

Principal Decomposition with Nested Submanifolds

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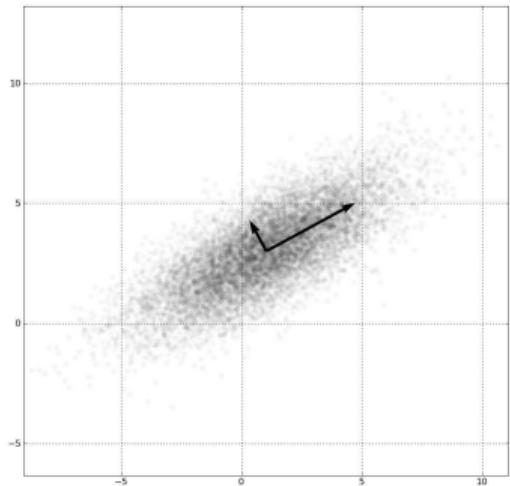
May 30, 2025
Yau Mathematical Sciences Center

Principal Component Analysis

- $\{x_1, \dots, x_n\} \subset \mathbb{R}^D$: points of interest
- $\mathcal{A}_{D-1} = \{z \in \mathbb{R}^D : v_D^\top(z - p) = 0\}$ with $\|V_D\| = 1$
- minimize $\sum_i d(x_i, \mathcal{A}_{D-1})^2 = \sum_i (v_D^\top(x_i - p))^2$
- One solution: $p = \bar{x}$,

$$v_D = \arg \min_{v: \|v\|=1} v^\top \sum_i (x_i - \bar{x})(x_i - \bar{x})^\top v$$

- Remaining components: $x'_i = x_i - v_D v_D^\top (x_i - \bar{x})$.
- Repeat with $\{x'_i\} \subset \mathcal{A}_{D-1}$...



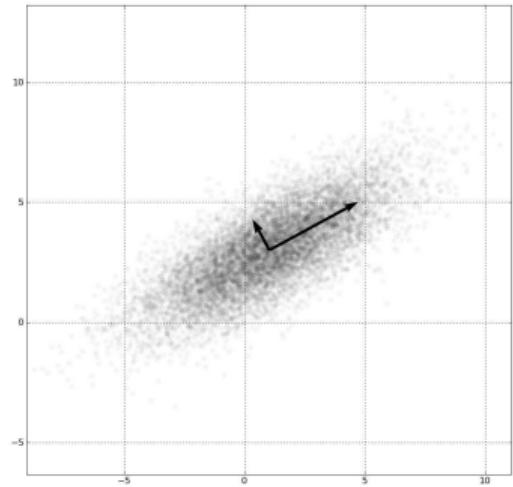
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- Remaining components: $x'_i = x_i - v_D v_D^\top (x_i - \bar{x})$.
- Repeat with $\{x'_i\} \subset \mathcal{A}_{D-1}$...
- $\hookrightarrow \mathcal{A}_d = \bar{x} + \text{span}(v_1, \dots, v_d)$

$\{\bar{x}\} \subset \mathcal{A}_1 \subset \dots \mathcal{A}_{D-1} \subset \mathbb{R}^D$: a *flag*.



Linear Decomposition can be Inadequate

- Data can take values on non-Euclidean spaces:
 - resides in known non-linear spaces:
 - ↪ compositional data; semi-positive definite matrices ...
 - has non-Euclidean topology:
 - ↪ directions; molecular geometry ...
- or distributed around lower dimensional structures
 - ↪ strongly nonlinear covariance structures ...

Additive Principal Component*

For $X = (X_1, \dots, X_D)^\top$, consider $\phi_i = \phi_i(X_i)$ s.t.

$$\phi_i \in H_i \subset \{\phi : \mathbb{E}[\phi(X)] = 0, \text{Var}[\phi(X)] < \infty\},$$

$$\Phi := (\phi_1, \dots, \phi_D) \in H_1 \times \dots \times H_D.$$

The first component: minimize $\text{Var}(\sum_i \phi_i)$ subject to $\sum_i \text{Var}(\phi_i) = 1$.

- Focus on the smallest PC/low-variance relationships
- Use $\sum \phi_i(X_i)$ instead of $\sum a_i X_i$
- Find $\sum \phi_i(X_i) \approx 0$
- $\{x = (x_1, \dots, x_D) \in \mathbb{R}^D : \sum \phi_i(x_i) = 0\}$: an *additive manifold with co-dimensional 1*

*Donnell, D.J., et al. (1994). *Analysis of additive dependencies and concurvities using smallest additive principal components*. AoS

Principal Curves[†]

Find a smooth curve passing the ‘middle’ of the data set/minimizing variation orthogonal to the curve

- $\gamma(t)$: a smooth curve with parameter t
- $\gamma^{-1}(x) = \arg \min_t \|x - \gamma(t)\|$
- Principal curve: $\mathbb{E}[X \mid \gamma^{-1}(X) = t] = \gamma(t)$
- Estimator:

Let $\gamma_0(t) = \bar{x} + vt$, define

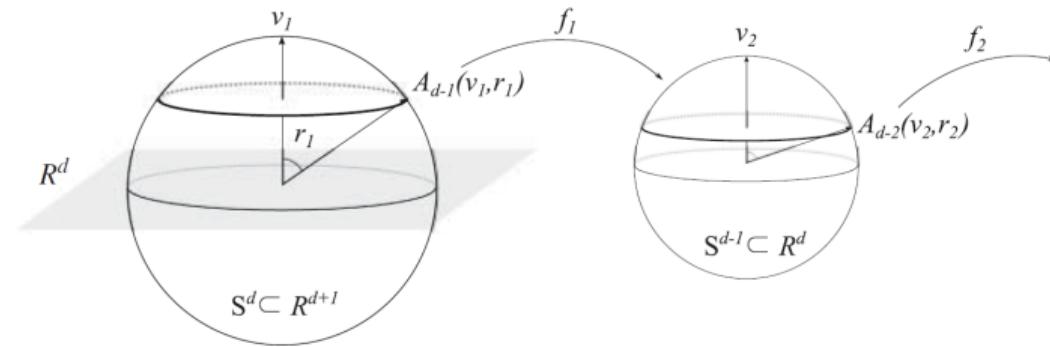
$$\gamma_j(t) = \mathbb{E}[X \mid \gamma_{j-1}^{-1}(X) = t]$$

[†]Hastie, T., & Stuetzle, W. (1989). *Principal curves*. JASA.

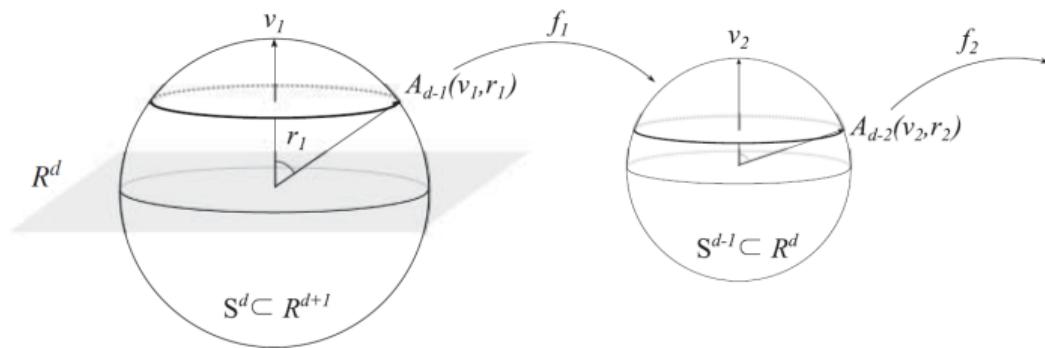
Principal Nested Spheres[†]

- $\{x_i^{(0)}\}_{i=1}^n \subset \mathcal{S}^D \subset \mathbb{R}^{D+1}$
- For $p, q \in \mathcal{S}^D$, $d(p, q) = \arccos(p^\top q)$
- With $v \in \mathcal{S}^D$ and $r \in (0, \pi/2]$, a sub-sphere of \mathcal{S}^D :

$$A_{D-1}(v, r) = \{x \in \mathcal{S}^D : d(v, x) = r\} = \mathcal{S}^D \cap \{x \in \mathbb{R}^{D+1} : v^\top x = \cos(r)\}$$



[†]Jung, S., Dryden, I. L., & Marron, J. S. (2012). *Analysis of principal nested spheres*. Biometrika.

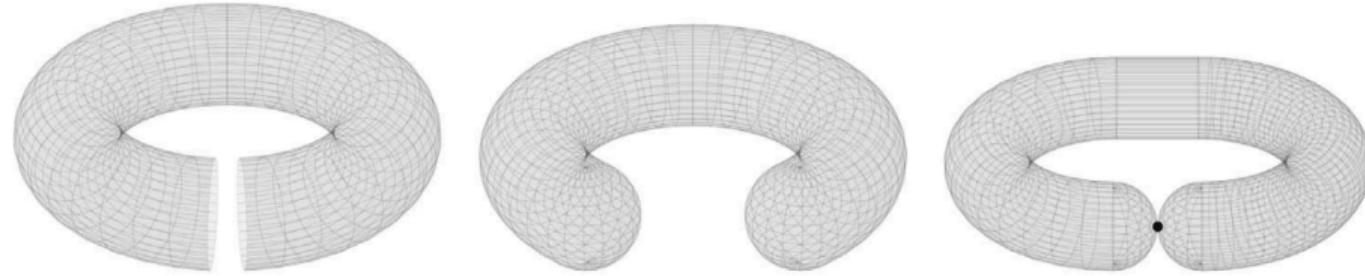


- Let $\mathcal{L}_j(v, r) = \sum_{i=1}^n \left(\cos^{-1}(v^\top x_i^{(j-1)}) - r \right)^2$, and

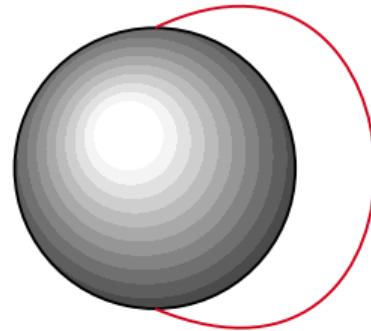
$$(\hat{v}_j, \hat{r}_j) = \arg \min_{v \in \mathcal{S}^{D-j+1}, r \in (0, 2\pi]} \mathcal{L}_{j-1}(v, r).$$

- $\hat{A}_{D-j} = A_{D-j}(\hat{v}_j, \hat{r}_j)$
- project $x_i^{(j-1)}$ along the geodesic to \hat{A}_{D-j}
- re-scale and rewrite coordinates to make $\{x_i^{(j)}\} \subset \mathcal{S}^{D-j}$

Torus PCA[§]

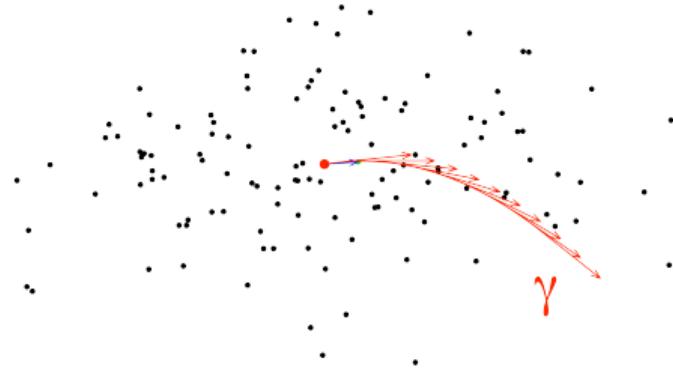


- Data on torus: $T^D = \mathcal{S}^1 \times \cdots \times \mathcal{S}^1$
- Have gaps on most dimensions
- Cut into special spheres and perform PNS



[§]Eltzner, B., Huckemann, S., & Mardia, K. V. (2018). *Torus principal component analysis with applications to RNA structure*. AoAS

Principal Flows[¶]

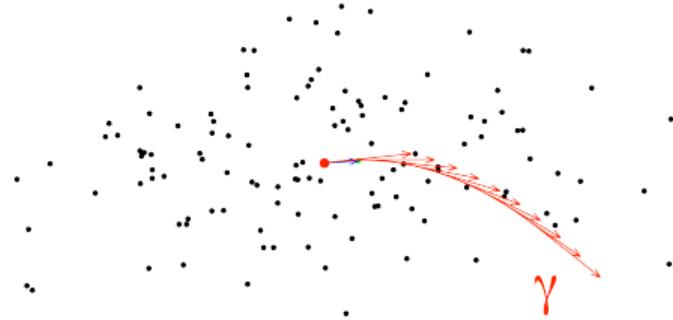


Find a smooth curve $\gamma(t)$ s.t.

- residing on known Riemannian manifold \mathcal{M}
- passing the 'middle' of data

[¶]Panaretos, V. M., Pham, T., & Yao, Z. (2014). *Principal flows*. JASA.

Principal Flows[¶]



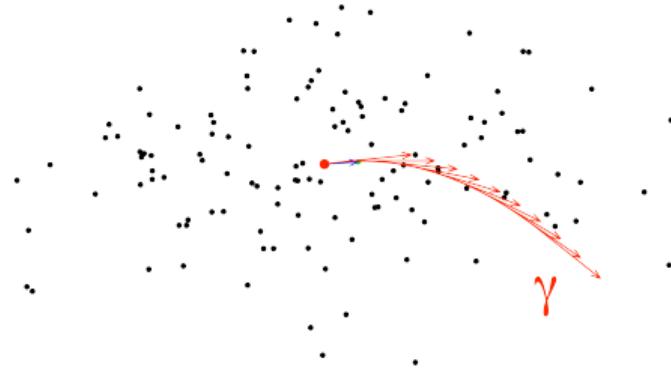
Find a smooth curve $\gamma(t)$ s.t.

- residing on known Riemannian manifold \mathcal{M}
- passing the 'middle' of data
- start from $\gamma(0)$, the *Fréchet mean*

On (\mathcal{M}, g) , $\Psi(p) = \sum_i g^2(p, x_i)$
Fréchet mean: $\arg \min_{p \in \mathcal{M}} \Psi(p)$
Fréchet variance: $\min_{p \in \mathcal{M}} \Psi(p)$

[¶]Panaretos, V. M., Pham, T., & Yao, Z. (2014). *Principal flows*. JASA.

Principal Flows[¶]



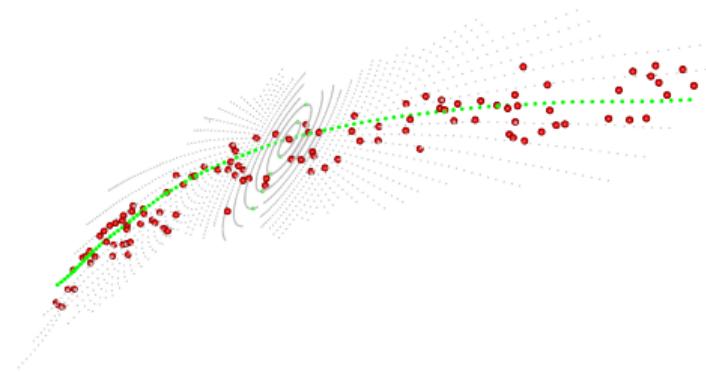
Find a smooth curve $\gamma(t)$ s.t.

- residing on known Riemannian manifold \mathcal{M}
- passing the 'middle' of data
- start from $\gamma(0)$, the *Fréchet mean*
- $\dot{\gamma}$ fits the first principal direction of the *tangent space PCA* at $\gamma(t)$.

Project x_i 's from \mathcal{M} to $T_{\gamma(t)}\mathcal{M}$;
Perform local PCA at $\gamma(t)$ in $T_{\gamma(t)}\mathcal{M}$.

[¶]Panaretos, V. M., Pham, T., & Yao, Z. (2014). *Principal flows*. JASA.

Principal Sub-manifold^{||}



Find a smooth sub-manifold s.t.

- residing on known Riemannian manifolds; passing the 'middle' of data
- start from the Fréchet mean
- the ray $\dot{\gamma}$ fits the principal direction derived from the tangent space PCA at $\gamma(t)$
- the collection of all such rays is the principal sub-manifold.

^{||}Yao, Z., Eltzner, B., & Pham, T. (2016–2024). *Principal sub-manifolds*. Accepted by Statistica Sinica.

Some Issues

The mean curves and surfaces:

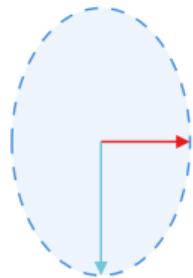
- Most of them are with dimension 1 or co-dimension 1
- Hard to extend, in terms of dimensionalities
- Lack of 'nested subspace' structure

The PCA on spheres, tori or *simplex*:

- Restricted by the form of data
- Inherit another form of 'linear constraint'

Better choice: principal directions from local covariance matrix

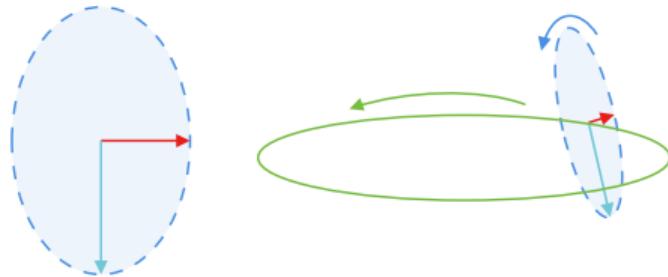
Intuitions: Decompose based on Smooth Covariance Structures



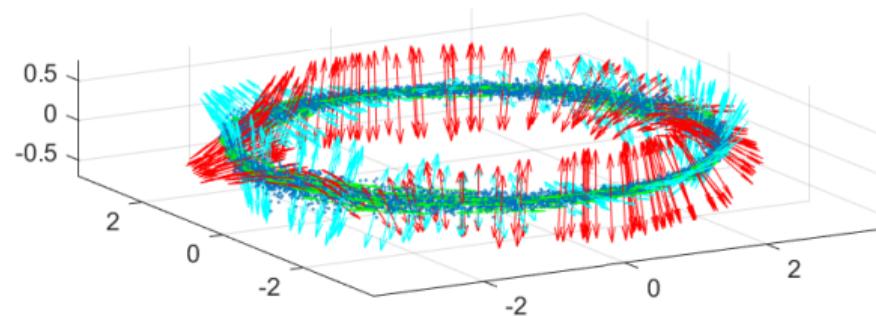
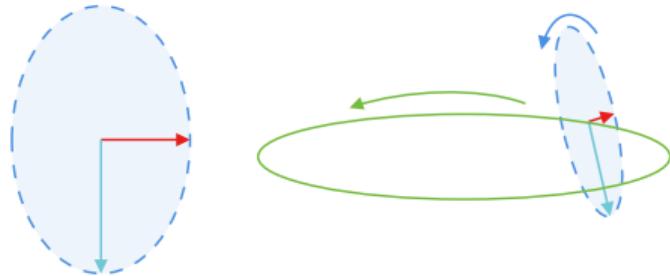
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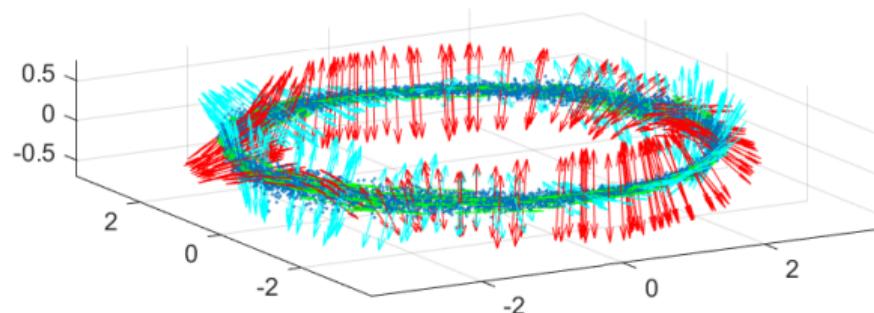
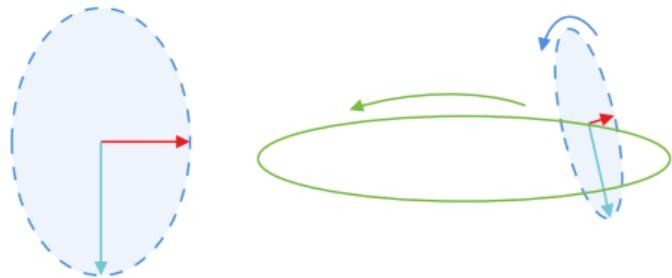
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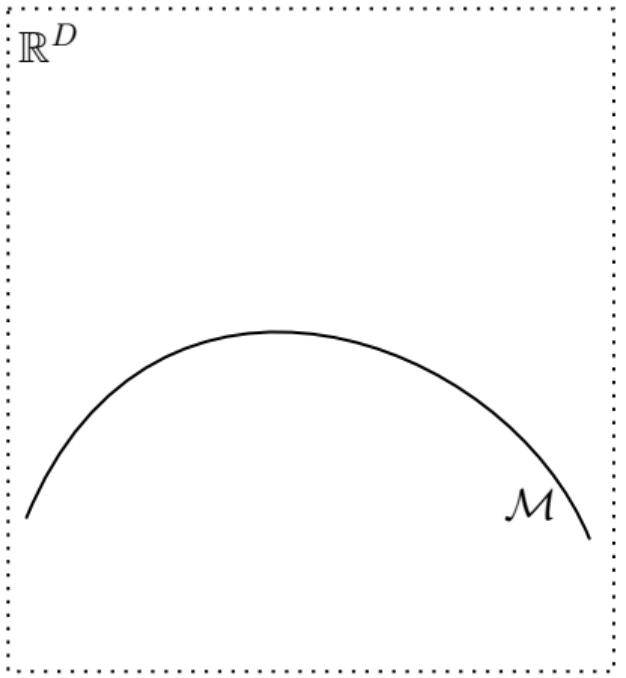
Intuitions: Decompose based on Smooth Covariance Structures



Find submanifolds such that

- tangent spaces approximate the linear space generated by principal directions
- passing through the 'middle' of the data clouds
- with different dimensionalities and a nested structure

Manifold Fitting Setup*



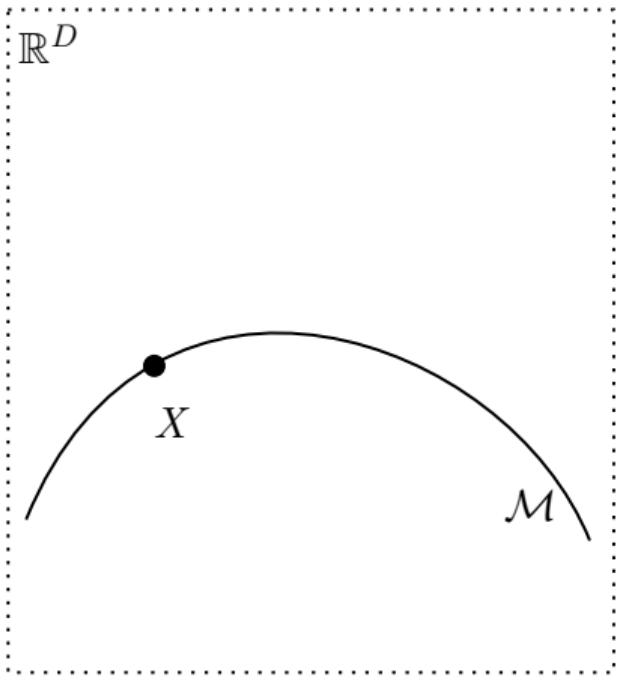
- $\mathcal{M} \subset \mathbb{R}^D$: smooth latent manifold
- $\dim(\mathcal{M}) = d$, $d < D$, $\text{reach}(\mathcal{M}) \geq \tau$

* Fefferman, C., et al. (2018). *Fitting a putative manifold to noisy data*. PMLR.

Yao, Z., & Xia, Y. (2019 – 2025). *Manifold fitting under unbounded noise*. JMLR, to appear.

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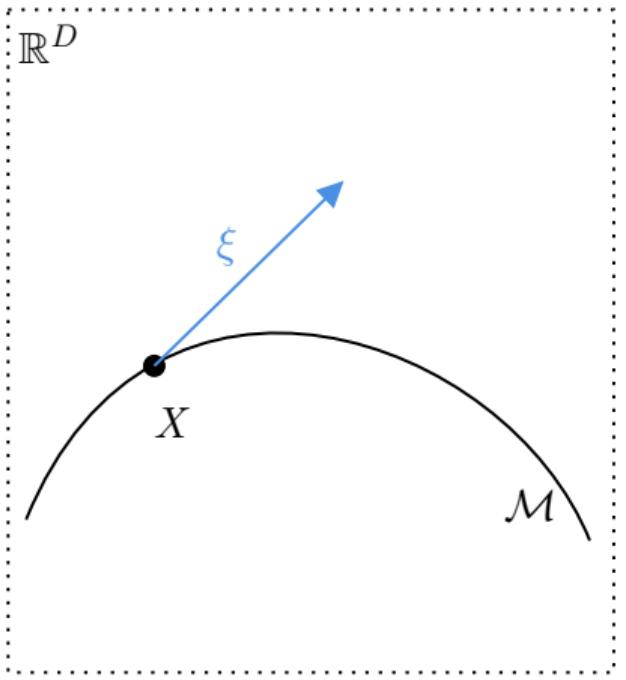
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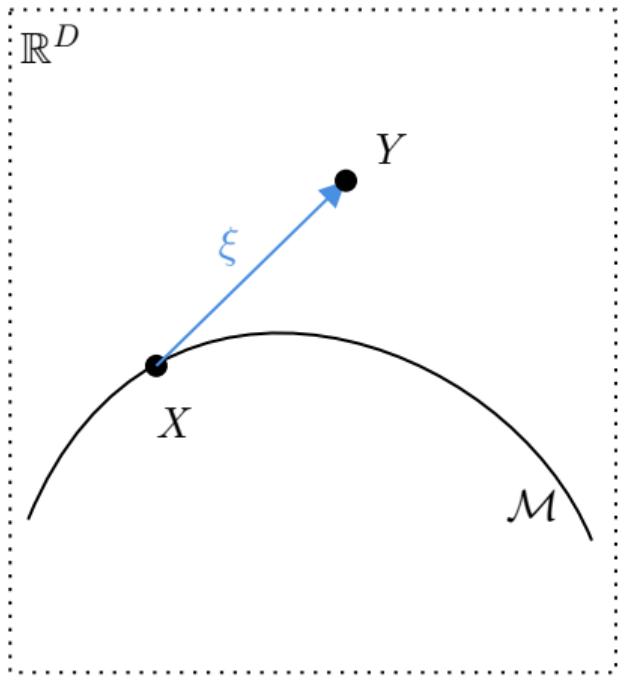
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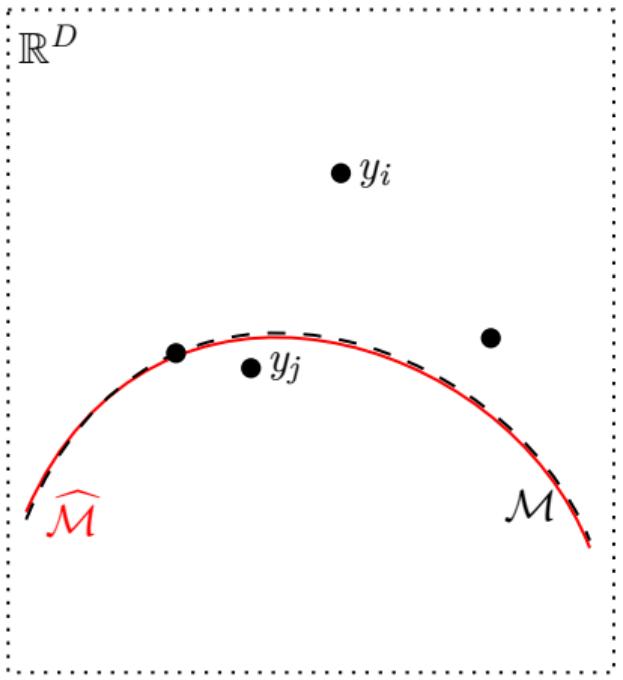
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- $Y = X + \xi \sim \nu = \mu \star \phi_\sigma^{(D)}$: observation

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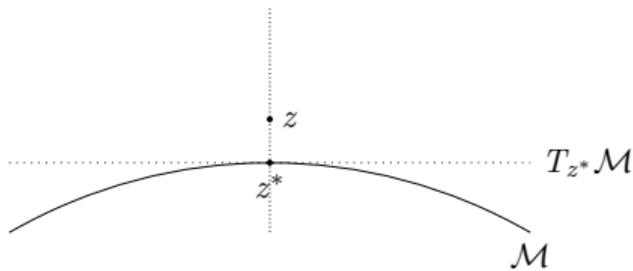
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- $Y = X + \xi \sim \nu = \mu \star \phi_\sigma^{(D)}$: observation
- Estimate \mathcal{M} with $\hat{\mathcal{M}}$ based on $\{y_i\}_{i=1}^N$

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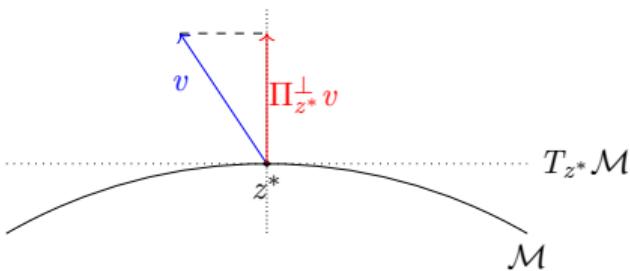
Fit the Latent Manifold[†]



- z : a point of interest
- $z^* = \arg \min_{z' \in \mathcal{M}} d(z, z')$: projection of z on \mathcal{M}
- $T_{z^*}\mathcal{M}$: tangent space of \mathcal{M} at z^*

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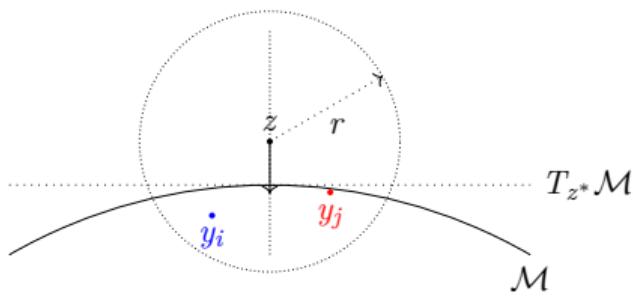
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- $T_{z^*}\mathcal{M}$: tangent space of \mathcal{M} at z^*
- $\Pi_{z^*}^\perp$: projection matrix onto the normal space of $T_{z^*}\mathcal{M}$
- $\widehat{\Pi}_z^\perp$: estimator of $\Pi_{z^*}^\perp$

[†]Yao, Z., & Xia, Y. (2019 – 2025). *Manifold fitting under unbounded noise*. JMLR, to appear.

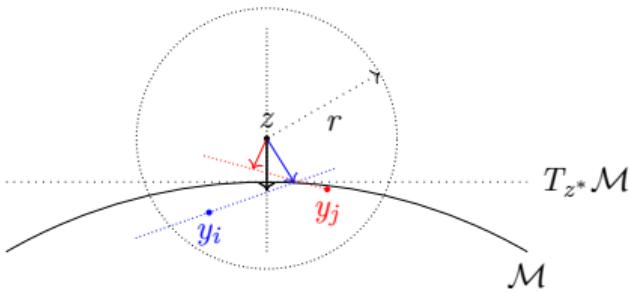
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- $r = \mathcal{O}(\sqrt{\sigma})$

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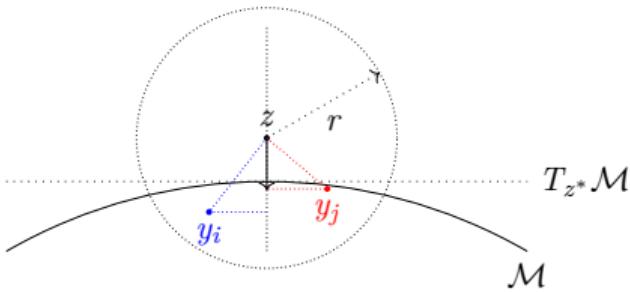
$$\tilde{\alpha}_i(z) = \left(1 - \frac{\|z - y_i\|^2}{r^2}\right)^\beta \mathbb{I}(\|z - y_i\| \leq r)$$

$$\alpha_i(z) = \frac{\tilde{\alpha}_i(z)}{\sum_{i=1}^n \tilde{\alpha}_i(z)}, \quad \beta > 2,$$

- $r = \mathcal{O}(\sqrt{\sigma})$
- $\widehat{\Pi}_{y_i}^\perp$: estimator of $\Pi_{y_i^*}^\perp$
- $\Psi_z = \mathbb{P}_{D-d} \left(\sum_i \alpha_i(z) \widehat{\Pi}_{y_i}^\perp \right)$: estimator of $\Pi_{z^*}^\perp$
- $\mathbb{P}_d(A)$: projection of matrix A on its leading d eigenvectors

[†]Yao, Z., & Xia, Y. (2019 – 2025). *Manifold fitting under unbounded noise*. JMLR, to appear.

Fit the Latent Manifold[†]



$$\widehat{\mathcal{M}} = \{z \in \mathbb{R}^D : d(z, \mathcal{M}) \leq cr, c < 1, f(z) = 0\}$$

$$\Rightarrow d(z, \mathcal{M}) \leq Cr^2 \text{ for any } z \in \widehat{\mathcal{M}}$$

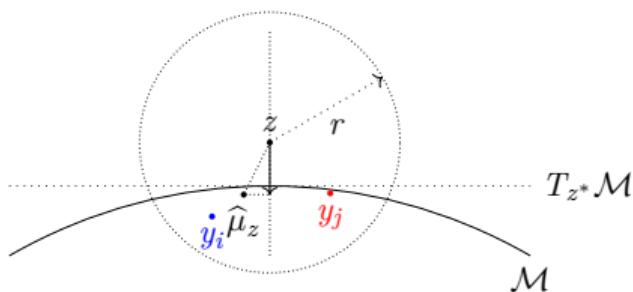
with probability

$$1 - d \exp\{-cNr^{d+2}\}.$$

- $\Psi_z = \mathbb{P}_{D-d} \left(\sum_i \alpha_i(z) \widehat{\Pi}_{y_i}^\perp \right)$
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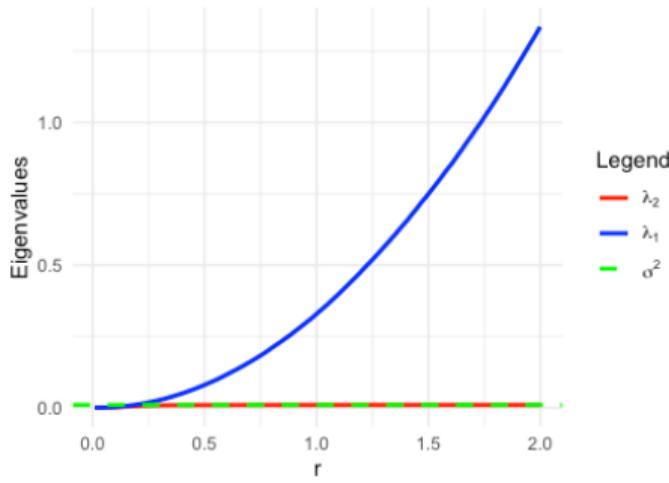
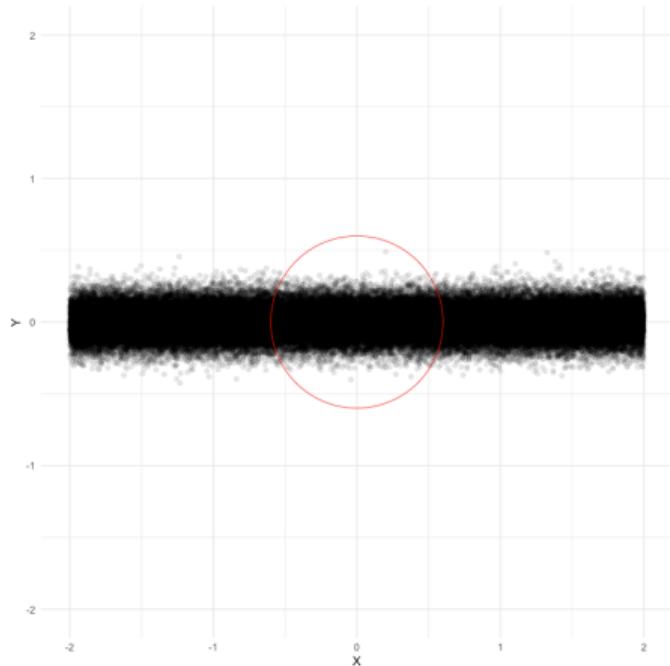
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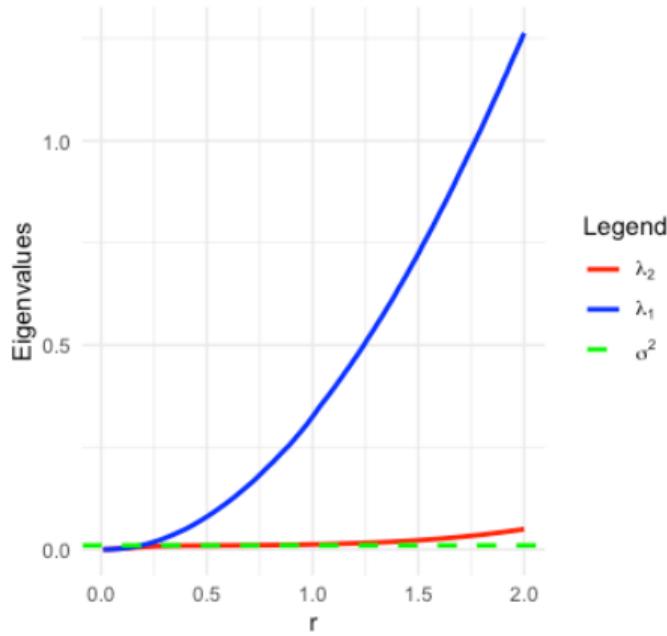
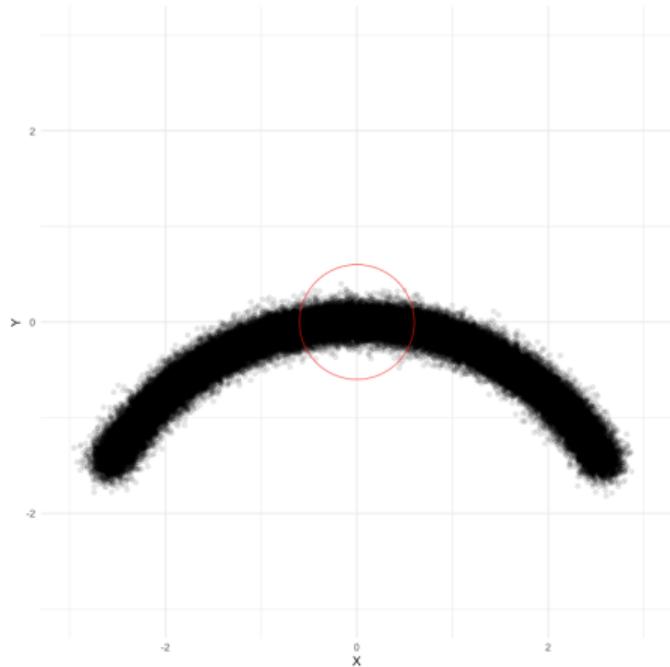
- $\Psi_z = \mathbb{P}_{D-d} \left(\sum_i \alpha_i(z) \widehat{\Pi}_{y_i}^\perp \right)$
- $\widehat{\mu}_z = \sum_i \alpha_i(z) y_i$: weighted mean of y_i
- $f(z) = \sum_i \alpha_i(z) \Psi_z(z - y_i) = \Psi_z(z - \widehat{\mu}_z)$

[†]Yao, Z., & Xia, Y. (2019 – 2025). *Manifold fitting under unbounded noise*. JMLR, to appear.

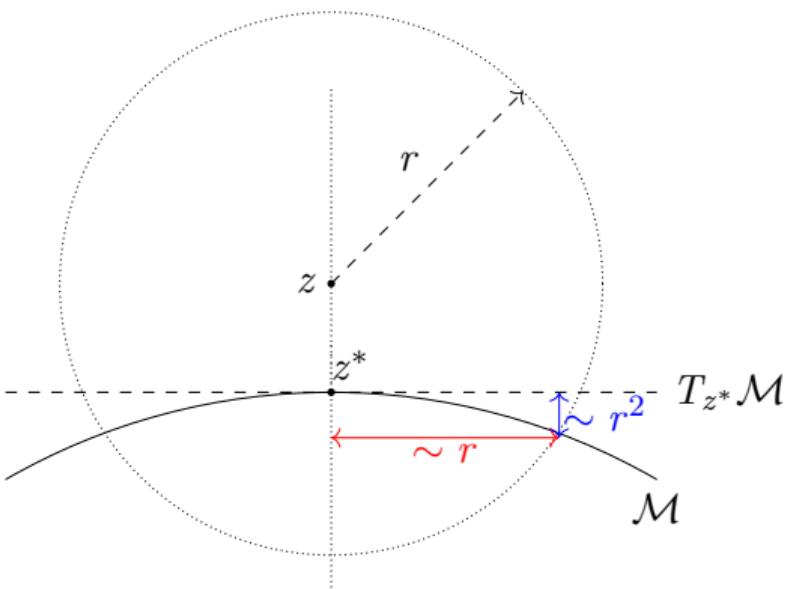
Difference with Kernels



Difference with Kernels



Difference with Kernels



By choosing a proper $r \gg \sigma$:

- $P(Y \in \mathcal{B}_D(z, r)) \propto r^d / \text{vol}(\mathcal{M})$
- Given $Y \in \mathcal{B}_D(z, r)$, the variance of Y :

$$\begin{aligned} &\leftrightarrow \sim r^2 + \sigma^2 \\ &\uparrow \sim r^4 + \sigma^2 \end{aligned}$$

→ allows estimating $\Pi_{z^*}^\perp$

How Does This Work?

With properly designed weighting functions:

$$\tilde{\alpha}_i(z) = \left(1 - \frac{\|z - y_i\|^2}{r^2}\right)^\beta \mathbb{I}(\|z - y_i\| \leq r), \quad \alpha_i(z) = \frac{\tilde{\alpha}_i(z)}{\sum_{i=1}^n \tilde{\alpha}_i(z)}, \quad \beta > 2,$$

- Ψ_z is second order smooth, and estimates $\Pi_{z^*}^\perp$ well;
- the Jacobian matrix $J_f(x)$ satisfies $\|J_f(x) - \Psi_z\|_F \leq C\sigma/r$

Together with the smoothness of \mathcal{M} , for $x \in \widehat{\mathcal{M}}$, in its neighbourhood

- construct $h(z) = V_x^\top f(z)$, which is rank $D - d$
- $f(z) = 0$ iff $h(z) = 0$

↪ $\widehat{\mathcal{M}}$ is d -dimensional locally. Reach can be derived from Hessian of f .

Principal Nested Submanifolds – Population

- $X \in \mathbb{R}^D$: random vector of interest
- \mathcal{X} : support of X
- r : a radius parameter
- z : point of interest, with $d(z, \mathcal{X}) < cr$
- Local average: $\mu_z = E\{X \mid X \in \mathcal{B}(z, r)\}$
- Local covariance matrix centered at z :

$$\Sigma_z = E\{(X - \mu_{r,z})(X - \mu_{r,z})^\top \mid X \in \mathcal{B}(z, r)\}$$

- SVD:

- $\lambda_{z,1} < \dots < \lambda_{z,D}$
- $v_{z,1}, \dots, v_{z,D}$, with $\|v_{z,j}\| = 1$

Principal Nested Submanifolds – Population

- $\Pi_{z,j} = v_{z,j}v_{z,j}^\top$: projection matrix onto the j -th principal direction at z
- $\mu_z = \mathbb{E}(X \mid \|X - z\| < r)$: reference point for z :

Consider bias vectors

$$f_j(z) = \Pi_{z,j}(\mu_z - z),$$

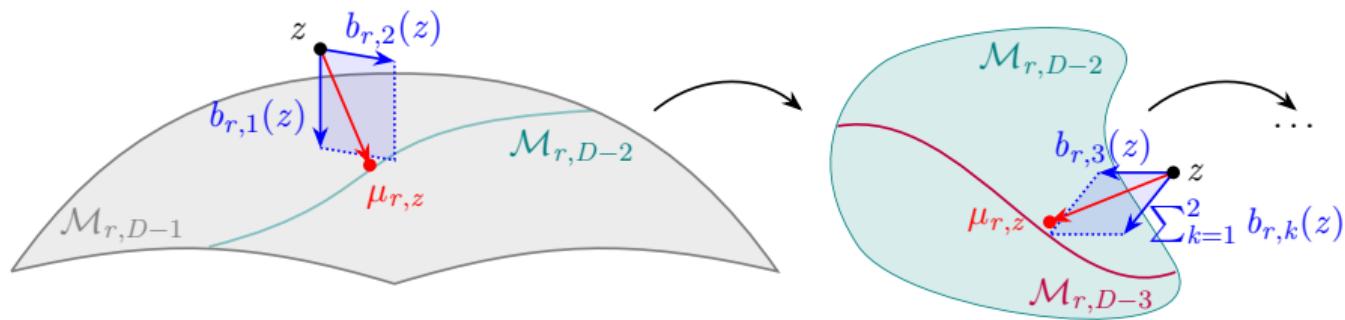
and let

$$\mathcal{M}_d = \{z \in \mathbb{R}^D : d(z, \mathcal{X}) \leq cr, \sum_{j=1}^{D-d} f_j(z) = 0\}.$$

Then, if X satisfies concentration, identifiability, and smoothness assumptions, there is

- $\dim(\mathcal{M}_d) = d$
- $\mathcal{M}_1 \subset \mathcal{M}_2 \subset \dots \subset \mathcal{M}_{D-1} \subset \mathbb{R}^D$

Intuition of Principal Nested Submanifolds



Empirical

- $\mathcal{X}_D = \{x_i\}_{i=1}^N \subset \mathbb{R}^D$
- Local covariance matrices:

$$\widehat{\Sigma}_i = \frac{\sum_j (x_i - x_j)(x_i - x_j)^\top \mathbb{I}(\|x_i - x_j\| < r)}{\sum_j \mathbb{I}(\|x_i - x_j\| < r)}$$

- $\widehat{\Pi}_{i,j}$: projection matrix onto the j -th smallest principal direction of $\widehat{\Sigma}_i$
- Weighting functions:

$$\tilde{\alpha}_i(z) = \left(1 - \frac{\|z - x_i\|^2}{r^2}\right)^\beta \mathbb{I}(\|z - x_i\| \leq r), \quad \alpha_i(z) = \frac{\tilde{\alpha}_i(z)}{\sum_{i=1}^n \tilde{\alpha}_i(z)}$$

with $\beta > 2$.

Empirical

Estimate

- $\widehat{\Pi}_{z,j} = \mathbb{P}_1 \left(\sum_i \alpha_i(z) \widehat{\Pi}_{i,j} \right)$
- $\widehat{\mu}_z = \sum_i \alpha_i(z) x_i$
- $\widehat{f}_j(z) = \widehat{\Pi}_{z,j} (\widehat{\mu}_z - z)$

and define the estimator for the nested d -dimensional submanifold as

$$\widehat{\mathcal{M}}_d = \{z \in \mathbb{R}^D : d(z, \mathcal{X}_D) \leq cr, \sum_{j=1}^{D-d} \widehat{f}_j(z) = 0\}.$$

Then, $\dim(\widehat{\mathcal{M}}_d) = d$, $\widehat{\mathcal{M}}_1 \subset \dots \subset \widehat{\mathcal{M}}_{D-1} \subset \mathbb{R}^D$, and $\widehat{\mathcal{M}}_d$ is close to \mathcal{M}_d with high probability.

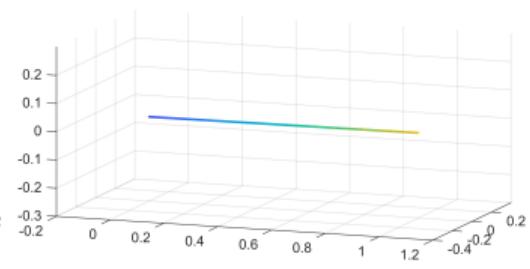
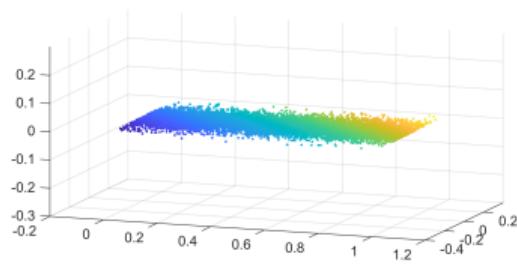
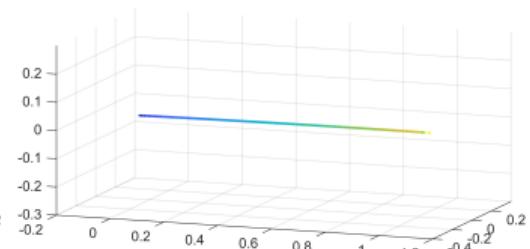
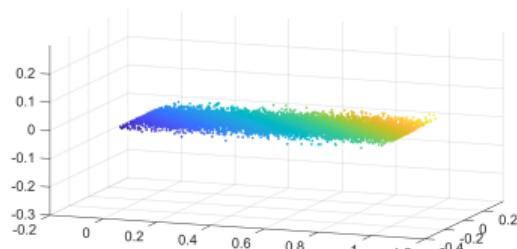
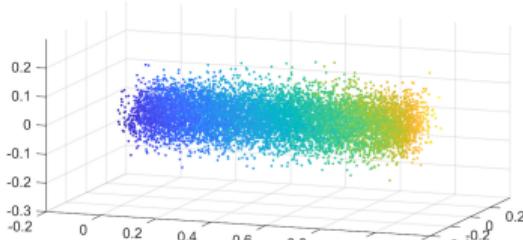
Estimation & Projection

- Embed data on \mathcal{M} in \mathbb{R}^D if needed
- Start with \mathcal{X}_D and calculate all $\widehat{\Pi}_{i,j}$'s
- for $d = \dim(\mathcal{M}) - 1 : 1$
 - for each element in \mathcal{X}_{d+1} , update with rule

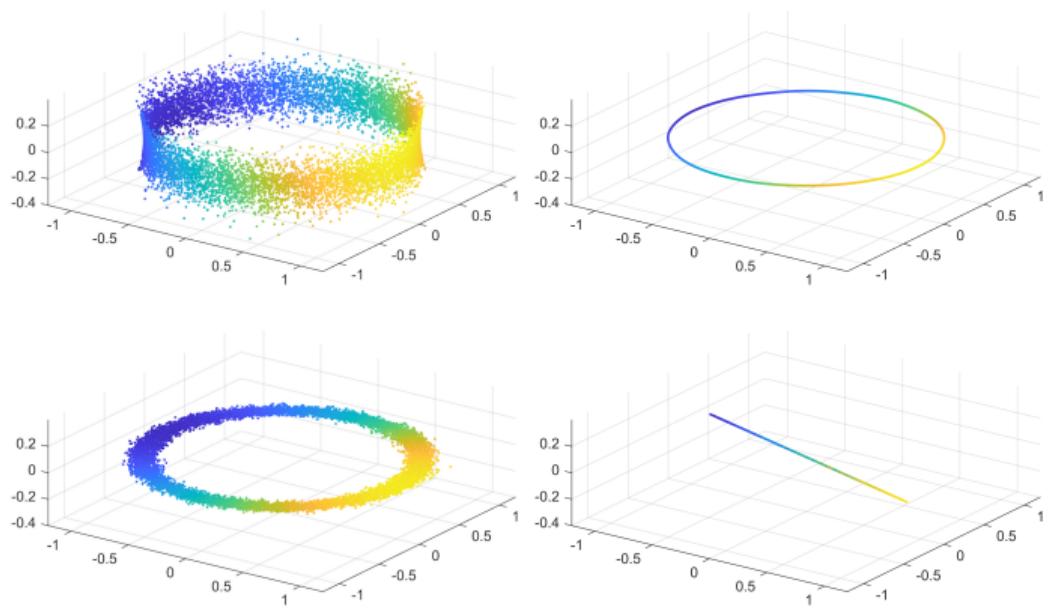
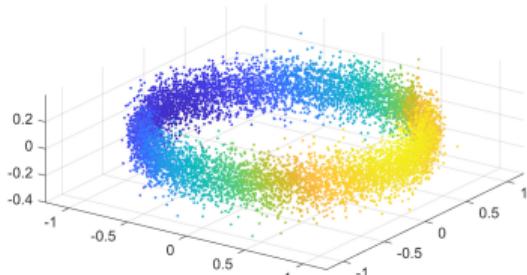
$$z' = z + \sum_{j=1}^{D-d} \widehat{f}_j(z)$$

- stop when $\|\sum_{k=1}^j \widehat{f}_j(z)\| < \epsilon$
- set the converge points as \mathcal{X}_d
- project \mathcal{X}_d on \mathcal{M} if needed.
- Return \mathcal{X}_d for $d = 1, \dots, \dim(\mathcal{M}) - 1$.

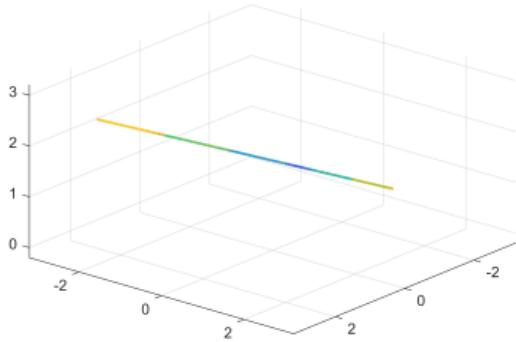
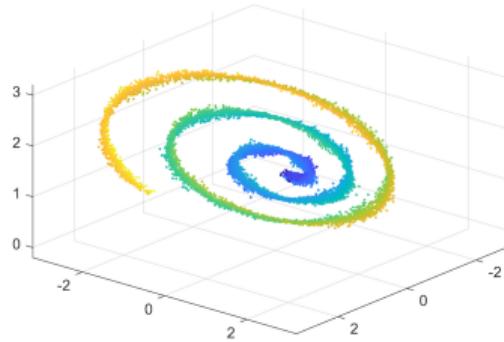
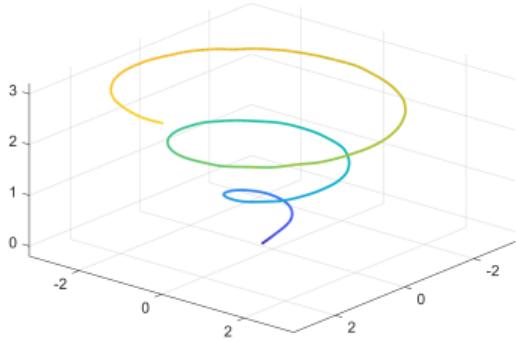
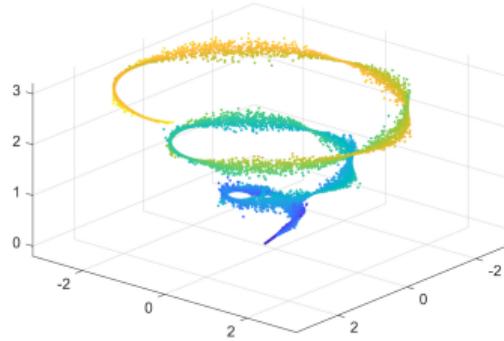
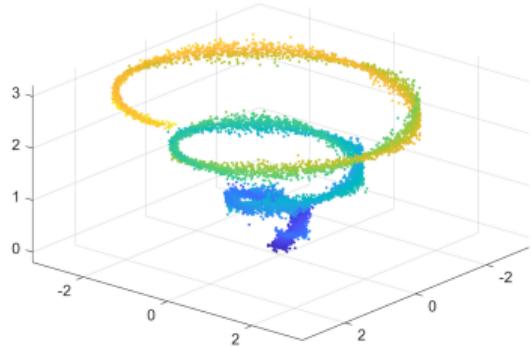
Simulation with Euclidean Space I



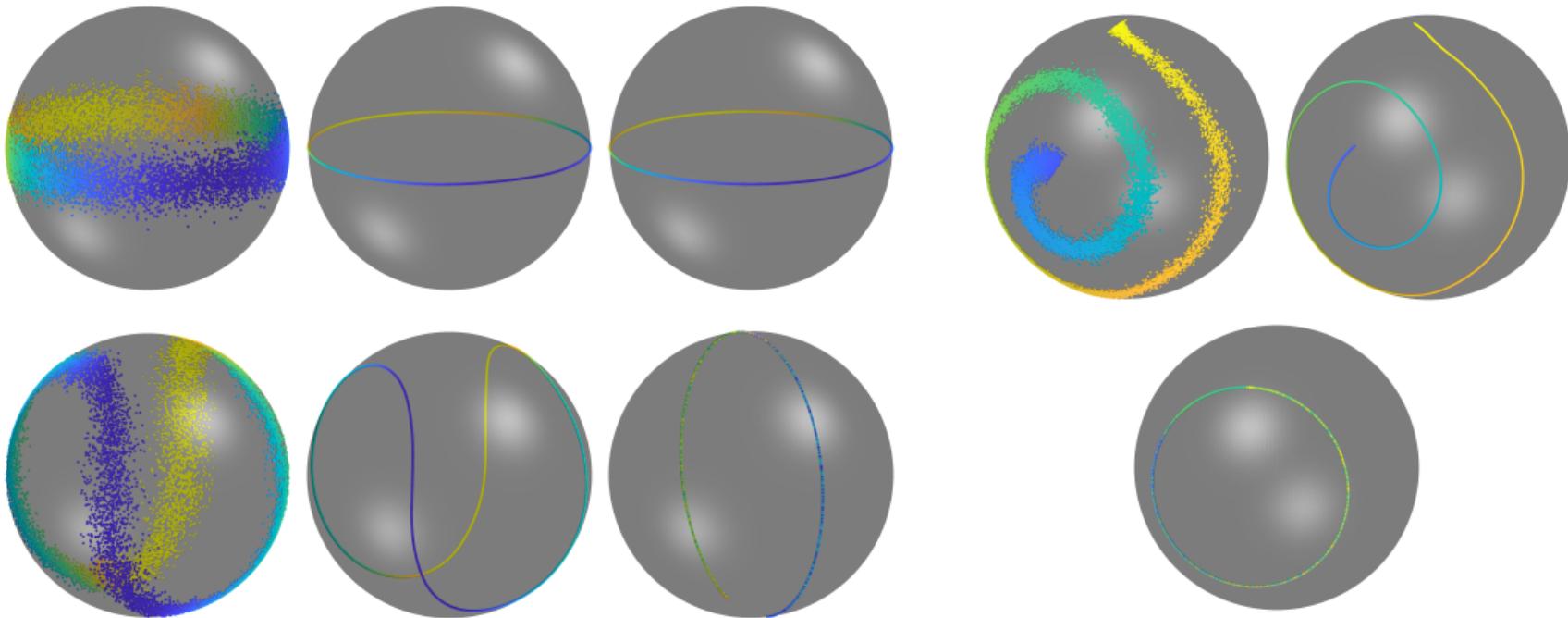
Simulation with Euclidean Space II



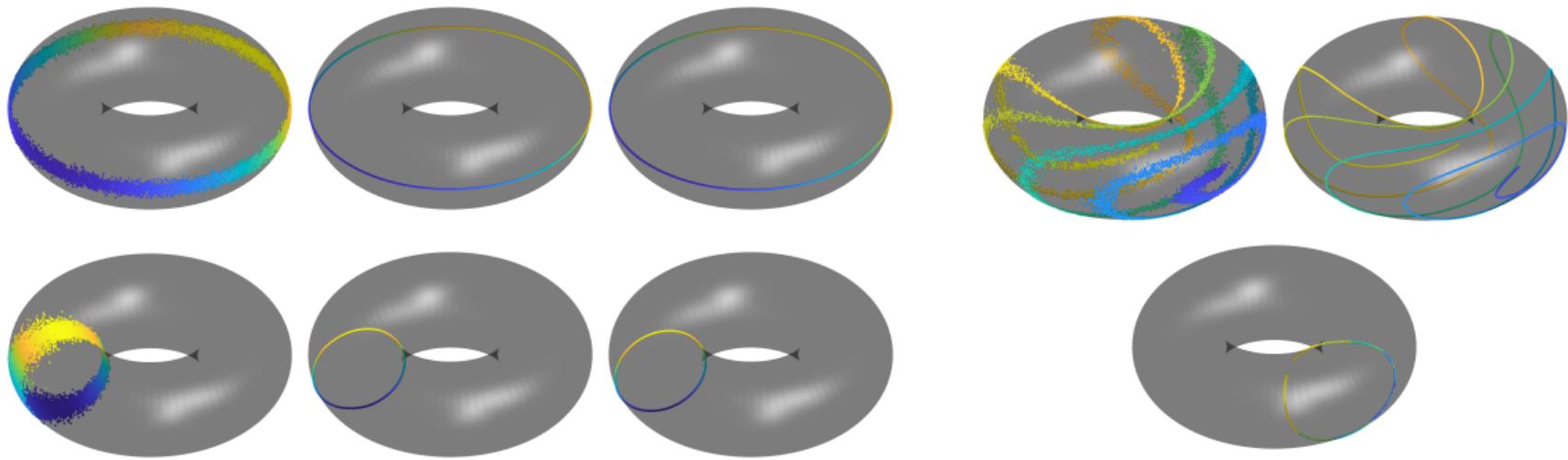
Simulation with Euclidean Space III



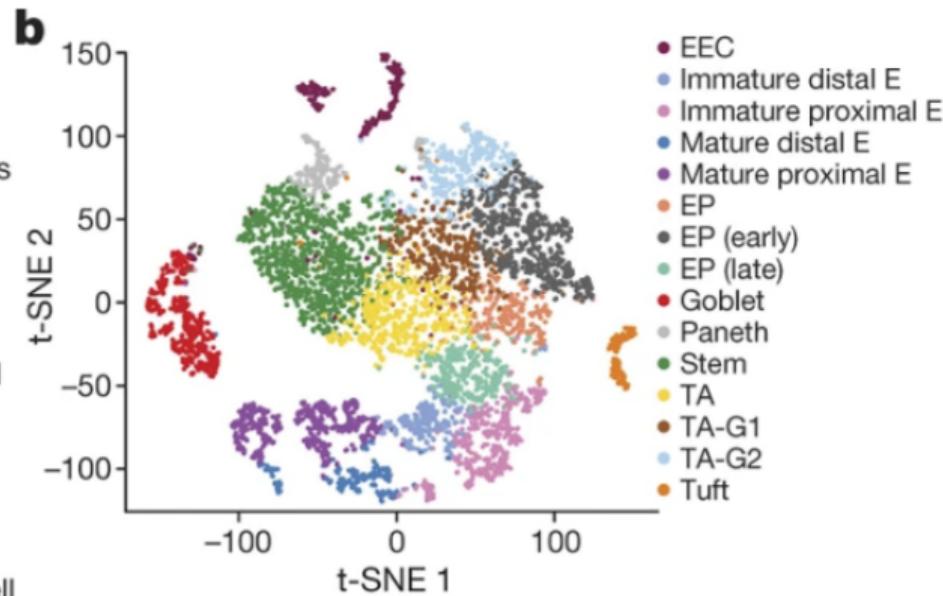
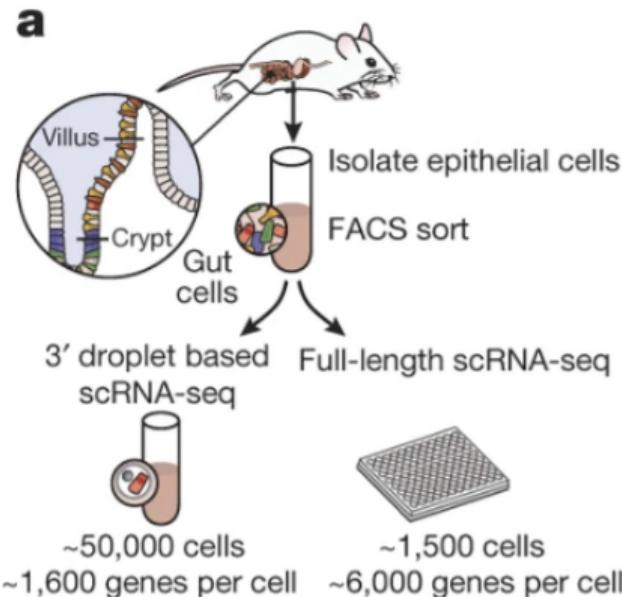
Simulation with Spheres



Simulation with Tori



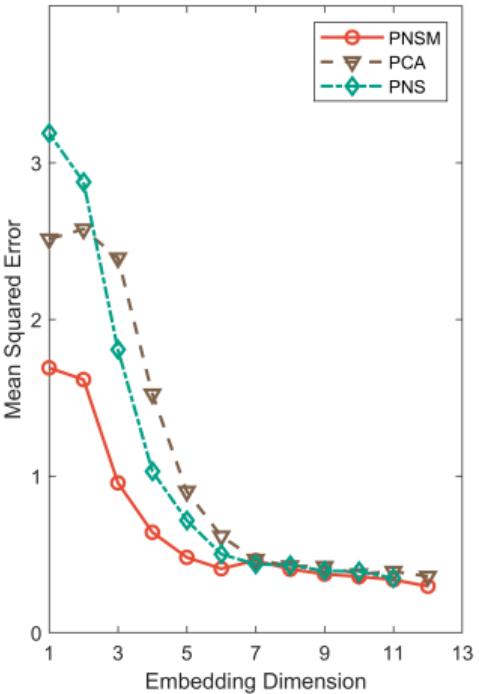
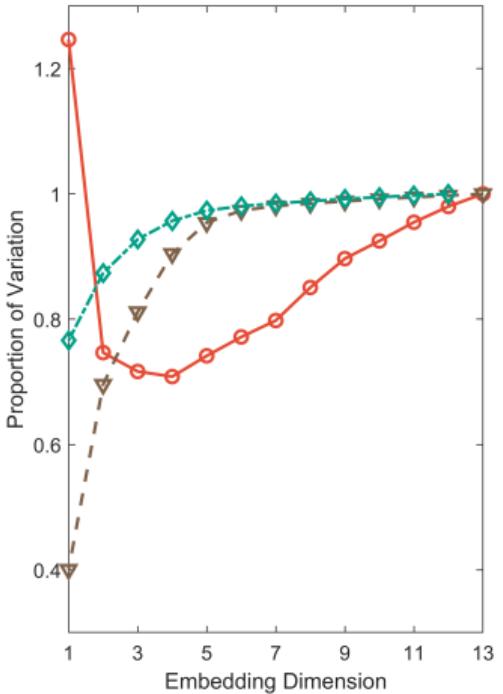
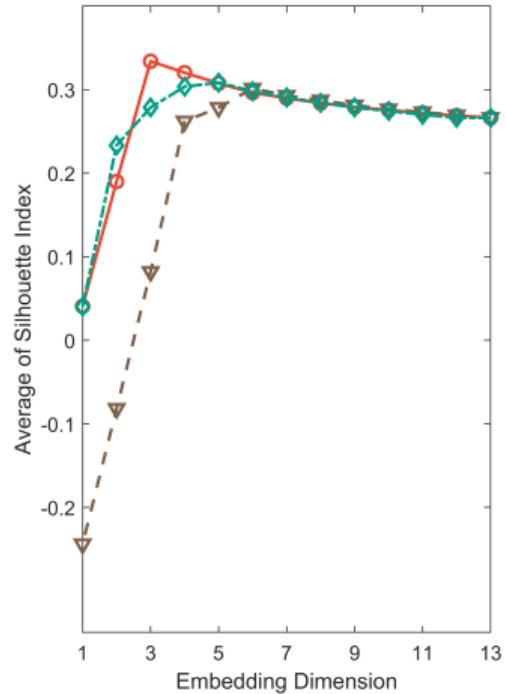
scRNA Data Set[†]



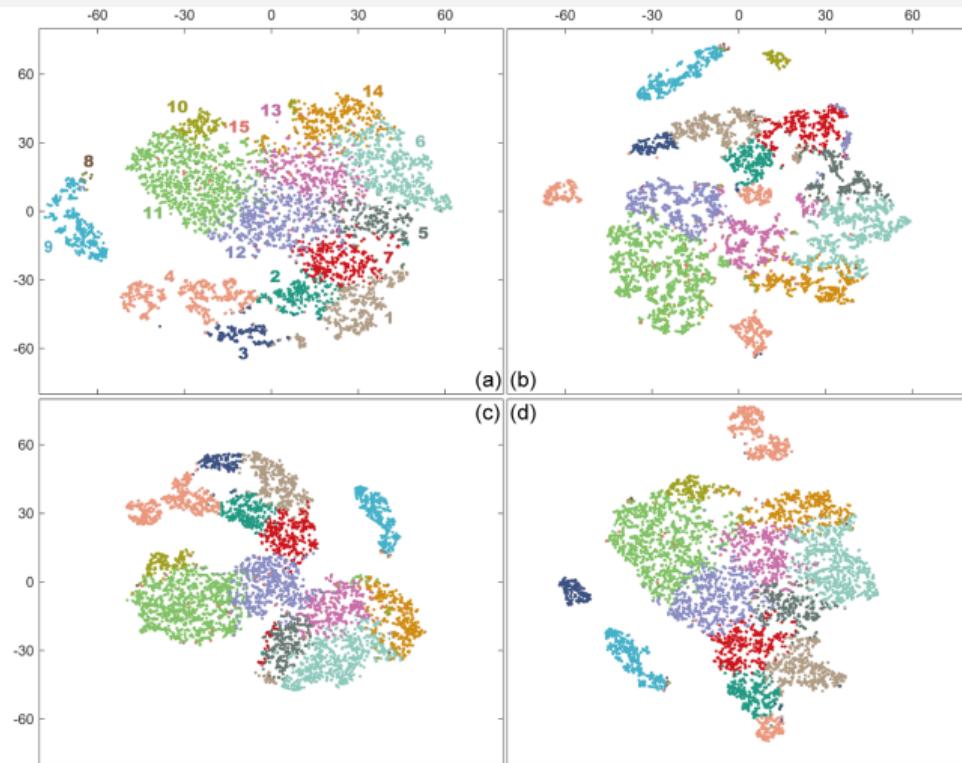
Totally 7,216 small intestinal epithelium cells from 6 mice, with the first 13 PCs.

[†]Haber, Adam L., et al. (2017). *A single-cell survey of the small intestinal epithelium*. Nature.

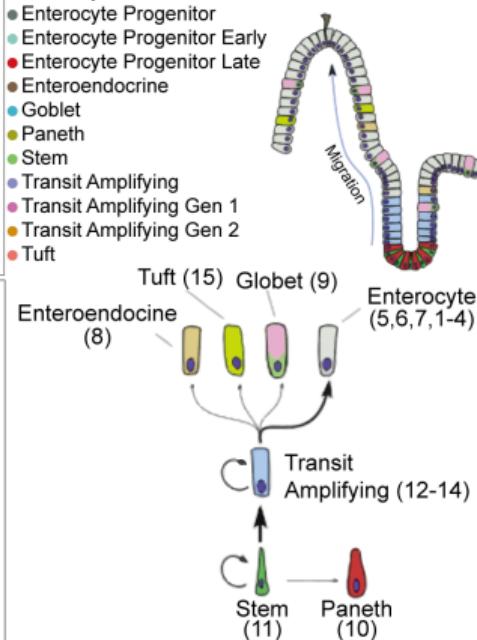
Compare



tSNE Visualization[§]

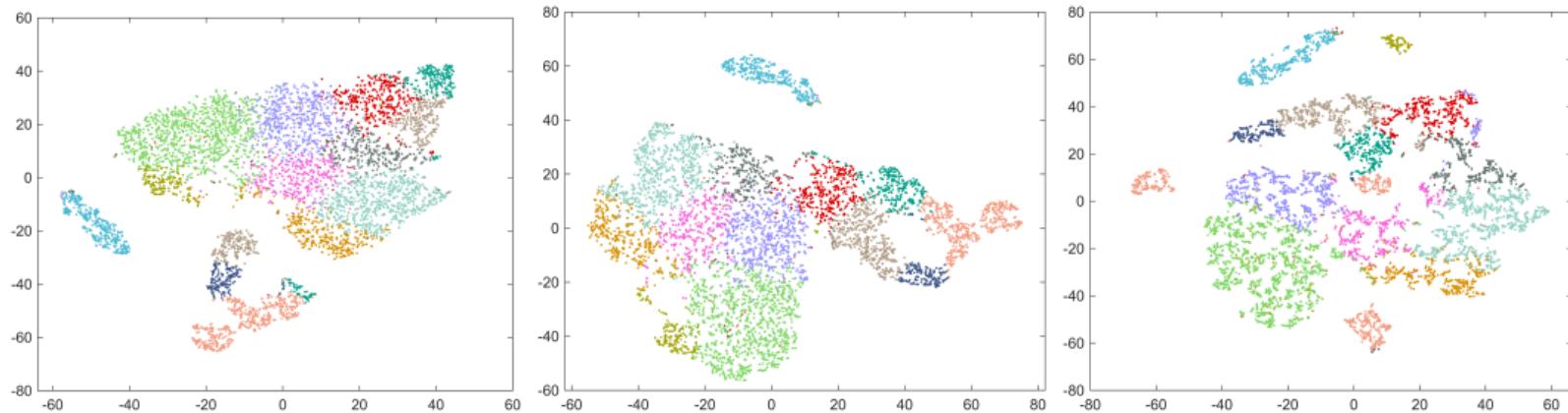


- Enterocyte Immature Distal
- Enterocyte Immature Proximal
- Enterocyte Mature Distal
- Enterocyte Mature Proximal
- Enterocyte Progenitor
- Enterocyte Progenitor Early
- Enterocyte Progenitor Late
- Enteroendocrine
- Goblet
- Paneth
- Stem
- Transit Amplifying
- Transit Amplifying Gen 1
- Transit Amplifying Gen 2
- Tuft



[§](a)Original Data; (b) PNSM with $d = 3$; (c) PCA with $d = 6$; (d) PNS with $d = 5$

tSNE Visualizations: $d \in \{13, 8, 3\}$



Conclusion & Outlook

- **Principal Nested Submanifolds:** a nonlinear, data-driven generalization of PCA.
 - Recovers nested low-dimensional structures from data
 - Applies to general spaces
 - Achieves superior performance in simulation and real single-cell data
- Future directions:
 - Scalable versions for large-scale omics data.
 - Integration into neural networks like generative models.

Thank you!
Questions are welcome.

Slides and preprint:



sujiaji.cn/nav