

Towards a generative model for Stochastic Neighbor Embedding

Julien Chiquet, Thibault Espinasse, Francois Gindraud, Franck Picard,
Hugues van Assel

Institut Camille Jordan, CNRS Univ. Lyon
AgroParisTech INRA - MIA, Paris
Laboratoire Biologie et Modélisation de la Cellule, CNRS ENS-Lyon

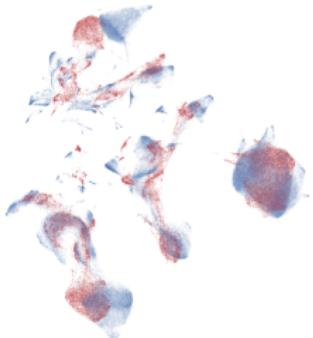
franck.picard@ens-lyon.fr

Outline

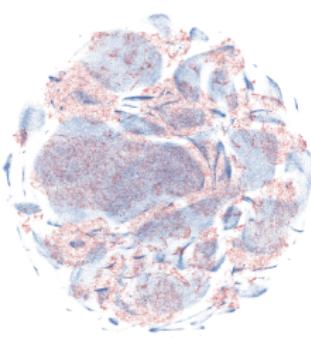
- 1 Presentation of Neighbor Embedding Methods
- 2 Empirical properties of tSNE
- 3 tSNE and Markov processes on Graphs
- 4 tSNE and Graph Coupling of Multivariate Gaussian Models
- 5 Open questions and research challenges

Beyond Linear methods

- Linear methods like PCA are robust but badly shaped for complex geometries
- High-dim. datas are characterized by multiscale properties (local / global structures)
- Non-Linear projection methods aim at preserving local characteristics of distances
- Many proposed methods such as LargeVis, tSNE, UMAP



(a) UMAP



(b) t-SNE

from [3]

Stochastic Neighbor Embedding (SNE) [4]

- (X_1, \dots, X_n) are the points in the high-dimensional space \mathbb{R}^p ,
- Consider a similarity between points:

$$p_{i|j} = \frac{\exp(-\|X_i - X_j\|^2/2\sigma_i^2)}{\sum_{\ell \neq i} \exp(-\|X_\ell - X_j\|^2/2\sigma_\ell^2)}$$

- Further symmetrized

$$p_{ij} = (p_{i|j} + p_{j|i})/2N$$

- Hyper-parameter σ_i locally smooths the data, to be tuned
- Linked to the regularity of the target manifold

tSNE and Student / Cauchy kernels

- Consider (Z_1, \dots, Z_n) are points in the low-dimensional space \mathbb{R}^2
- Consider a similarity between points in the new representation:

$$q_{i|j} = \frac{\exp(-\|Z_i - Z_j\|^2)}{\sum_{\ell \neq i} \exp(-\|Z_\ell - Z_j\|^2)}$$

- Robustify this kernel by using Student(1) kernels (ie Cauchy)

$$q_{i|j} = \frac{(1 + \|Z_i - Z_j\|^2)^{-1}}{\sum_{\ell \neq i} (1 + \|Z_i - Z_\ell\|^2)^{-1}}$$

Optimizing tSNE by Gradient descent

- Minimize the KL between p and q to find $Z \in \mathbb{R}^2$ such that:

$$C(Z) = \sum_{ij} KL(p_{ij}, q_{ij})$$

$$\left[\frac{\partial C(Z)}{\partial Z} \right]_i = \sum_j (p_{ij} - q_{ij})(Z_i - Z_j)$$

- Gradient update (adaptive learning rate η)

$$Z^{(t)} = Z^{(t-1)} + \eta \frac{\partial C(Z)}{\partial Z} + \alpha(t)(Z^{(t-1)} - Z^{(t-2)})$$

- $\alpha(t)$ momentum to speed up and improve convergence
- Initialization $Z_i^{(0)} \sim \mathcal{N}(0, \delta I)$, δ small.

Uniform Manifold Approximation and Projection [3]

$$\forall (i, j) \in [n]^2, \quad p_{j|i} = \exp \left(-\frac{\|X_i - X_j\|_2^2 - \rho_i}{\sigma_i} \right)$$

with $\rho_i = \min_{j \neq i} \|X_i - X_j\|^2$. Let us define

$$p_{ij} = p_{j|i} + p_{i|j} - p_{j|i}p_{i|j}$$

and:

$$\forall (i, j) \in [n]^2, \quad q_{ij} = \left(1 + a \|X_i - X_j\|_2^{2b} \right)^{-1}$$

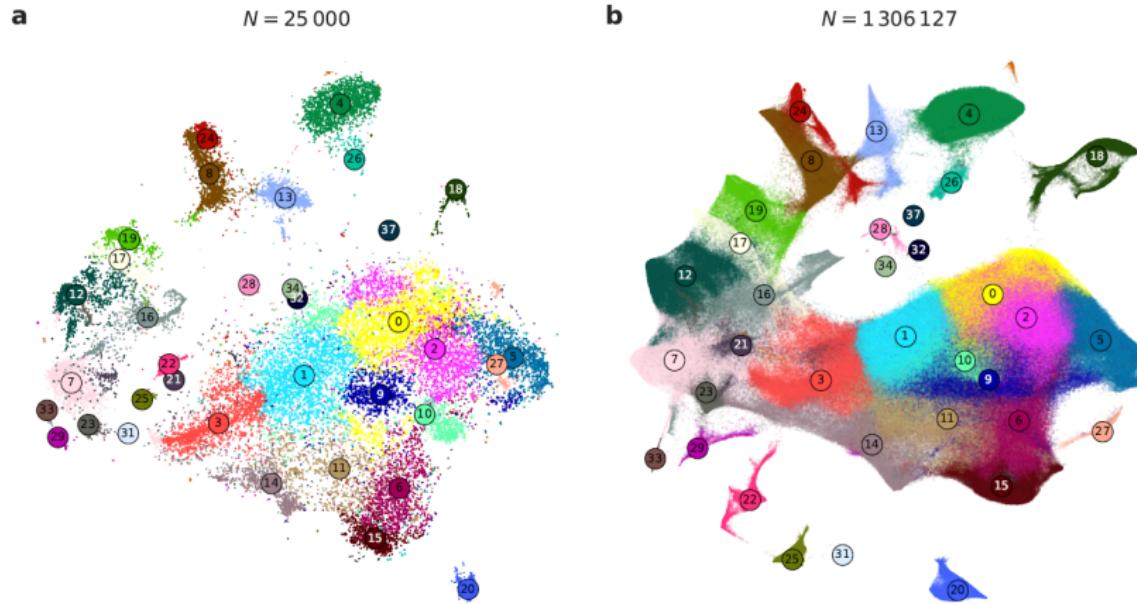
UMAP solves the following problem:

$$\min_{Z \in \mathbb{R}^{n \times d}} - \sum_{i < j} p_{ij} \log q_{ij} + (1 - p_{ij}) \log(1 - q_{ij})$$

Outline

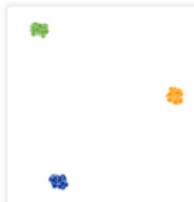
- 1 Presentation of Neighbor Embedding Methods
- 2 Empirical properties of tSNE
- 3 tSNE and Markov processes on Graphs
- 4 tSNE and Graph Coupling of Multivariate Gaussian Models
- 5 Open questions and research challenges

tSNE on single cell Gene Expression data [1]

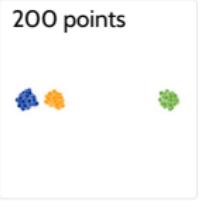
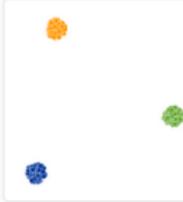


tSNE does not account for between-cluster distance

50 points

A scatter plot showing 50 points in a 2D space. The points are colored into three distinct clusters: blue, orange, and green. The clusters are somewhat compact and well-separated.*Original*Perplexity: 2
Step: 5,000Perplexity: 5
Step: 5,000Perplexity: 30
Step: 5,000Perplexity: 50
Step: 5,000Perplexity: 100
Step: 5,000

200 points

A scatter plot showing 200 points in a 2D space. The points are colored into three distinct clusters: blue, orange, and green. The clusters are somewhat compact and well-separated.*Original*Perplexity: 2
Step: 5,000Perplexity: 5
Step: 5,000Perplexity: 30
Step: 5,000Perplexity: 50
Step: 5,000Perplexity: 100
Step: 5,000

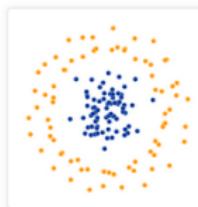
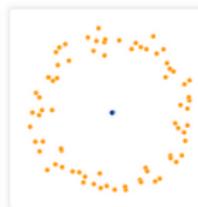
What about random noise ?



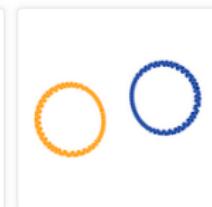
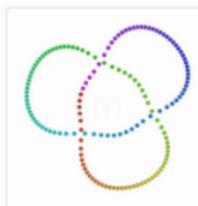
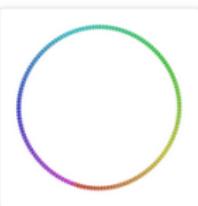
Catching Complex Geometries



Original

Perplexity: 2
Step: 5,000Perplexity: 5
Step: 5,000Perplexity: 30
Step: 5,000Perplexity: 50
Step: 5,000Perplexity: 100
Step: 5,000

Original

Perplexity: 2
Step: 5,000Perplexity: 5
Step: 5,000Perplexity: 30
Step: 5,000Perplexity: 50
Step: 5,000Perplexity: 100
Step: 5,000

Properties of t-SNE

- Good at preserving local distances (intra-cluster variance)
- Not so good for global representation (inter-cluster variance)
- Good at creating clusters of points that are close, but bad at positioning clusters wrt each other
- Does not handle well high dimensional data (preliminary PCA and feature selection)
- Sensitive to the calibration of the hyperparameter (smoothing)
- Reproducibility of results due to stochastic optimization

→ What are the statistical / probabilistic foundations of Stochastic Neighbor Embedding ?

Outline

- ① Presentation of Neighbor Embedding Methods
- ② Empirical properties of tSNE
- ③ tSNE and Markov processes on Graphs
- ④ tSNE and Graph Coupling of Multivariate Gaussian Models
- ⑤ Open questions and research challenges

Motivations

- tSNE is defined by a quantity to optimize: Minimize the KL between p and q so that the data representation z minimizes:

$$C(z) = \sum_{ij} KL(p_{ij}, q_{ij})$$

- What is the underlying model ? p_{ij} proba of ?
- Could we improve the optimization algorithm if the underlying model was better defined ?
- Could we estimate the hyperparameters (smoothing) using ML ?
- Could we perform model selection ?

Markov Processes on a Graph for X

- Consider $G_X = (\mathcal{V}, \mathcal{E}_X)$ with $\mathcal{V} = \{1, \dots, n\}$ a set of nodes
- Nodes have attributes (X_1, \dots, X_n) in \mathbb{R}^p
- **Main idea:** to any reversible Markov Process one can associate a symmetric graph, (reciprocal true).
- Introduce Y_X , a MP taking values in \mathcal{V} , s.t.

$$\mathbb{P}(Y_X(t+1) = j \mid Y_X(t) = i, X = x) = \Pi_X(i, j)$$

- X is fixed, no distribution assumption (kernel method)

Gaussian Transition Kernel on X

- We suppose that the transition kernel is of the form

$$\Pi_X(i, j) = \frac{k(x_i, x_j)}{d_X(i)}, \quad d_X(i) = \sum_{j=1}^n k(x_i, x_j)$$

- Π_X is not symmetric but has the conservation property:

$$\sum_{j=1}^n \Pi_X(i, j) = 1.$$

- Π_X is the 1-step transition matrix between points
- Stationary distribution of Y_X :

$$\mu_X \Pi_X = \mu_X, \quad \mu_X(i) = \frac{d_X(i)}{\bar{d}_X}, \quad \bar{d}_X = \sum_j d_X(j)$$

Markov Process on a Graph for Z

- Consider another graph $G_Z = (\mathcal{V}, \mathcal{E}_Z)$ with $\mathcal{V} = \{1, \dots, n\}$ (same)
- Z is the set of new attributed in \mathbb{R}^q (unknown).
- Introduce a new MP Y_Z defined on $\{1, \dots, n\}$ s.t.

$$\mathbb{P}(Y_Z(t+1) = j \mid Y_Z(t) = i, Z = z) = \frac{h(z_i, z_j)}{d_Z(i)} = \Pi_Z(i, j)$$

- Z is fixed and considered as a parameter, but the form of the transition is specified

Gaussian or Student transition kernel on Z

- Suppose the new transition is of the form (Z unknown)

$$\Pi_Z(i, j) = \frac{h(z_i, z_j)}{d_Z(i)}$$

- We get close to tSNE by choosing

$$\begin{aligned} k(x_i, x_j) &= \exp\left(-\frac{1}{2\sigma}\|x_i - x_j\|^2\right) \\ h(z_i, z_j) &= \frac{1}{1 + \|z_i - z_j\|^2} \end{aligned}$$

- Suppose the two chains are conditionally independent

$$Y_X \perp Y_Z | X, Z$$

Maximum Coupling between Markov Processes

- Once the two chains specified, find Z by coupling the two processes

$$Z(X) = \max_Z \left(\log \mathbb{P}(Y_X = Y_Z \mid X, Z) \right)$$

- Maximizing the coupling between Y_X and $Y_Z \Leftrightarrow$ Minimizing the KL between Y_X and Y_Z

$$\mathbb{E}_{Y_X \sim \mu_X} \left(\log \mathbb{P}(Y_Z = Y_X \mid X, Z) \right) = \mathbb{E}_{Y \sim \mu_X} \left(\log \mathbb{P}(Y_Z = Y \mid X, Z) \right)$$

Minimum KL and Maximum Coupling

- The KL divergence between Markov Process

$$KL(Y_X, Y_Z) = \mathbb{E}_{Y \sim \mu_X} \left(\log \mathbb{P}(Y_X = Y) \right) - \mathbb{E}_{Y \sim \mu_X} \left(\log \mathbb{P}(Y_Z = Y) \right)$$

- Connection with the probability of coupling

$$\mathbb{E}_{Y_X \sim \mu_X} \left(\log \mathbb{P}(Y_Z = Y_X) \right) = \mathbb{E}_{Y \sim \mu_X} \left(\log \mathbb{P}(Y_Z = Y) \right)$$

- Minimizing the KL between chains wrt Z maximizes the probability of coupling

$$KL(Y_X, Y_Z) = -H_{\mu_X}(Y_X) - \mathbb{E}_{Y_X \sim \mu_X} \left(\log \mathbb{P}(Y_Z = Y_X \mid X, Z) \right)$$

Empirical Maximum Coupling

- To retrieve the hidden components:

$$Z_n(X) = \arg \max_Z \left[\hat{H}_{\mu_X}(Y_Z | X) \right],$$

- $H_{\mu_X}(Y_Z | X, Z)$ stands for the entropy of chain Y_Z under μ_X with empirical version (fixed X)

$$\begin{aligned} \hat{H}_{\mu_X}(Y_Z | X) &= \sum_{i=1}^n \mu_X(i) \log \mu_Z(i) \\ &+ \sum_{i=1}^n \mu_X(i) \left(\sum_{j=1}^n \Pi_X(i, j) \log \Pi_Z(i, j) \right) \end{aligned}$$

Specified transitions induce simplifications

$$d_X(i) = \sum_{j=1}^n k(x_i, x_j), \quad d_Z(i) = \sum_{j=1}^n h(z_i, z_j)$$

$$\mu_X(i) = d_X(i)/\bar{d}_X \quad \bar{d}_X = \sum_i d_X(i)$$

$$\mu_Z(i) = d_Z(i)/\bar{d}_Z \quad \bar{d}_Z = \sum_i d_Z(i)$$

and

$$\Pi_X(i, j) = \frac{k(X_i, X_j)}{d_X(i)}, \quad \Pi_Z(i) = \frac{h(Z_i, Z_j)}{d_Z(i)}$$

Then

$$\widehat{H}_{\mu_X}(Y_Z | X) = \sum_{i,j} \frac{k(X_i, X_j)}{\bar{d}_X} \log \frac{h(Z_i, Z_j)}{\bar{d}_Z}$$

tSNE maximizes the coupling between Markov Processes

- If considering only KL minimization, the new representation would be such that:

$$\hat{Z}_n(X) = \arg \max_Z \left[\sum_{i,j} \frac{k(X_i, X_j)}{\bar{d}_X} \log \frac{h(Z_i, Z_j)}{\bar{d}_Z} \right],$$

- \bar{d}_X, \bar{d}_Z are normalization terms (different in tSNE - for now)
- The criterion is conditional to X
- interpretability of Z ? Representation of new X s ?

Outline

- ① Presentation of Neighbor Embedding Methods
- ② Empirical properties of tSNE
- ③ tSNE and Markov processes on Graphs
- ④ tSNE and Graph Coupling of Multivariate Gaussian Models
- ⑤ Open questions and research challenges

Hidden Graph to structure observations

- Let us suppose that observations (rows) are structured thanks to a hidden random Graph
- $G = (V, E)$ with $V = \{1, \dots, n\}$ the vertices

$$A_{ij} = \sum_{(k, \ell) \in E} \mathbb{1}_{(i, j) = (k, \ell)}, \quad L_G = D - A, \quad \text{where} \quad D_{ii} = \sum_j A_{ij}$$

- L_G , the Laplacian of G has the following property:

$$\forall X \in \mathbb{R}^{n \times p}, \quad \sum_{i, j} A_{ij} \|X_i - X_j\|^2 = \text{tr}(X^\top L_G X).$$

Conditional distribution of X on a graph

- Conditional model of the observations given the graph

$$X | G \sim \mathcal{MN}\left(0, L_G^{-1}, R^{-1}\right),$$

- L_G^{-1} between-cell variability, R^{-1} between-genes correlation.
- Consider the Gaussian kernel for X

$$k(X_i, X_j) = \exp\left(-\frac{1}{2}\|X_i - X_j\|_R^2\right),$$

- Conditional distribution of $X | G$:

$$\mathbb{P}(X | G) \propto |L_G|^{p/2} \prod_{i,j=1}^n k(X_i, X_j)^{A_{ij}}$$

Conditional distribution of Z on a graph

- Consider that the low-dimensional representation is also structured according to a graph
- Consider the Gaussian kernel for Z

$$k(Z_i, Z_j) = \exp\left(-\frac{1}{2}\|Z_i - Z_j\|_{I_q}^2\right),$$

- Conditional distribution of $Z \mid G$:

$$\mathbb{P}(Z \mid G) \propto |L_G|^{q/2} \prod_{i,j=1}^n k(Z_i, Z_j)^{A_{ij}}$$

Embedding with Graph Coupling

- Consider two graphs G_X and G_Z
- Coupling with $G_X = G_Z$

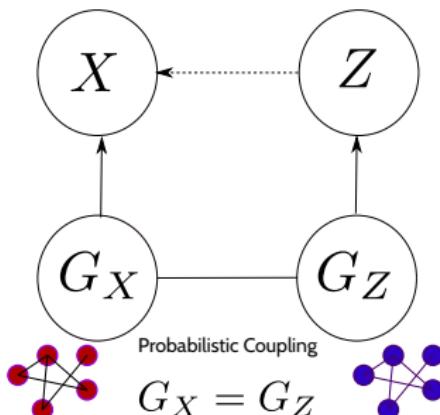
$$\mathbb{E}_{G \sim G_X} \left(\log \mathbb{P}(G_Z = G_X \mid X, Z) \right)$$

- which is equivalent to

$$\mathbb{E}_{G \sim G_X} \left(\log \mathbb{P}(G_Z = G \mid X, Z) \right)$$

- which is the entropy of G_Z under G_X

$$H_{G_X}(G_Z \mid X, Z)$$



Graph Coupling with Z as a parameter

- Find the best Z such that the two graphs G_X and G_Z are as close as possible:

$$Z(X) = \arg \min_Z \left[H_{G_X}(G_Z | X, Z) \right]$$

- The cross entropy between distribution of G_X and G_Z , which writes

$$H_{G_X}(G_Z) = - \sum_g \mathbb{P}(G_X = g | X) \log \mathbb{P}(G_Z = g | Z).$$

- Challenge : define a prior distribution and deduce the posterior

Bernoulli prior distribution for G_X

- Let A_X be the adjacency matrix of G_X , with $A_{X,ij} \in \{0, 1\}$

$$\mathbb{P}(G_X; \pi_X) = \frac{|L_X|^{-a_X/2} \times \prod_{i,j} \pi_{X,ij}^{A_{X,ij}}}{\sum_{A' \in \{0,1\}} |L_X(A')|^{-a_X/2} \times \prod_{i',j'} \pi_{X,i'j'}^{A'_{X,i'j'}}}$$

- $|L_{G_X}|^{-a_X/2}$ catches the dependency of connections wrt the graph.
- Retrieves conjugacy with the Gaussian conditional model
- Setting $a_X = 0$ leads to an independent Bernoulli prior

$$\mathbb{P}(A_{X,ij} = 1; \pi_X) = \frac{\pi_{X,ij}}{1 + \pi_{X,ij}}$$

Induced Posterior Distribution for G_X

- The posterior writes

$$\begin{aligned}\mathbb{P}(G_X | X; \pi_X) &\propto \mathbb{P}(G_X; \pi_X) \mathbb{P}(X | G_X; R) \\ &\propto |L_X|^{(p-a_X)/2} \prod_{ij} \left(\pi_{X,ij} k(X_i, X_j; R) \right)^{A_{X,ij}}\end{aligned}$$

- When $a_X = p$ we get independent Bernoulli posteriors

$$\mathbb{P}(A_{ij} = 1 | X; \pi) = \frac{\pi_{ij} k(X_i, X_j)}{1 + \pi_{ij} k(X_i, X_j)} = q_B(X_i, X_j)$$

- When $a_X = 0$ we get an independent prior, but an intractable posterior

Maximum Coupling with the Bernoulli prior

$$\begin{aligned}\text{KL}(G_X, G_Z) &= \sum_{ij} p_{\mathcal{B}}(X_i, X_j) \log \frac{p_{\mathcal{B}}(X_i, X_j)}{q_{\mathcal{B}}(Z_i, Z_j)} \\ &+ \sum_{ij} \left(1 - p_{\mathcal{B}}(X_i, X_j)\right) \log \frac{1 - p_{\mathcal{B}}(X_i, X_j)}{1 - q_{\mathcal{B}}(Z_i, Z_j)} \\ &= \mathsf{H}_{G_X}^{\mathcal{B}}(G_Z) \\ &+ \sum_{ij} p_{\mathcal{B}}(X_i, X_j) \log p_{\mathcal{B}}(X_i, X_j) \\ &+ \sum_{ij} \left(1 - p_{\mathcal{B}}(X_i, X_j)\right) \log \left(1 - p_{\mathcal{B}}(X_i, X_j)\right)\end{aligned}$$

→ UMAP computes a KL (and not a cross entropy)

Fixed-degree prior distribution for G_X

- Denote by $D_{X,i}$ the degree of node i , consider

$$\mathbb{P}(G_X; \pi, D_X) \propto |L_{G_X}|^{-\alpha_X/2} \prod_{i=1}^n \prod_{\ell=1}^{D_i} \pi_{i, e_{i\ell}}, \quad A_{X,ij} = \sum_{\ell=1}^{D_i} \mathbb{1}_{\{e_{i\ell}=j\}}$$

- Choosing $\alpha_X = 0$ corresponds to a multinomial model:

$$A_{X,i1}, \dots, A_{X,in}; D_{X,i} \sim \mathcal{M}\left\{ D_{X,i}; \left(\frac{\pi_{X,ij}}{\sum_{\ell=1}^n \pi_{X,i\ell}} \right)_j \right\},$$

- Choosing $\alpha_X = p$ leads to

$$A_{X,i1}, \dots, A_{X,in} | X; D_{X,i} \sim \mathcal{M}\left\{ D_{X,i}; \left(\frac{\pi_{X,ij} k(X_i, X_j)}{\sum_{\ell=1}^n \pi_{X,ik} k(X_i, X_{\ell})} \right)_j \right\},$$

tSNE and the Fixed-degree model

- In the following we will write:

$$p_D(X_i, X_j) = \frac{\pi_{ij} k(X_i, X_j)}{\sum_{\ell=1}^n \pi_{ij} k(X_i, X_\ell)}, \quad q_D(Z_i, Z_j) = \frac{\pi_{ij} k(Z_i, Z_j)}{\sum_{\ell=1}^n \pi_{ij} k(Z_i, Z_\ell)}.$$

- We retrieve the non-symmetric normalization term (Markov-like)
- With this prior we obtain the tSNE-like criterion

$$H_{G_X}^D(G_Z) = - \sum_{i,j} D_{Xi} \left\{ p_D(X_i, X_j) \log q_D(Z_i, Z_j) \right\}$$

tSNE is defined for fixed X

- In the original method, the distribution of X is not modelled
- All quantities are defined conditionally to X
- This helps to choose $a_X = p$ and $a_z = q$ so that the posteriors p and q are factorized
- This allows to compute the cross entropy (sum)
- Master's internship:
 - impact on Z of the different priors
 - induced momentum algorithms for each prior

Outline

- ① Presentation of Neighbor Embedding Methods
- ② Empirical properties of tSNE
- ③ tSNE and Markov processes on Graphs
- ④ tSNE and Graph Coupling of Multivariate Gaussian Models
- ⑤ Open questions and research challenges

Symmetrization and directed graphs

- In the original formulation : $p_{ij} = (p_{i|j} + p_{j|i})/2N$
- What probabilistic model should we consider to obtain the same symmetrization with our posteriors ?
- Considering an oriented graph with symmetrized Laplacian

$$\begin{cases} L_{ij} = -(A_{ij} + A_{ji})/2 & \text{if } i \neq j \\ L_{ii} = (A_{i+} + A_{+i})/2 & \end{cases}$$

- How to get to a symmetrized posterior from here ?
- interpretation of the underlying directed graph ?

Kernel calibration and Perplexity

- tSNE strongly depends on the calibration of the kernel

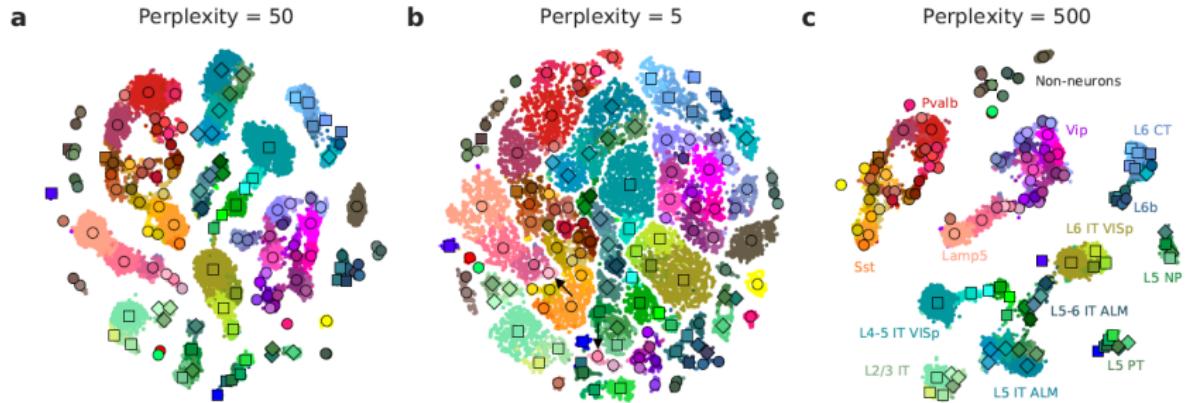
$$k(X_i, X_j; \sigma_i) = \exp\left(-\frac{1}{2\sigma_i}\|X_i - X_j\|_R^2\right),$$

- σ_i should adjust to local densities (neighborhood of point i)
- In practice, the method is tuned by fixing a given amount of entropy

$$H(p_i) = - \sum_{j=1}^n p_{ij} \log_2 p_{ij}$$

- Find σ_i such that $2^{H(p_i)} = \text{perp}$ (user defined)
- Interpreted as the smoothed effective number of neighbors.

Visual inspection of the influence of $\sigma[1]$



Connecting the kernel bandwidth with the graph model

- Consider $D = \text{diag}(d_1, \dots, d_n)$ the matrix of degrees
- Consider the random walk laplacian is defined by:

$$L^{RW} = D^{-1}L$$

- The following property holds:

$$\forall X \in \mathbb{R}^n, \text{tr}(X^T L^{RW} X) = \frac{1}{2} \sum_{i,j} A_{i,j} \frac{\|X_i - X_j\|^2}{d_i}$$

- Hence we can consider

$$X_{n,p} \mid G_X \sim \mathcal{MN}_{n,p} \left(0, \left(L^{RW} \right)^{-1}, R^{-1} \right)$$

Back to the coupling strategy

- Maximizing the probability of coupling by minimizing the KL

$$\text{KL}(G_X, G_Z) = H_{G_X}(G_Z) - H_{G_X}(G_X)$$

- $H_{G_X}(G_X)$ is exactly the perplexity parameter
- Constrained coupling with a given degree of entropy

$$\begin{aligned} Z(X) &= \arg \min_{Z, H_{G_X}(G_X) = \text{Perp}} \left[\text{KL}(G_X, G_Z) \right] \\ &= \arg \min_{Z, H_{G_X}(G_X) = \text{Perp}} \left(H_{G_X}(G_Z) - \text{Perp} \right) \end{aligned}$$

Connection with Nearest Neighbors Graphs and Manifold Learning

- The method is based on a preliminary smoothing of the data to retrieve a graph with controlled complexity
- This is related (how ?) to manifold learning and density estimation on manifolds
- The output $\widehat{Z}(X)$ strongly depends on this preliminary step

$$\widehat{Z}_{\text{Perp}}(X) = \arg \min_Z \left(H_{\widehat{G}_{X, \text{Perp}}} (G_Z) \right)$$

Maximum Likelihood inference for SNE ?

- Define the observed X and hidden G, Z variables
- Define the observed-data likelihood : $\mathbb{P}(X)$
- Define the conditional distribution : $\mathbb{P}(X | G, Z)$
- Define the prior distribution $\mathbb{P}(G, Z)$
- Compute the conditional expectation of the complete-data loglik

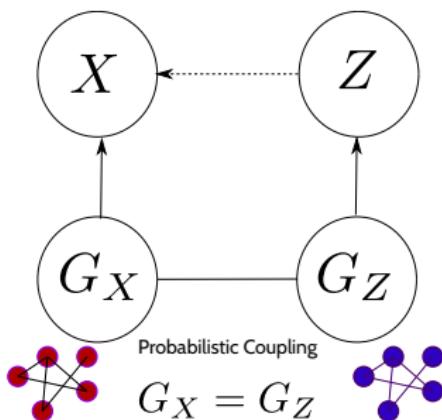
$$\mathcal{Q} = \mathbb{E}_{G, Z | X} \left(\log \mathbb{P}(X, G, Z) \right)$$

- Compute the posterior

$$\log \mathbb{P}(G, Z | X)$$

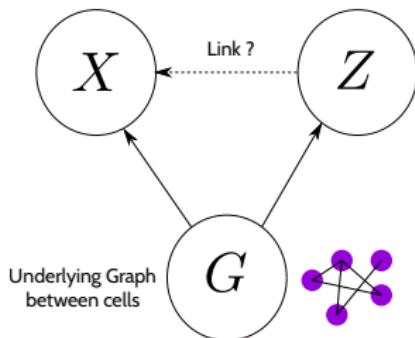
The two-graph model is not identifiable

- Coupling with $G_X = G_Z$
 $\log \mathbb{P}(X, Z, G_X, G_Z, G_X = G_Z)$
- Discrepancy between two priors and posterior
- Difficult to model a link between X and Z
- Non identifiable model



The one-graph model

- One prior that rules them all
- Different priors for G (Bernoulli, fixed number of edges, fixed degree)
- Identifiable model but computational issues
- tSNE strategy : Z is a parameter



When a_X and a_Z come back

- The joint likelihood of the model:

$$\log \mathbb{P}(X, G | Z) = \log \mathbb{P}(X | G, Z) + \log \mathbb{P}(G | Z)$$

- In the EM framework, \mathcal{Q} becomes

$$\mathcal{Q}_Z = \mathbb{E}_{G|X} \left(\log \mathbb{P}(X | G, Z) + \log \mathbb{P}(G | Z) \right)$$

- \hat{Z} maximizes the posterior probability of connection

$$\hat{Z} = \arg \max_Z \left(\mathcal{Q}_Z \right) = \arg \max_Z \left\{ \mathbb{E}_{G|X} \left(\log \mathbb{P}(G | Z) \right) \right\}$$

- Involves the tricky term

$$\mathbb{E}_{G|X} \left(|L_G| \right)$$

Connections with the fixed graph model [2]

- Consider the Multivariate Gaussian Model

$$X_i \sim \mathcal{N}(\mu_i, \Sigma), \quad \mu_i \in \mathbb{R}^p \quad \Sigma \in \mathcal{S}_+^p \quad i = 1, 2, \dots, n$$

- Consider that the observations are connected by a given graph G
- Regularized Mean estimation problem:

$$\hat{M}_\alpha = \underset{M}{\operatorname{argmin}} \|X - M\|_F^2 + \alpha \operatorname{tr}(M^T \mathcal{L}_S M)$$

$$\text{where } \mathcal{L}_S = \frac{D - A}{\frac{1}{n} \sum_i d_i}$$

- In our setting, would it be $X \mid \mu, \mu \sim \mathcal{N}(0, \tau)$?

References

- [1] Dmitry Kobak and Philipp Berens. The art of using t-sne for single-cell transcriptomics. *bioRxiv*, 2018.
- [2] Tianxi Li, Cheng Qian, Elizaveta Levina, and Ji Zhu. High-dimensional gaussian graphical models on network-linked data. *Journal of Machine Learning Research*, 21(74):1–45, 2020.
- [3] L. McInnes, J. Healy, and J. Melville. Umap: Uniform manifold approximation and projection for dimension reduction. *Arxiv*, (1802.03426):1–63, 2018.
- [4] Laurens van der Maaten and Geoffrey Hinton. Visualizing Data using t-SNE. *Journal of Machine Learning Research*, 9(Nov):2579–2605, 2008.