + 2\langle r, x\rangle + \|x\|^2)r + (1 - \|r\|^2)x}{1 + 2\langle r, x\rangle + \|r\|^2\|x\|^2}$$

4.9 Phylogenetic tree

A simple phylogenetic tree is visualized by plotting low-dimensional Poincaré distances between the cells (as summarized in Equation 4.1) against the embryonic stage. For some of the datasets, individual cells were grouped into lineages. This serves multiple purposes — (i) it helps in understanding the evolutionary trend in different datasets, (ii) it reveals the density of cells at each embryonic stage, (iii) it reveals the diversity within each lineage or cell type.

4.10 Poincaré Half-Plane Model and Geodesic Calculation

We can transition from the Poincaré ball model to the Poincaré half-plane model using an isometry known as the Cayley transform. The Cayley transform preserves the hyperbolic distances and angles between points, ensuring the integrity of the underlying geometrical structures of the embeddings during the transformation. The Cayley transform is given by

$$C : \mathbb{P}^d \to \mathbb{H}^d, \quad C(x) = \frac{x + i}{ix + 1}, \tag{4.9}$$

where $x \in \mathbb{P}^d$ is a point in the Poincaré ball model, i is the imaginary unit, and $\mathbb{H}^d$ is the Poincaré half-plane model.

In the Poincaré half-plane model, geodesics are represented as either vertical lines (when they pass through the point at infinity) or semi-circles that are orthogonal to the boundary line (the x-axis). The geodesic $\gamma : [0, 1] \to \mathbb{H}^d$ connecting two points $x, y \in \mathbb{H}^d$ is given by:

$$\gamma(t) = a\cosh(t) + b\sinh(t), \tag{4.10}$$

where a and b are computed to satisfy the boundary conditions $\gamma(0) = x$ and $\gamma(1) = y$. By utilizing these equations, we can compute the geodesic in the half-plane model that connects any two given points.

In a similar manner to our previous experiment, we select pairs of root and leaf nodes and map these points into the half-plane model.

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A Background

A.1 Single-cell RNA sequencing

Single-cell RNA sequencing (scRNA-seq) is a transformative technique that allows for transcriptomic profiling at the resolution of individual cells, enabling researchers to characterize cellular heterogeneity, identify rare cell populations, and reconstruct developmental trajectories (Tang et al., 2009; Kolodziejczyk et al., 2015). Unlike bulk RNA-seq, which averages gene expression across many cells, scRNA-seq captures cell-specific transcriptional signatures, crucial for understanding complex biological systems, especially during dynamic processes such as development and differentiation (Trapnell, 2015).

In multicellular organisms, cell differentiation is the process through which progenitor or stem cells acquire specialized functions and identities. This is a tightly regulated process involving coordinated changes in gene expression, often orchestrated by lineage-specific transcription factors, epigenetic modifications, and signaling pathways (Morris, 2019). scRNA-seq offers a unique opportunity to capture these dynamic changes at high resolution, enabling the identification of intermediate cell states and transient gene expression programs that are otherwise obscured in population-level analyses (La Manno et al., 2018b).

One of the most critical applications of scRNA-seq in the context of cell differentiation is lineage detection, which is the inference or experimental tracing of the developmental history of individual cells. Accurate lineage reconstruction provides insight into the hierarchy of cell fate decisions and the molecular determinants that guide them. Computational approaches such as pseudotime analysis (Trapnell et al., 2014), trajectory inference (Saelens et al., 2019), and RNA velocity (Bergen et al., 2020) have been developed to infer the progression of differentiation from transcriptomic data. These methods attempt to order cells along a continuum reflecting a temporal or developmental progression, based on similarities in gene expression patterns.

Understanding lineage relationships is particularly vital in developmental systems biology, regenerative medicine, and cancer research, where the misregulation of differentiation programs can lead to developmental disorders. For example, in hematopoiesis, scRNA-seq has revised the classical view of hierarchical differentiation into a more continuous landscape of lineage priming and bifurcations (Paul et al., 2015). Similarly, in cancer, lineage tracing with scRNA-seq has elucidated how tumors recapitulate developmental programs and acquire resistance through plastic differentiation (Quinn et al., 2021).

In summary, scRNA-seq has become an indispensable tool for dissecting the cellular basis of differentiation. Lineage detection is essential for interpreting scRNA-seq data in a developmental context and for uncovering the principles that govern cell fate decisions.

A.2 Single nucleus RNA sequencing

Single nucleus RNA sequencing (snRNA-seq) has emerged as a powerful alternative to single-cell RNA sequencing (scRNA-seq) for transcriptomic profiling of individual cells, particularly in tissues that are difficult to dissociate or where intact cell isolation is impractical (Habib et al., 2017). Unlike scRNA-seq, which relies on whole-cell dissociation, snRNA-seq isolates and profiles RNA from individual nuclei, thereby minimizing stress-induced transcriptional artifacts and enabling the study of archived or frozen specimens (Bakken et al., 2018; Lake et al., 2016). This approach preserves the native transcriptional landscape of cells from complex or fragile tissues

such as the adult brain, fibrotic tissue, and solid tumors (Grindberg et al., 2013). Moreover, snRNA-seq captures both nuclear-retained transcripts and nascent RNA species, offering insights into transcriptional regulation and splicing dynamics (Kim et al., 2020). These advantages make snRNA-seq an indispensable tool for characterizing cellular heterogeneity in contexts where conventional scRNA-seq is limited.

A.3 Euclidean Embedding Methods

Analyzing complex biological datasets derived from next-generation sequencing technologies is often challenging, given their high-dimensional nature. To make exploratory analysis more tractable, dimension reduction techniques are commonly used to generate a low-dimensional representation of the data (Kharchenko (2021)) that approximates pairwise distances in the original high-dimensional space. For instance, multidimensional scaling (MDS) (Kruskal and Wish, 1978) projects the original data $X \in \mathbb{R}^{n \times m}$ with n observations and m dimensions onto a low-dimensional space $Y \in \mathbb{R}^{n \times p}, p << m$ so that pairwise Euclidean distances in the embedding space $\|y_i - y_j\|_{\mathbb{E}}$ approximate the distances $d_{ij} = \|x_i - x_j\|$ in the input space:

$$\arg\min_{y_1,\ldots,y_n} \sum_{i<j} (\|y_i - y_j\|_{\mathbb{E}} - d_{ij})^2.$$

Principal component analysis (PCA) (Ringnér, 2008) is a special case of MDS with the Euclidean metric used in the input space. In practice, PCA is computed via the eigendecomposition of the covariance matrix $\mathrm{cov}(X) = \frac{1}{n-1} X^{\mathrm{T}} X = V \Sigma V^{\mathrm{T}}$. By applying PCA, the data is linearly transformed $T = XV_p$ with $V_p \in \mathbb{R}^{m \times p}$, resulting in the alignment of the first p principal components with the axes of maximal variation.

While PCA reveals the global structure of the data, its linearity assumption makes it inadequate to accurately represent nonlinear low-dimensional structure in complex biological data sets. As a result, nonlinear dimension reduction techniques t-SNE (Maaten and Hinton, 2008)) and UMAP (McInnes et al., 2018) have garnered popularity in single-cell transcriptome analyses. Unlike PCA, t-SNE and UMAP favor the preservation of local distances at the cost of global distances. To achieve this, t-SNE approximates Gaussian kernel similarities p_{ij} in the input space using Student's t-distribution similarities q_{ij} in the embedding space. Similarly, UMAP constructs a k-nearest neighbor (KNN) graph in the input space and approximates the manifold spanned by this graph using the low-dimensional map. Both t-SNE and UMAP rely on Euclidean distances $\|y_i - y_j\|_{\mathbb{E}}$ in the embedding space to determine pairwise similarities and fuzzy set memberships, respectively. Thus, the Euclidean intuition indirectly influences the geometry of t-SNE and UMAP embeddings.

Another class of algorithms extensively used to visualize single-cell data is based on the diffusion process (Coifman et al., 2005; Nadler et al., 2005), representing a random walk along the KNN graph, which models the underlying data manifold. Within this framework, the edges in the KNN graph are assigned weights corresponding to pairwise similarities p_{ij}, allowing the construction of a transition matrix P, the diffusion operator, for the random walk process. The conventional diffusion map emerges through the eigendecomposition of this transition matrix P (Coifman et al., 2005). Advancements in this research field led to the development of diffusion pseudotime (DPT) (Haghverdi et al., 2016)) and PHATE (Moon et al., 2019) algorithms, both of which are widely used for single-cell lineage tracing. However, even in sophisticated methods such as PHATE, the reliance on Euclidean distances in the embedding space persists.

Despite their advantages and well-established methodologies, Euclidean embedding methods may face challenges in effectively capturing hierarchical structures, often present in biological data. Leveraging non-Euclidean geometries can address some of these challenges.

A.4 Representing Data in Hyperbolic Space

A.4.1 Hyperbolic Embeddings

In this work, we focus on representing data in two-dimensional hyperbolic space, by learning a map $\phi : \mathcal{X} \to \mathbb{P}^2$ between data space $\mathcal{X}$ and hyperbolic representation space $\mathbb{P}^2$, which maps a data point $x \in \mathcal{X}$ to $\phi(x) \in \mathbb{P}^2$. Classical mathematics literature provides theoretical guarantees on the accuracy of representing trees in low-dimensional Euclidean or hyperbolic space. Here, representation error refers to the extent to which pairwise distances among the data points are preserved between the data space and the representation space. Gupta (1999) demonstrated that a tree with L leaves (i.e., number of nodes in the last level of the tree) cannot be represented in d-dimensional Euclidean space with representation error better than a multiplicative factor of $O(L^{1/(d-1)})$. In contrast, Sarkar (2011) showed that trees of *any* size can be embedded into the two-dimensional hyperbolic space with near-exact distance preservation, i.e., with representation error no worse than a multiplicative factor of $O(1+\epsilon)$.

Hierarchical or tree-structured data are common in machine learning, and the complexity of algorithms often scales with the dimension of the data space. Hyperbolic geometry is particularly appealing because it allows for faithful representation of hierarchical data in low dimensions, making it promising for efficient data analysis. A growing line of work explore methods for computing hyperbolic representations of data (Nickel and Kiela, 2017; Chamberlain et al., 2017; Chami et al., 2019). Throughout this work, we focus on the two-dimensional Poincaré disk setting, $\mathbb{P}^2$. In some cases, we will represent data using a second parametrization, the closely related *Poincaré half-plane model*. In two dimensions, it is given by

$$\mathbb{H}^2 = \{x \in \mathbb{R}^2 \,:\, x_1 > 0\}$$
$$d_{\mathbb{H}}(x, x') = \operatorname{acosh}\left(1 + \frac{(x_0' - x_0)^2 + (x_1' - x_1)^2}{2x_1 x_1'}\right) .$$

Importantly, the two parameterizations are isometric, i.e., we can map point configurations from $\mathbb{P}^2$ to $\mathbb{H}^2$ distortion-free.

A.4.2 Geodesic interpolation

In order to investigate the intrinsic structure of hyperbolic embeddings, it can be beneficial to interpolate between points along geodesics, which constitute the shortest paths in this space. In the hyperbolic geometry of the Poincaré ball model, geodesics are arcs of circles that intersect the boundary of the ball orthogonally. For any two points in the Poincaré ball, there exists a unique geodesic connecting them. To validate the utility of our hyperbolic embeddings, we conduct an experiment involving geodesic interpolation. Specifically, we select pairs of root and leaf nodes in our hierarchical tree-like data, and compute the unique geodesic path that connects these two points in the hyperbolic space.

This interpolation experiment allows us to examine the relationship between data points and the underlying structure of the embedded data. By considering the root and leaf nodes, we are effectively exploring the extremes of the hierarchical structure encoded by our hyperbolic

embeddings. The intermediate points along the geodesic offer valuable insights into the transition from the root to the leaf, and potentially reflect the tree's structure (Fig. 8).

For each pair of root and leaf nodes, we perform the following steps:

1. Compute the coordinates of the root and leaf nodes in the hyperbolic embedding space.
2. Compute the unique geodesic $\gamma(t)$ that connects the root to the leaf.
3. Select a set of t values to sample intermediate points along the geodesic.
4. For each intermediate point, compute its hyperbolic distance to the geodesic.

We expect that if the hyperbolic embeddings have captured the tree structure well, then the distances from the intermediate points to the geodesic should be relatively small, reflecting a high consistency of the tree structure with the geodesic path in the embedding space. On the other hand, if these distances are large, it would suggest that the embedding may not fully capture the hierarchical relationships in the original data. The results from this experiment provide us with a quantitative measure of the quality of our embeddings and the effectiveness of hyperbolic space in capturing the hierarchical structure of tree-like data.

The computation of geodesics is as follows: Given two points $x, y \in \mathbb{P}^d$, the geodesic $\gamma : [0,1] \to \mathbb{P}^d$ from x to y is formulated by

$$\gamma(t) = \mathrm{Exp}_x(t \cdot \mathrm{Log}_x(y)) \ , \tag{A.1}$$

where $\mathrm{Exp}_x(v)$ and $\mathrm{Log}_x(y)$ refer to the exponential and logarithm maps at x, respectively. Both maps can be expressed in terms of hyperbolic cosine and sine functions and the Minkowski product. In particular,

$$\mathrm{Exp}_x(v) = \cosh(\|v\|_M)x + \sinh(\|v\|_M)\frac{v}{\|v\|_M} \ , \tag{A.2}$$

and

$$\mathrm{Log}_x(y) = \frac{d_{\mathbb{P}}(x,y)}{\sinh(d_{\mathbb{P}}(x,y))}(y - \cosh(d_{\mathbb{P}}(x,y))x) \ . \tag{A.3}$$

These equations allow for the calculation of a point along the geodesic from x to y at any parameter $t \in [0,1]$. For $t = 0$, $\gamma(t)$ returns x; for $t = 1$, it returns y. For values of t in between, it yields a point along the geodesic from x to y.

Geodesic interpolation thus provides a meaningful mechanism to traverse the learnt representation space, enabling a better understanding and visualization of the structure and relationship of the embedded data in the hyperbolic space.

A.5 Contrastive Learning

Contrastive learning is a self-supervised learning paradigm that aims to learn an embedding space in which similar data pairs (positive samples) are mapped to nearby points and dissimilar pairs (negative samples) are mapped far apart. It is grounded in the idea of learning by comparison, drawing from concepts in metric learning and information theory (Hadsell et al., 2006; Oord et al., 2018).

Let $\mathcal{X}$ denote the input space and $f_\theta : \mathcal{X} \to \mathbb{R}^d$ be an encoder parameterized by θ that maps inputs to a d-dimensional representation space. For a given anchor sample $x_i \in \mathcal{X}$, a positive sample x_i^+ (e.g., an augmented version of x_i) and a set of negative samples $\{x_j^-\}_{j=1}^{N-1}$ are used to define the contrastive objective.

A common objective function is the InfoNCE loss (Oord et al., 2018), given by:

$$\mathcal{L}_i = -\log \frac{\exp\left(\mathrm{sim}(f_\theta(x_i), f_\theta(x_i^+))/\tau\right)}{\sum_{j=1}^{N} \exp\left(\mathrm{sim}(f_\theta(x_i), f_\theta(x_j^-))/\tau\right)}$$

where $\mathrm{sim}(u, v) = \frac{u^\top v}{\|u\|\|v\|}$ is the cosine similarity, and $\tau > 0$ is a temperature parameter.

Contrastive learning has demonstrated strong performance in various domains. Unsupervised pre-training of image encoders such as SimCLR (Chen et al., 2020), MoCo (He et al., 2020) provides competitive performance on downstream tasks such as image classification, object detection, and segmentation, compared to supervised baselines. In Natural Language Processing, sentence embeddings (Gao et al., 2021) and document retrieval benefit from contrastive objectives using positive pairs from natural augmentations or dropout noise. In general, contrastive learning has emerged as a key technique for effective representation learning in the absence of labels, enabling models to leverage large unlabeled datasets and generalize well to downstream supervised tasks.

SCARF The lack of suitable and meaningful augmentation strategies is a key limitation for applying contrastive learning to tabular data. SCARF (Bahri et al., 2022) introduces a contrastive learning framework specifically designed for tabular data, addressing this key limitation in the domain. While contrastive learning has achieved remarkable success in modalities like vision and language through domain-specific augmentations like image cropping or token masking, such techniques do not transfer directly to tabular formats. SCARF tackles this by proposing a novel data augmentation method based on random feature corruption. For each data instance, a positive pair is generated by randomly replacing a subset of its features with values sampled from the empirical marginal distributions of those features. This ensures the augmented sample remains in-distribution while introducing variability necessary for contrastive training.

This corruption-based augmentation is domain-agnostic, making it highly applicable across diverse tabular datasets without requiring handcrafted feature engineering. The learning objective encourages the model to generate invariant representations between the original and corrupted views, enabling robust representation learning. Notably, this approach is well-suited to challenges typical in tabular data, such as noise, missing values, and high feature heterogeneity.

B Baselines

t-SNE T-distributed stochastic neighbor embedding (t-SNE) is a non-linear dimensionality reduction method (Van der Maaten and Hinton, 2008) that approximates Gaussian kernel similarities p_{ij} in the input space using heavier-tailed Student's t-distribution similarities q_{ij} in the lower-dimensional map:

$$p_{ij} = \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$$

$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_{k \neq l}(1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}$$

Perplexity is the key parameter in t-SNE that determines the dispersion of the Gaussian kernel and indirectly influences the balance between preserving the local and global structure of the data. We used the Scikit-learn v1.0.2 (Pedregosa et al., 2011) implementation of t-SNE with the Barnes-Hut approximation and varied perplexity as the main hyperparameter. The perplexity values tested were $[5, 10, 20, 30, 40, 50]$.

UMAP Uniform manifold approximation and projection (UMAP) is a non-linear dimensionality reduction method that combines manifold learning and topological data analysis techniques (McInnes et al., 2018). It constructs a fuzzy topological representation by transforming the high-dimensional data into a k-nearest neighbor (KNN) graph with edges weighted by the normalized Gaussian kernel similarities:

$$p_{ij} = \frac{\exp\left(-\frac{\|x_i - x_j\|^2}{\sigma_i}\right)}{\sum_{k \neq i} \exp\left(-\frac{\|x_i - x_k\|^2}{\sigma_i}\right)}$$

The low-dimensional embedding in UMAP is obtained by minimizing the cross-entropy between the high-dimensional (p_{ij}) and low-dimensional (q_{ij}) fuzzy topological representations:

$$C = -\sum_{i \neq j} p_{ij} \log(q_{ij}) + (1 - p_{ij}) \log(1 - q_{ij})$$

The key hyperparameters of UMAP are the number of nearest neighbors k and minimum distance d_{min} between the points in the low-dimensional embedding space. We used the python implementation UMAP v0.5.3 (McInnes et al., 2018).

PHATE PHATE is a diffusion-based method commonly used for single-cell trajectory analysis (Moon et al., 2019). Similar to UMAP, PHATE constructs a KNN graph with edges weighted by normalized kernel similarities $p_{ij} = K_{ij} / \sum_{k \neq i} K_{ik}$. Unlike UMAP, PHATE uses an alpha-decaying Gaussian kernel:

$$K_{ij} = \frac{1}{2} \exp\left(-\left(\frac{||x_i - x_j||}{\sigma_i}\right)^{\alpha}\right) + \frac{1}{2} \exp\left(-\left(\frac{||x_i - x_j||}{\sigma_j}\right)^{\alpha}\right)$$

PHATE differs from the classical diffusion maps by using the diffusion potential $D_{ij}(t) = [P^t]_{ij}$ instead of the diffusion operator P itself. The exponent t, automatically chosen by the algorithm, represents the number of steps taken in a random walk and the powers of the diffusion operator P^t capture structure of the data at different scales. To obtain a low-dimensional embedding Y, PHATE applies multidimensional scaling (MDS) to the diffusion potential D.

Poincare Maps Klimovskaia et al. (Klimovskaia et al., 2020) propose Poincaré maps, a dimensionality reduction technique that embeds single-cell RNA sequencing (scRNA-seq) data into a hyperbolic space to better capture hierarchical relationships. Unlike conventional methods such as t-SNE or UMAP that operate in Euclidean spaces and often struggle with representing branching or hierarchical structures, Poincaré maps utilize the Poincaré disk model of hyperbolic geometry to preserve both local and global topological features.

The method begins by constructing a k-nearest neighbor graph over d-dimensional expression data $\mathcal{X} = \{\mathbf{x}_i\}_{i=1}^n$, where $\mathbf{x}_i \in \mathbb{R}^d$. Geodesic distances are then approximated via shortest paths within this graph to reflect the manifold structure of the data. These distances are used to guide the embedding of the data into the two-dimensional Poincaré disk $\mathbb{D}^2$ by minimizing the Kullback–Leibler divergence between the geodesic distances in the input space and the hyperbolic distances in the embedded space.

Empirical results demonstrate that Poincaré maps outperform standard techniques in representing branching structures in various scRNA-seq datasets. However, Poincaré maps are a shallow embedding method, meaning that the embedding is computed directly from pairwise distance relationships without the use of deep neural networks or hierarchical feature extraction layers. This inhibits the model to capture complex nonlinear transformations compared to deep embedding methods.

C Additional results: Model robustness

We evaluated the performance of all embedding methods across all datasets without applying PCA-based dimensionality reduction (Supplementary Fig. 10). For the chicken cardiogenesis dataset, batch correction with Scanorama (Hie et al., 2024) was omitted. Performance declined for all methods except CPM, which remained robust in the absence of additional pre-processing.

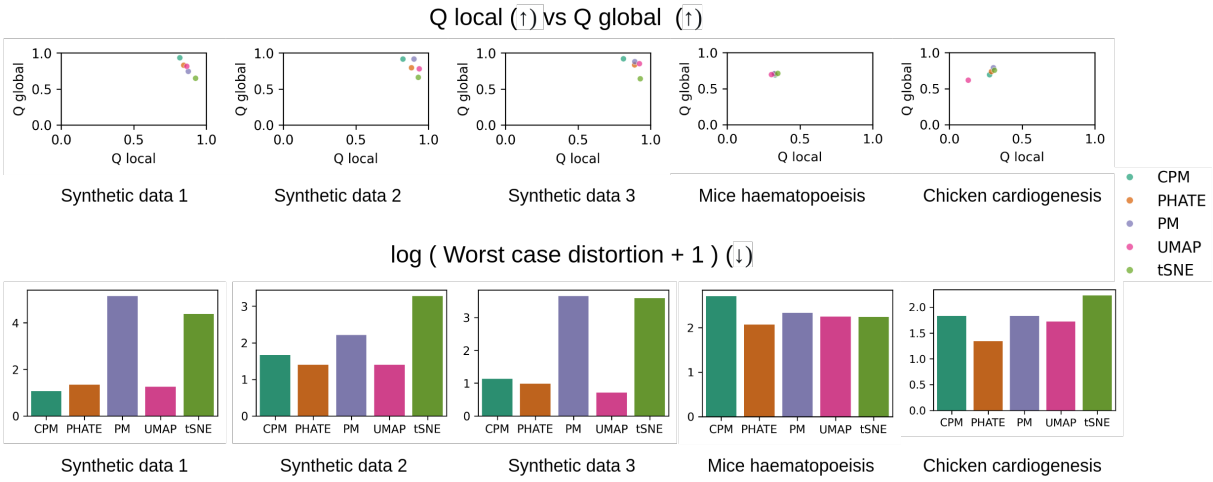

Figure 10: **Robustness to pre-processing** Performance of all embedding methods evaluated without PCA-based dimensionality reduction across all datasets. For the chicken cardiogenesis dataset, batch correction using Scanorama was also omitted.

We also evaluated the performance of Contrastive Poincaré Maps under varying model hyperparameters (Supplementary Fig. 11). The quality metrics remain largely consistent across different configurations, demonstrating the robustness of the model to hyperparameter choices.

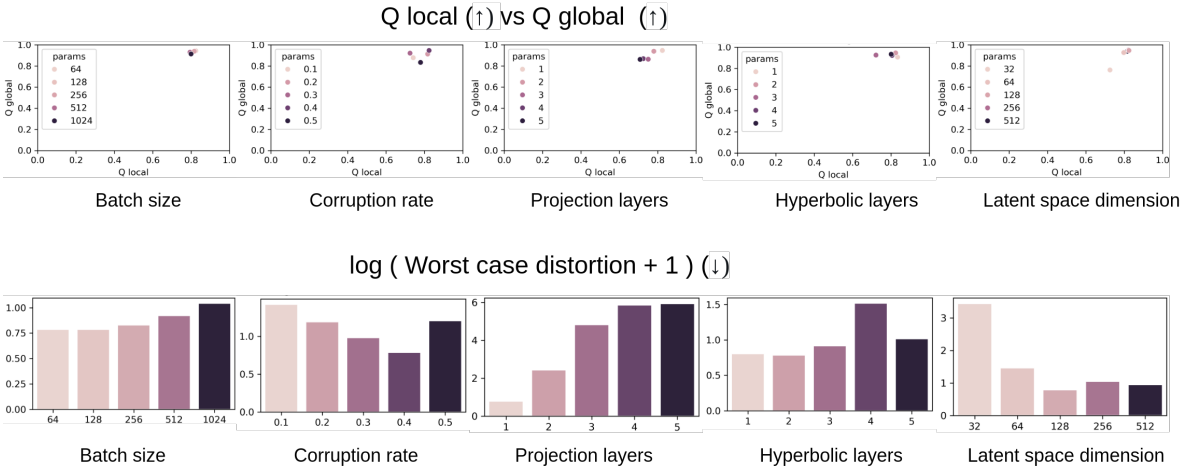

Figure 11: **Robustness of Contrastive Poincaré Maps to hyperparameter variation** Performance of Contrastive Poincaré Maps across a range of model hyperparameter configurations.

D Additional results: Visualizations of embeddings

This section presents visualizations of embeddings generated by all methods across all datasets. For synthetic datasets, visualizations are colour-coded by branch, with the corresponding ground truth tree structure included for reference. For real datasets, embeddings are colour-coded by cell type to reflect known biological annotations. There is no continuous progression between hierarchical levels in Poincaré maps, as demonstrated in CPM. All hierarchical levels beyond the root appear to be pushed toward the horizon, resulting in an unnatural representation that fails to preserve the inherent hierarchical structure. On closer inspection, we also see an unnatural intersection between branches on some of the visualizations produced by PHATE, t-SNE and UMAP.

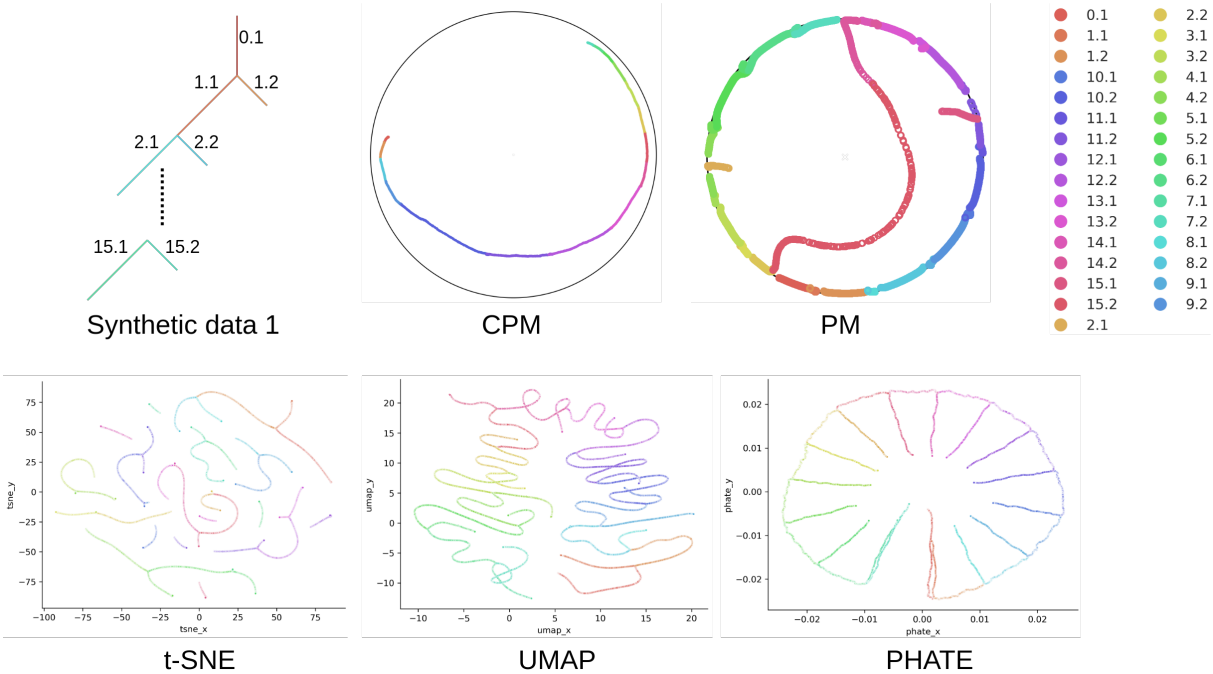

Figure 12: Visualization of embeddings for synthetic data 1, a deep binary tree with 15 hierarchical levels, where each node branches into two children.

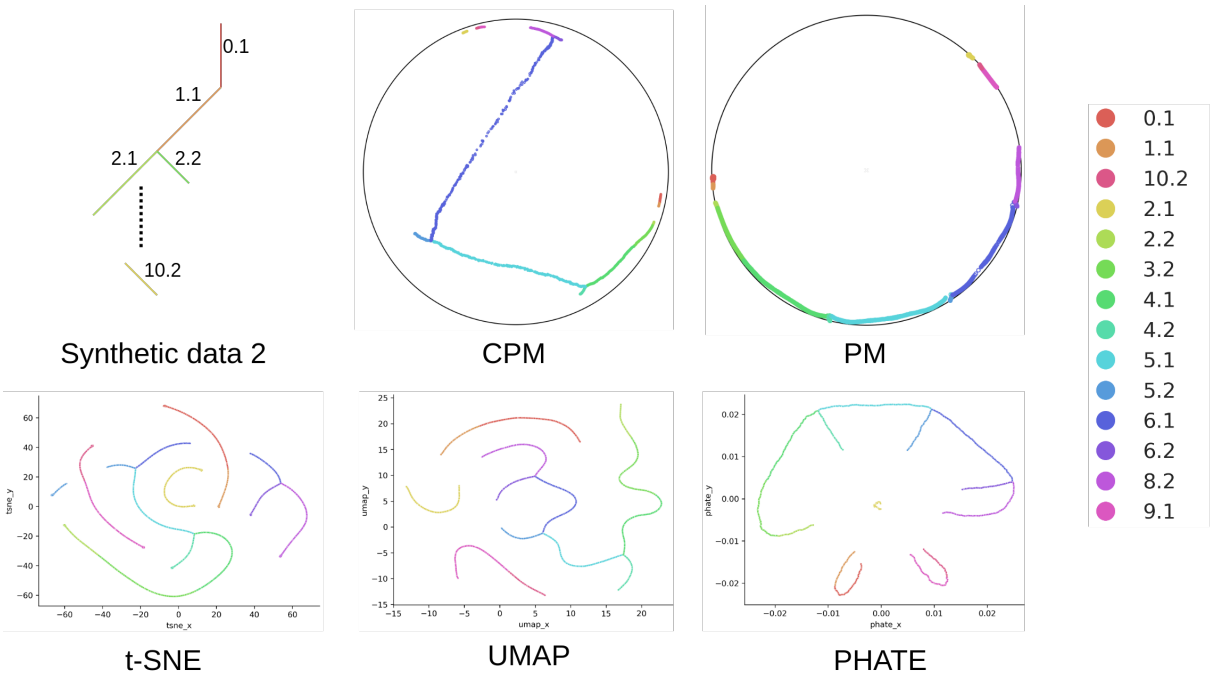

Figure 13: Visualization of embeddings for synthetic data 2, an imbalanced binary tree with 10 levels, in which each node also has two children, but branches are sampled randomly to introduce structural irregularity.

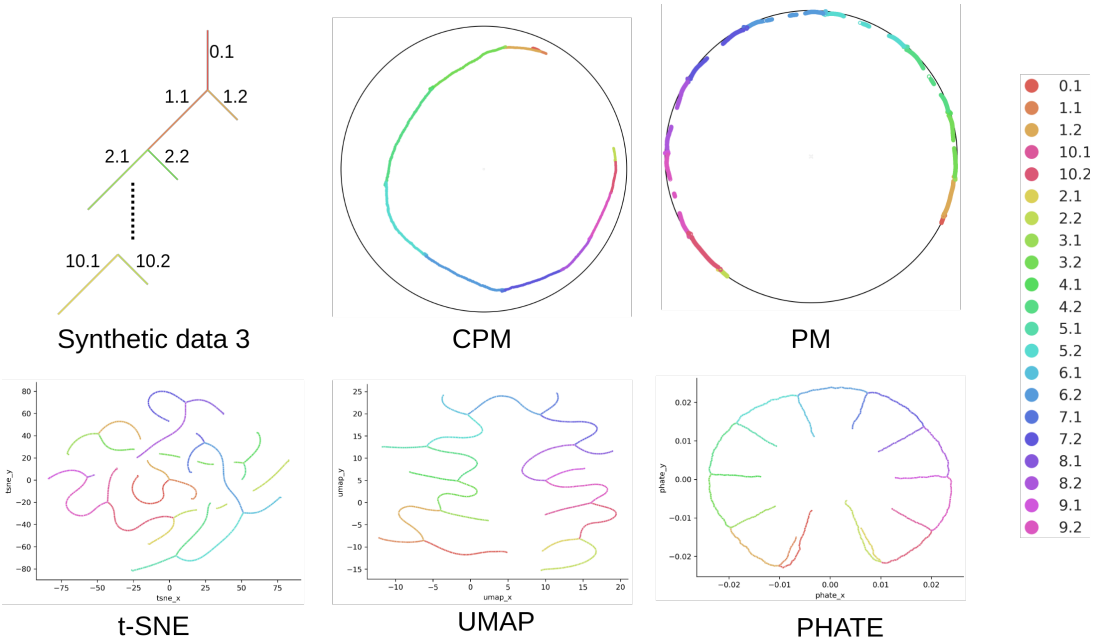

Figure 14: Visualization of embeddings for synthetic data 3, a balanced binary tree with 10 levels, each node branching into two children, with no randomness in structure.

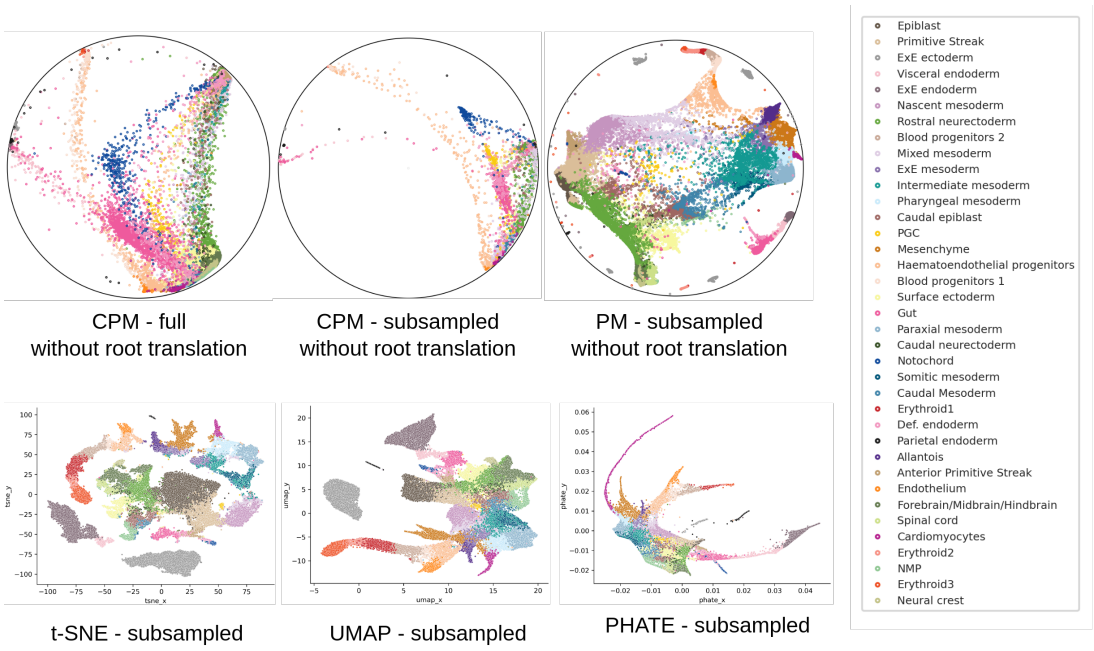

Figure 15: Visualization of embeddings for the subsampled mouse gastrulation dataset, comprising 58,156 cells across nine developmental stages. For Contrastive Poincaré Maps, the visualization for the full dataset, comprising 116,312 cells is also provided.

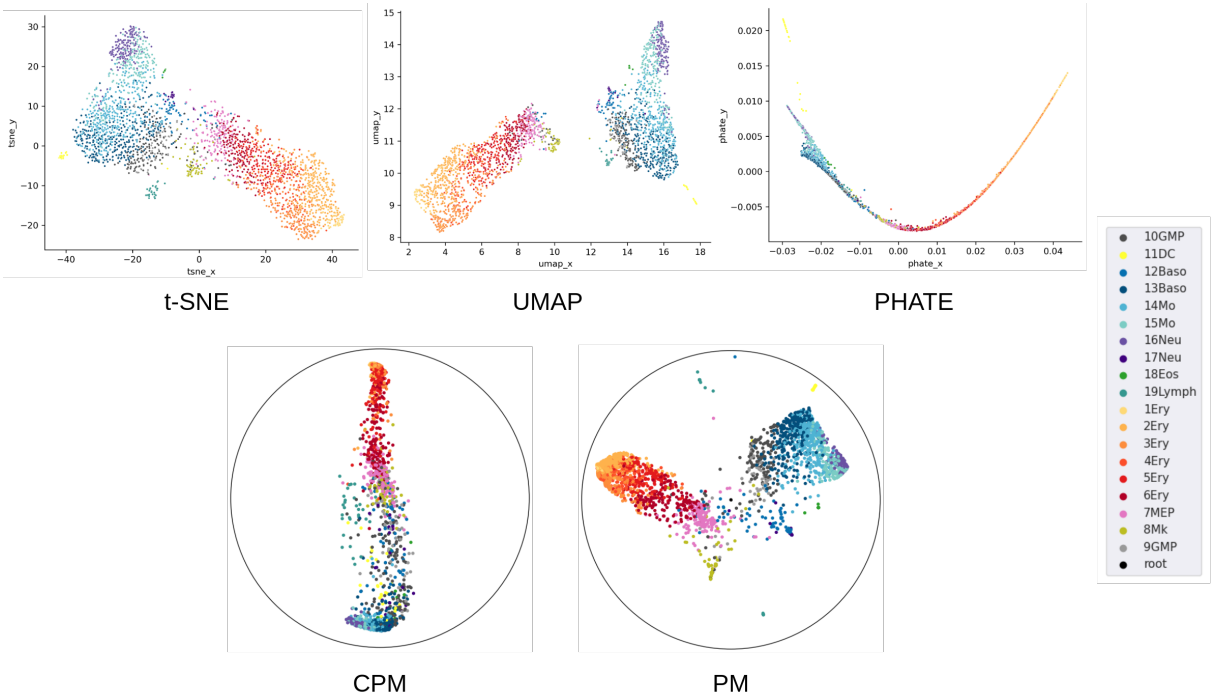

Figure 16: Visualization of embeddings for the Mice haematopoiesis dataset, comprising 2,730 myeloid progenitor cells.

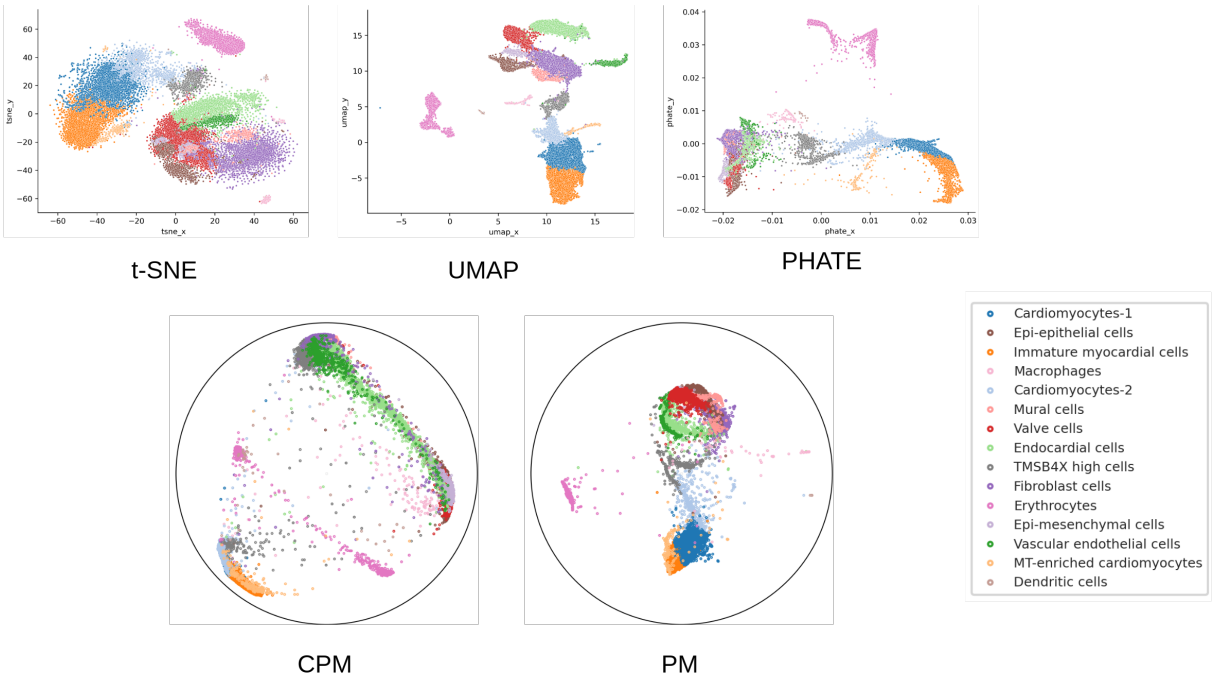

Figure 17: Visualization of embeddings for the Chicken cardiogenesis dataset, comprising 22,315 cells from multiple lineages across four developmental stages.

E Additional results: Mouse gastrulation

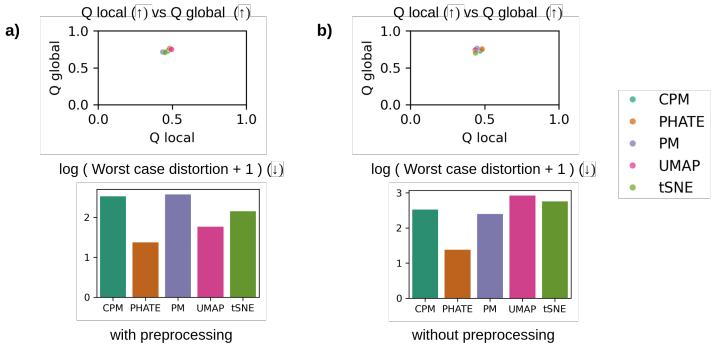

Figure 18: **Quantitative evaluation on subsampled mouse gastrulation data.** Performance of all embedding methods evaluated on a subsample of 58,156 cells from the full mouse gastrulation dataset. Due to computational constraints associated with pairwise distance calculations on the full dataset, metrics were computed on the subsample. Additional results with PCA-based dimensionality reduction are included for all methods except Contrastive Poincaré Maps.

F Additional results: Translation to single nucleus RNA sequencing dataset

We analyze single-nucleus RNA sequencing (snRNA-seq) data from mouse brain generated by (Russell et al., 2024), who developed the Slide-tags method to achieve spatially resolved transcriptomics at single-nucleus resolution. This dataset comprises of spatially resolved transcriptomes from 4,584 nuclei, with a median of 4,594 UMIs per nucleus. These data were derived from a 7mm^2 sagittal section of the mouse brain at embryonic day 14 (E14). While previous results were primarily focused on scRNA-seq datasets, we use this dataset to demonstrate capabilities of CPM in resolving cellular hierarchies from snRNA-seq data as well. Specifically, we use it to show that CPM can resolve localized differentiation hierarchies within a single embryonic stage.

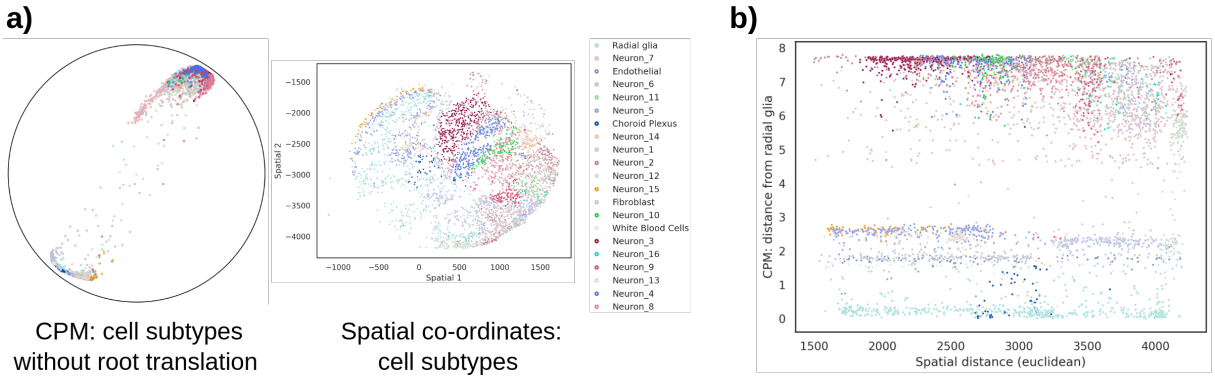

Figure 19: **Mouse brain development at E14** (a) Embedding learned by Contrastive Poincaré Maps and the corresponding spatial coordinates from the dataset, colour-coded by cell subtype. (b) Distances from radial glia in the embedding plotted against spatial distances. The plot reveals discrete tiers of differentiation, indicating that Contrastive Poincaré Maps captures global transcriptional hierarchies, independent of spatial proximity.

Figure 19a presents the embedding generated by CPM, alongside the original spatial coordinates from the dataset. Three key observations emerge from these results: (i) CPM partitions the data into two principal clusters - one comprising radial glia, choroid plexus, white blood cells, endothelial cells, fibroblasts, and a subset of neurons, and the other consisting predominantly of neurons; (ii) Inferred developmental trajectories place Neuron 13, Neuron 5, and Neuron 15 closer to progenitor populations (Radial glia). (iii) Neuron 6 and Neuron 12 appear to originate early in the differentiation process but remain transcriptionally abundant at both early and late stages (see Fig. 20), indicating sustained expression across developmental time as inferred from CPM embedding. Figures 21 and 22 illustrate the quantitative and qualitative evaluation of all embedding methods.

Figure 19b shows a scatter plot of embedding distances from radial glia versus spatial distances provided in the dataset. The lack of correlation between these two distance measures highlights that CPM captures global differentiation hierarchies based on transcriptional cell states, rather than spatial proximity. Specifically, the plot reveals discrete waves or tiers of cell differentiation, as inferred from the embedding. While spatial distances reflect the physical adjacency of cell types within the tissue, the embedding distances generated by CPM reflect

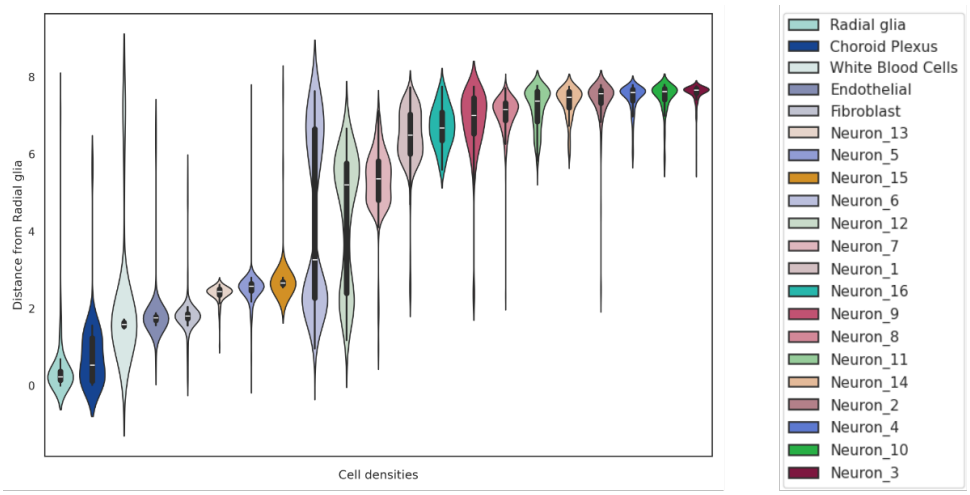

Figure 20: **Cell densities in mouse brain development** Cell subtype densities in the mouse brain development dataset visualized as a function of distance from radial glia in the Contrastive Poincaré Maps embedding. This analysis supports inference of cell ordering along developmental trajectories while cross-validating with local cell density distributions.

their relative maturation along the differentiation trajectory.

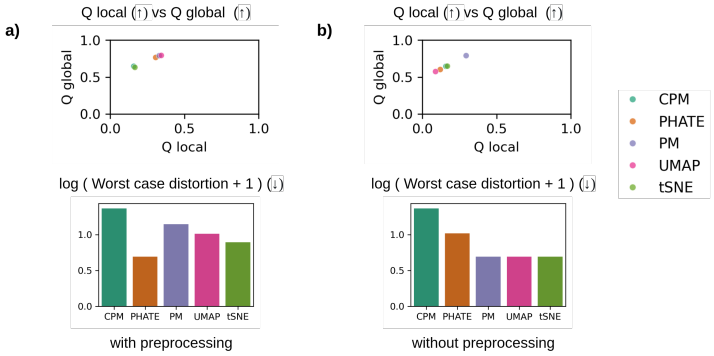

Figure 21: **Quantitative evaluation on mouse brain development dataset.** Performance of all embedding methods on mouse brain development dataset evaluated (a) with and (b) without PCA-based dimensionality reduction. The results of Contrastive Poincaré Maps (CPM) in both (a) and (b) are without PCA-based dimensionality reduction.

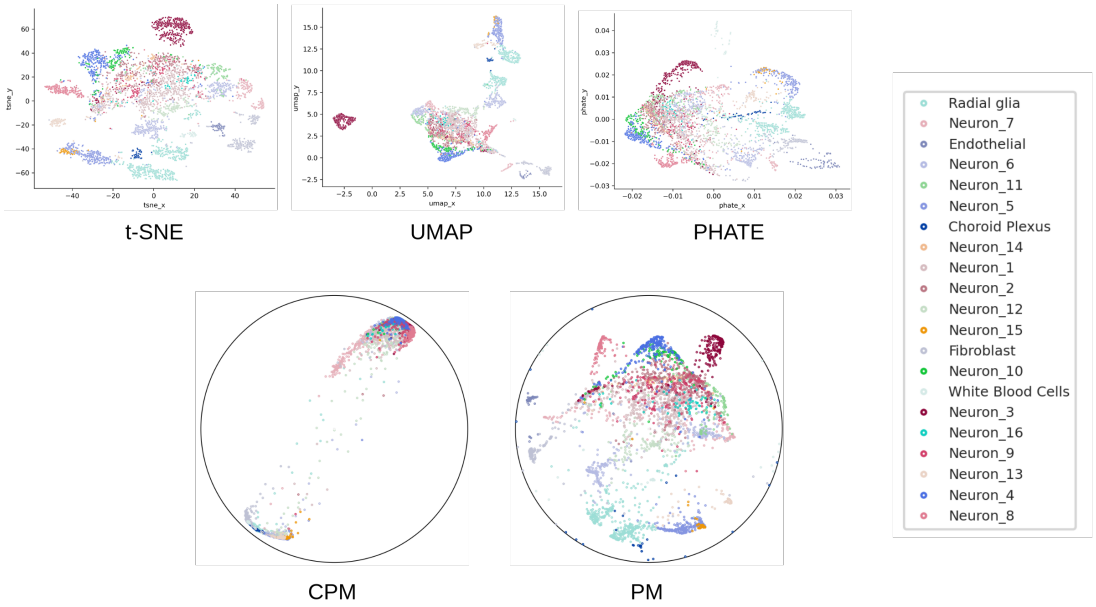

Figure 22: Visualization of embeddings for the mouse brain development dataset, comprising single-nucleus RNA sequencing data from 4,853 nuclei at embryonic day E14.

G Additional results: Analysis of gene expression profiles

This section presents gene expression profiles of key marker genes across all real datasets. Expression values are min–max normalized to facilitate comparison and overlaid on the CPM embedding. The overlays reveal transcriptional gradients and global hierarchical organization of cell states, reflecting underlying differentiation trajectories.

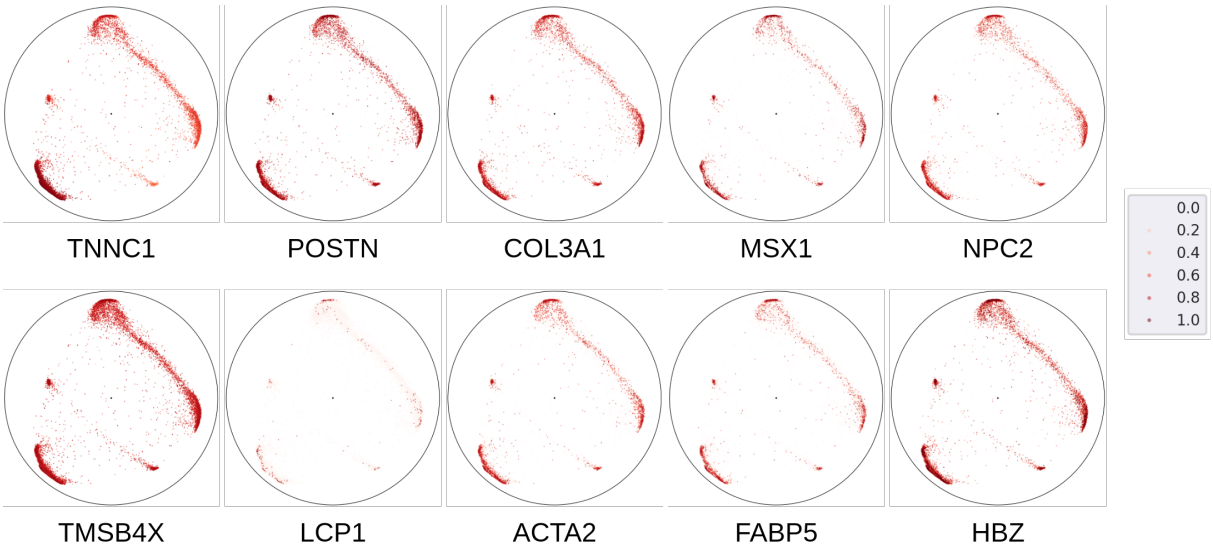

Figure 23: **Gene expression patterns overlaid on CPM embeddings** Min–max normalized expression profiles of representative marker genes for the chicken cardiogenesis dataset, visualized on CPM embeddings.

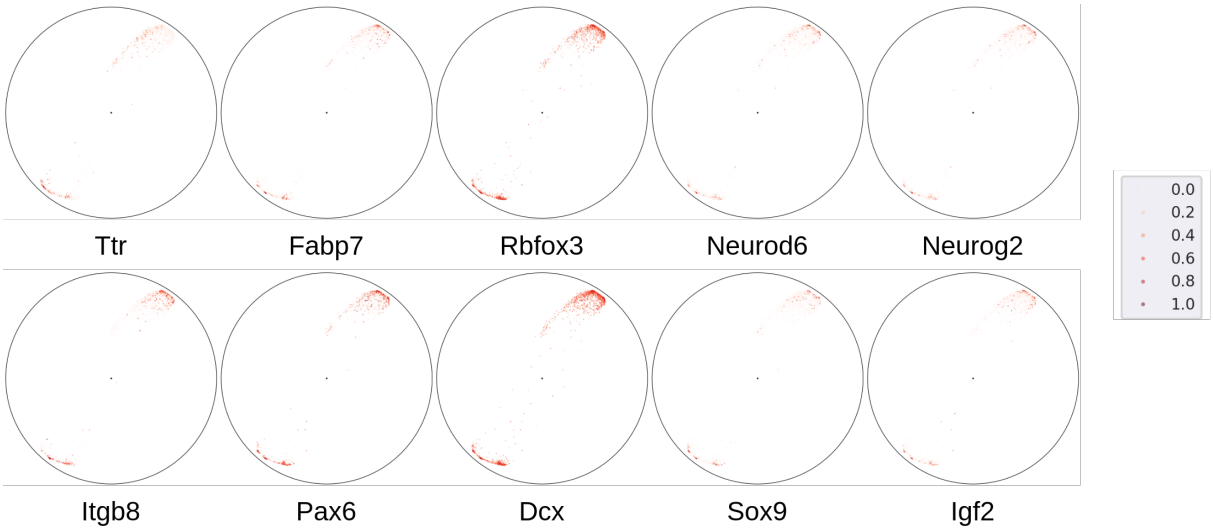

Figure 24: **Gene expression patterns overlaid on CPM embeddings** Min–max normalized expression profiles of representative marker genes for the mouse brain development dataset, visualized on CPM embeddings.

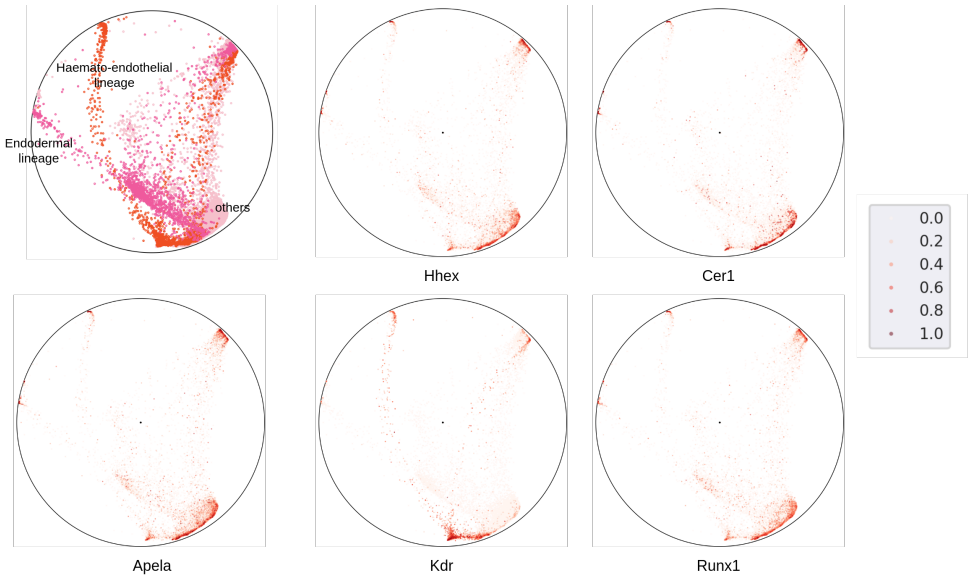

Figure 25: **Gene expression patterns overlaid on CPM embeddings** Min–max normalized expression profiles of representative marker genes for the mouse gastrulation dataset, visualized on CPM embeddings.

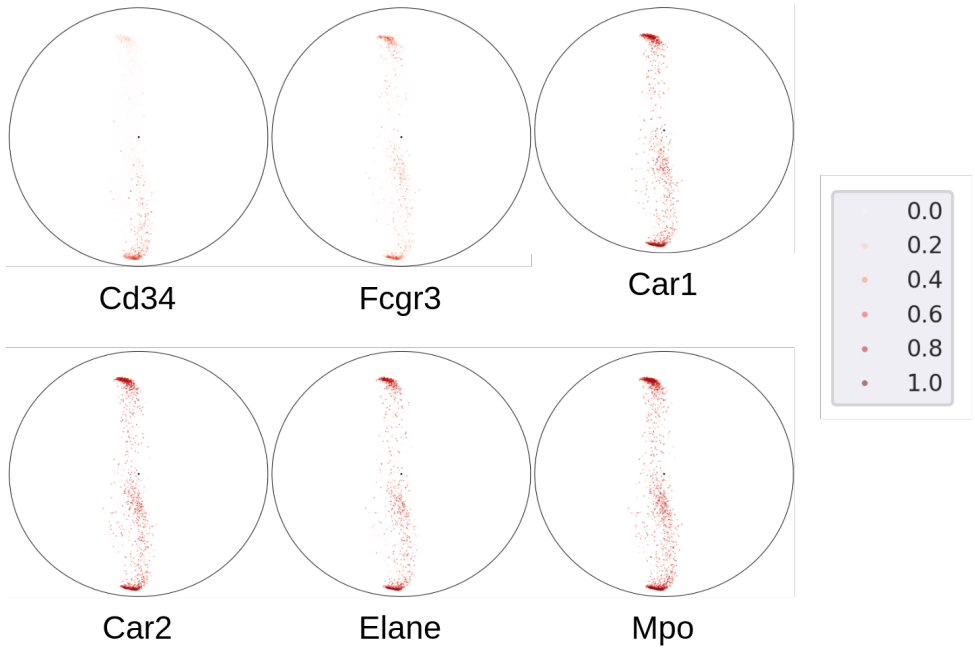

Figure 26: **Gene expression patterns overlaid on CPM embeddings** Min–max normalized expression profiles of representative marker genes for the mouse haematopoeisis dataset, visualized on CPM embeddings.

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