

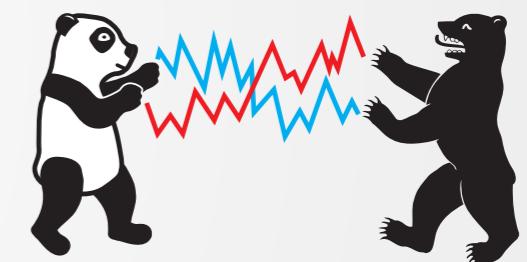
# Dim Reduction VizTech

Elizaveta Zinovyeva

Lucas Umann

Bingling WANG

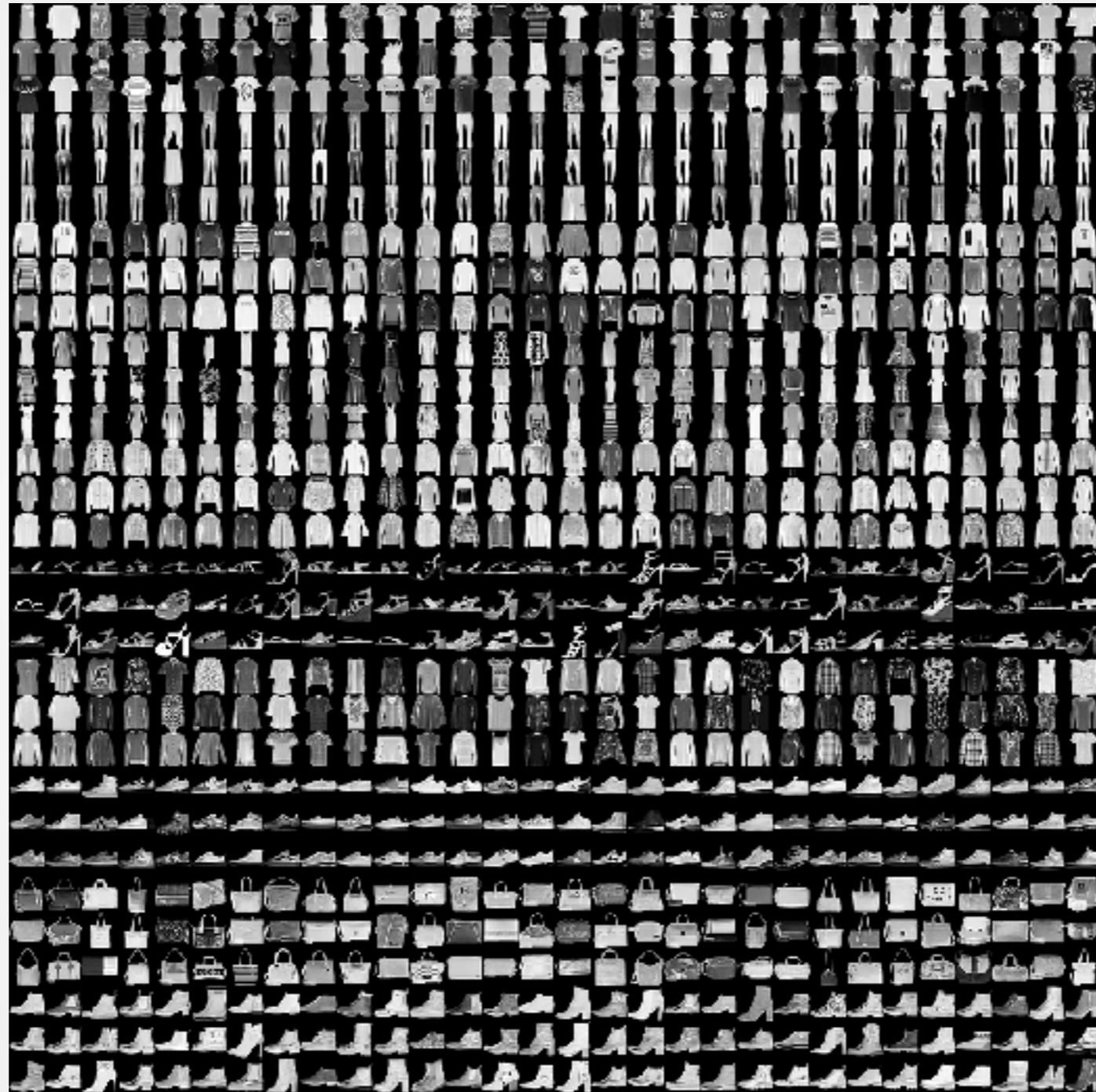
Wolfgang Karl Härdle



Ladislaus von Bortkiewicz Professor of Statistics  
Humboldt-Universität zu Berlin  
[lvb.wiwi.hu-berlin.de](http://lvb.wiwi.hu-berlin.de)

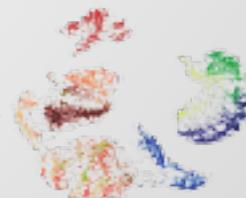


# Fashion-MNIST

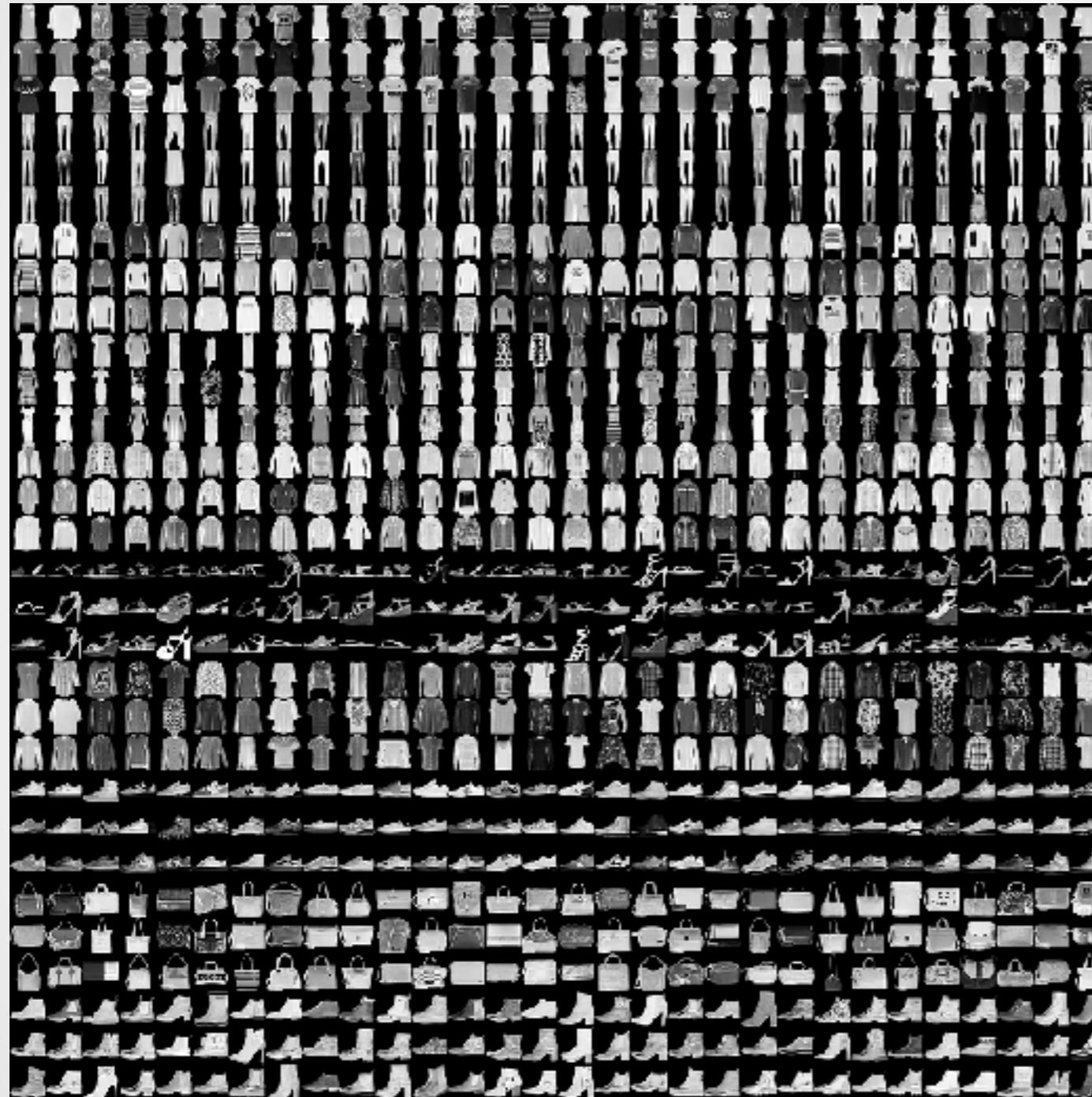


Fashion MNIST dataset

Source: [Zalando Research](#)



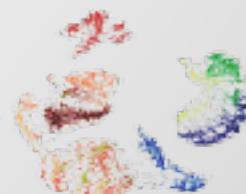
# Fashion-MNIST



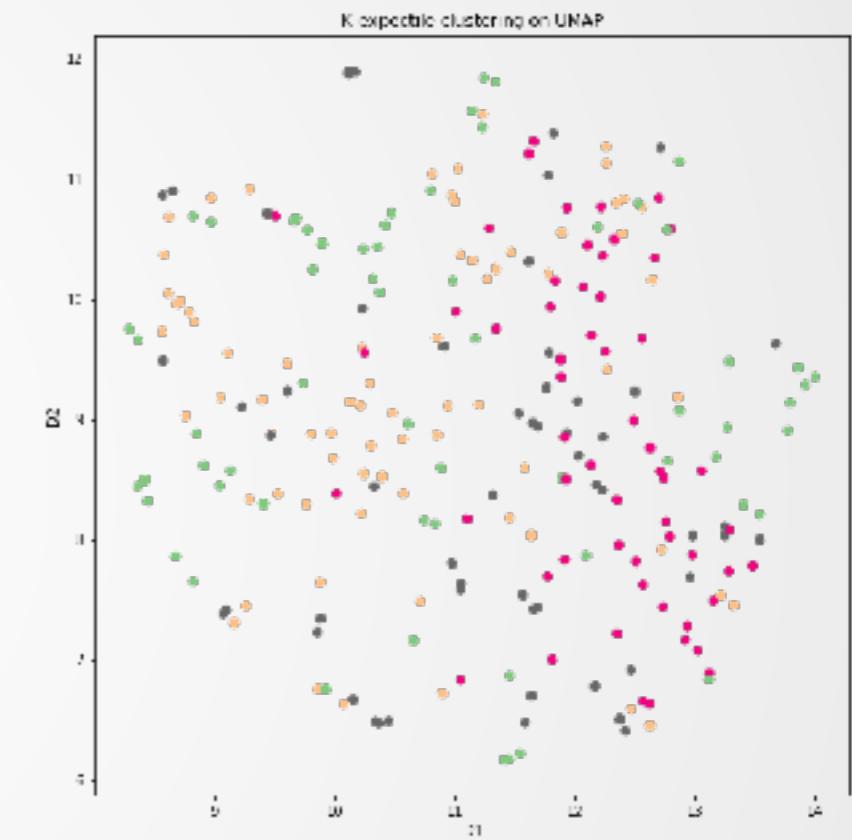
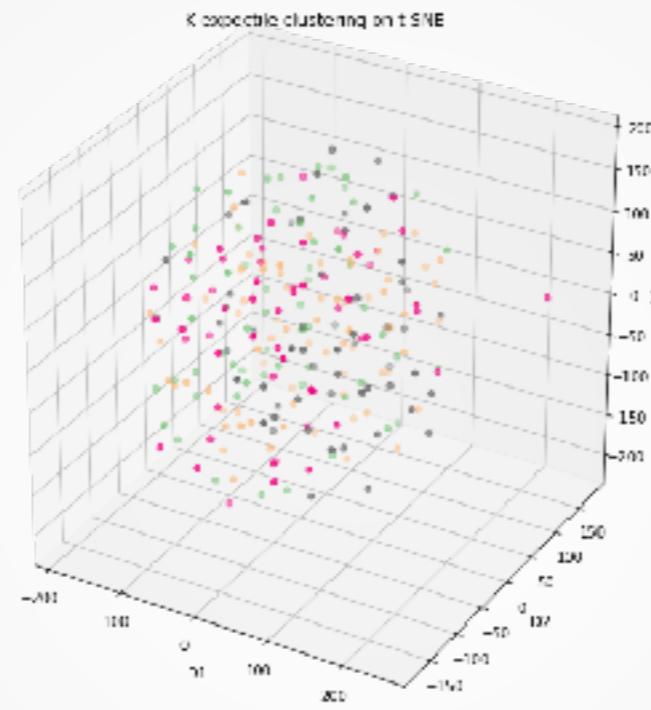
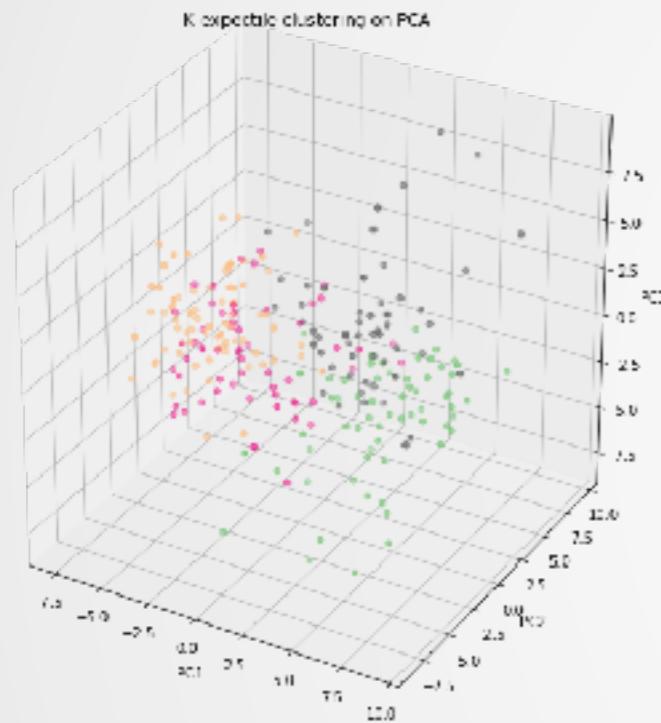
Fashion MNIST dataset

Source: [Zalando Research](#)

- Zalando article images
- 60.000 training, 10.000 test
- 28x28 grayscale
- dim = 784
- No interpretability of raw data by human observer



# Classification



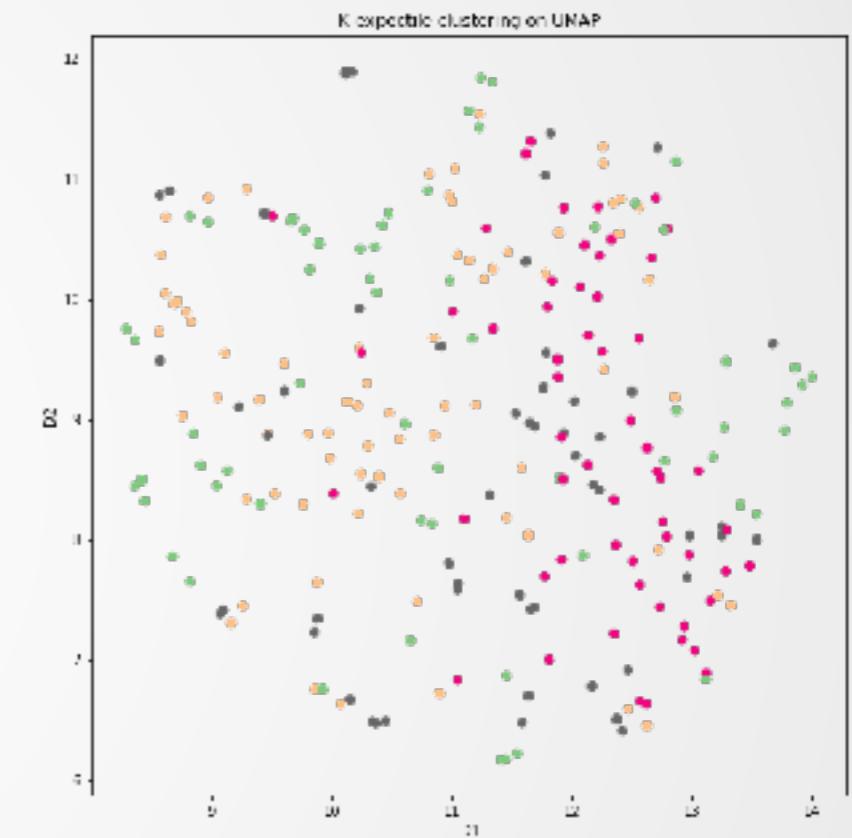
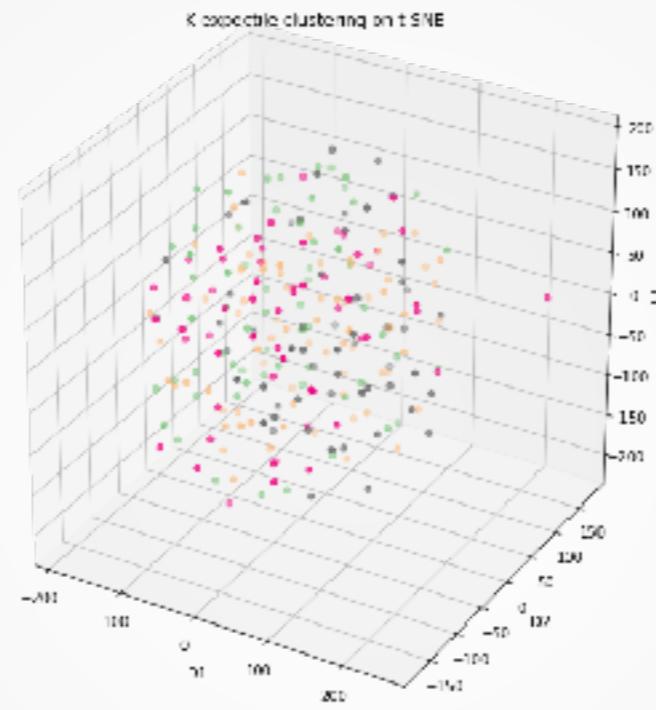
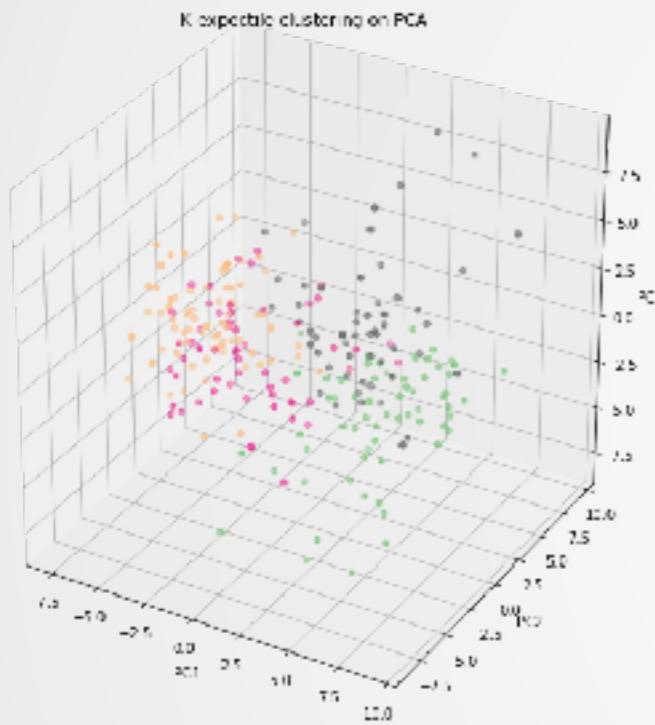
n\_neighbors=5, min\_dist =0.1

Data Source: CoinGecko crypto returns 20190730-20200117

248 observations, 998 dimensions reduced to 3



# Classification

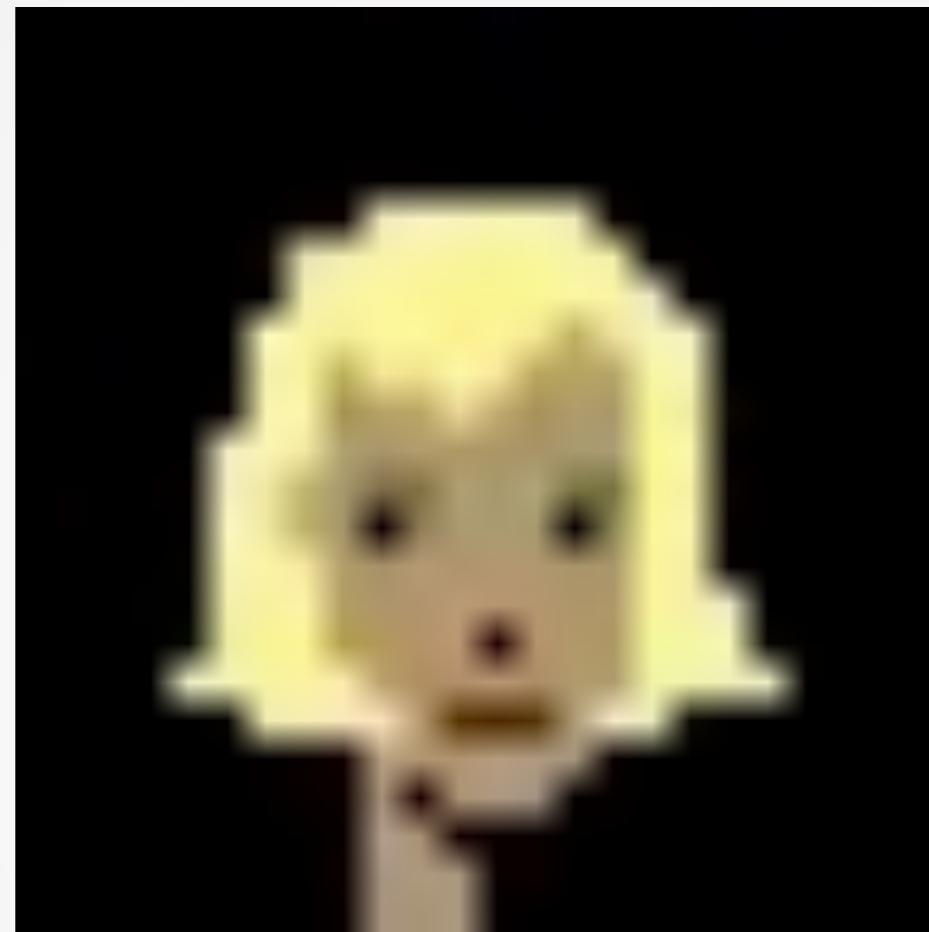


n\_neighbors=5, min\_dist =0.1

- Pattern similarities between crypto returns are hard to describe in high dim
- Dim reduction helps to describe them in different ways

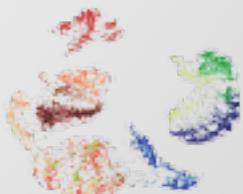


# CryptoPunk



CryptoPunk Images  
Source: [larvalabs.com](https://larvalabs.com)

- Cryptopunk a NFT non-fungible token
- Are there clusters in high dim?
- Dim reduction provides good start



# Clustering in High Dimensions: 4 problems

Curse of dimensionality



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Curse of dimensionality

Distances less precise:

$$\lim_{dim \rightarrow \infty} \frac{dist_{max} - dist_{min}}{dist_{min}} = 0$$



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$dist_{min}/dist_{max}$  min/max distance  
between all data points



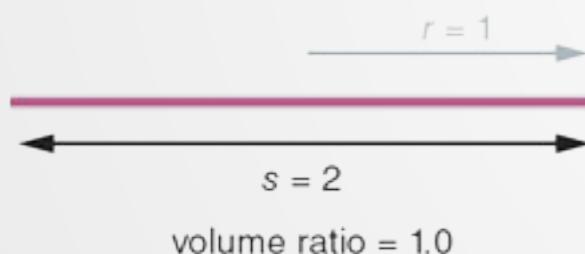
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1-ball in 1-cube

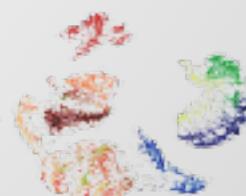
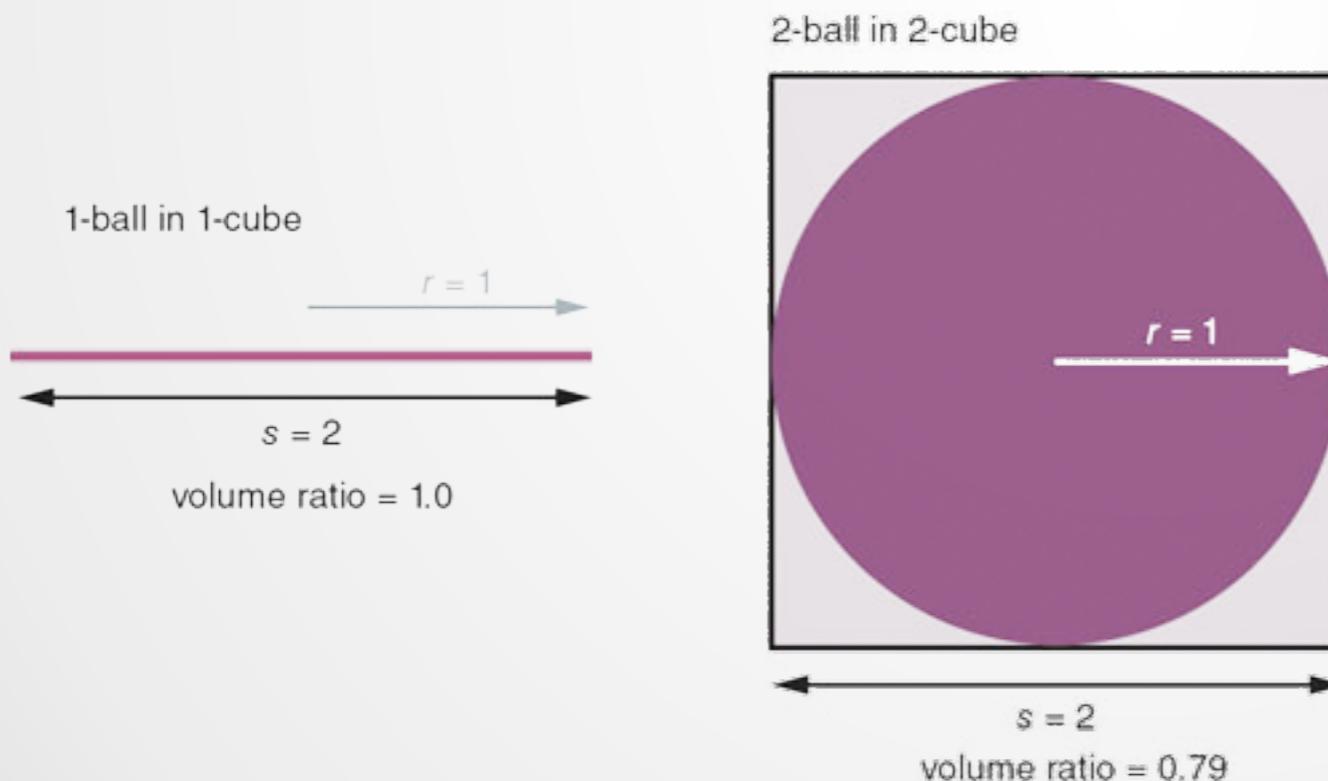


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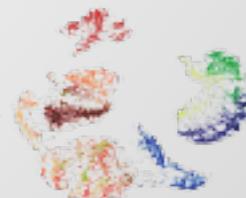
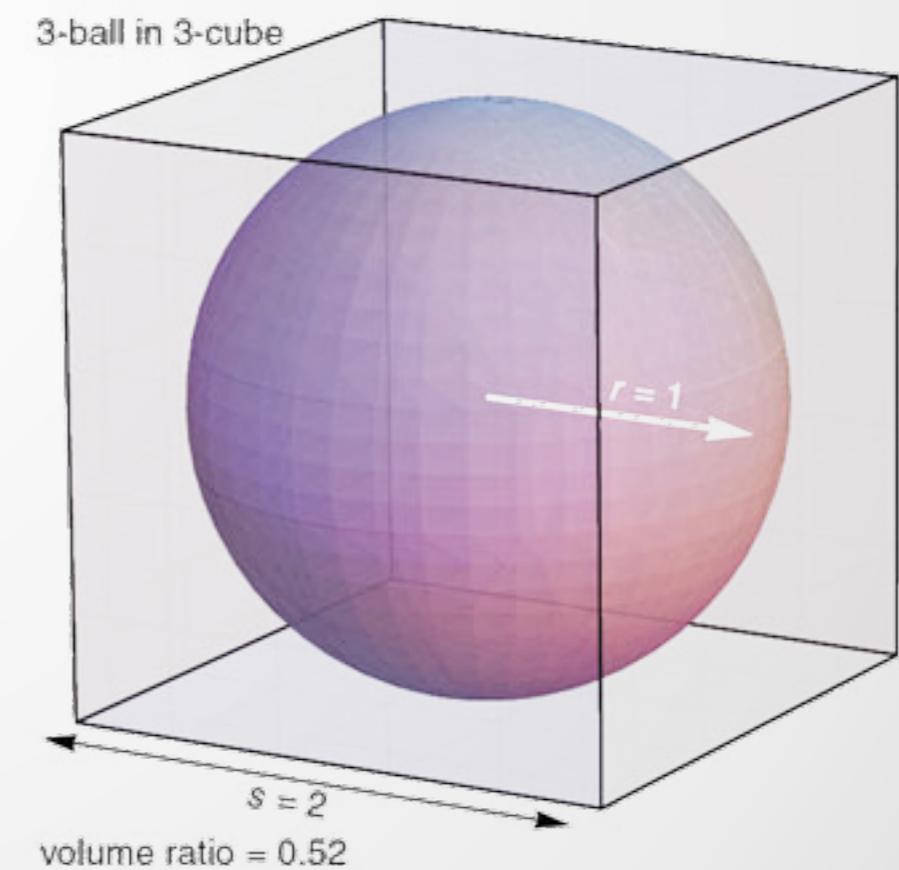
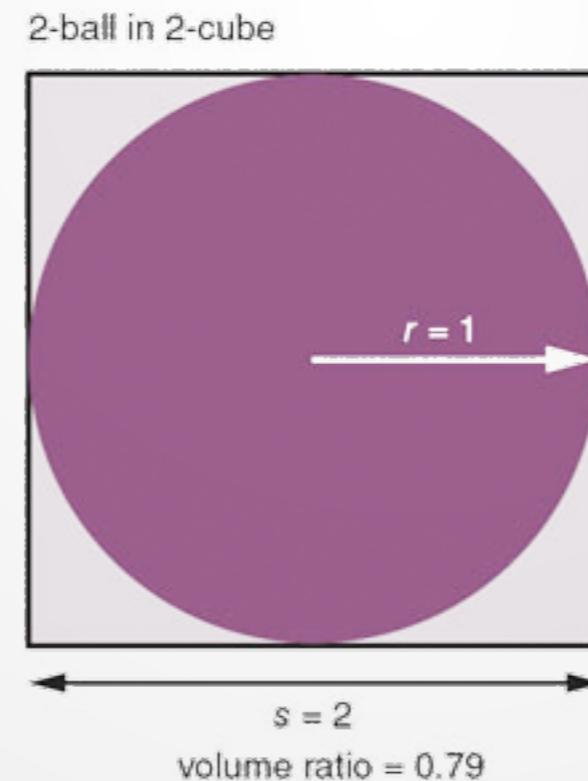
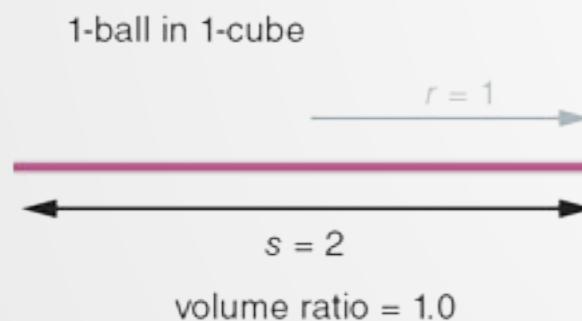


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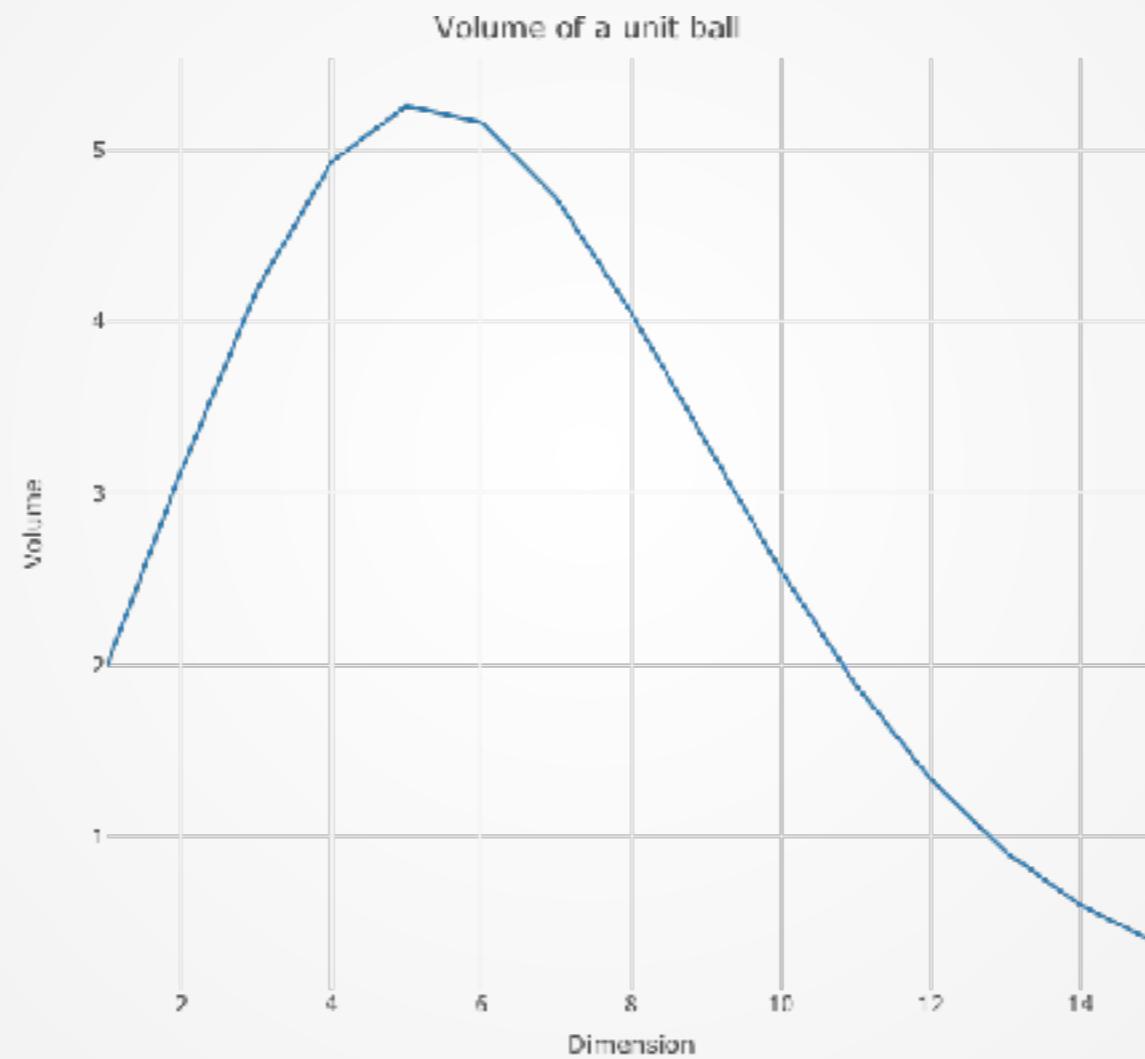
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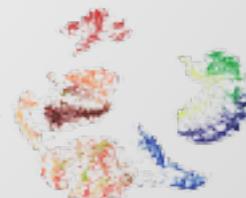
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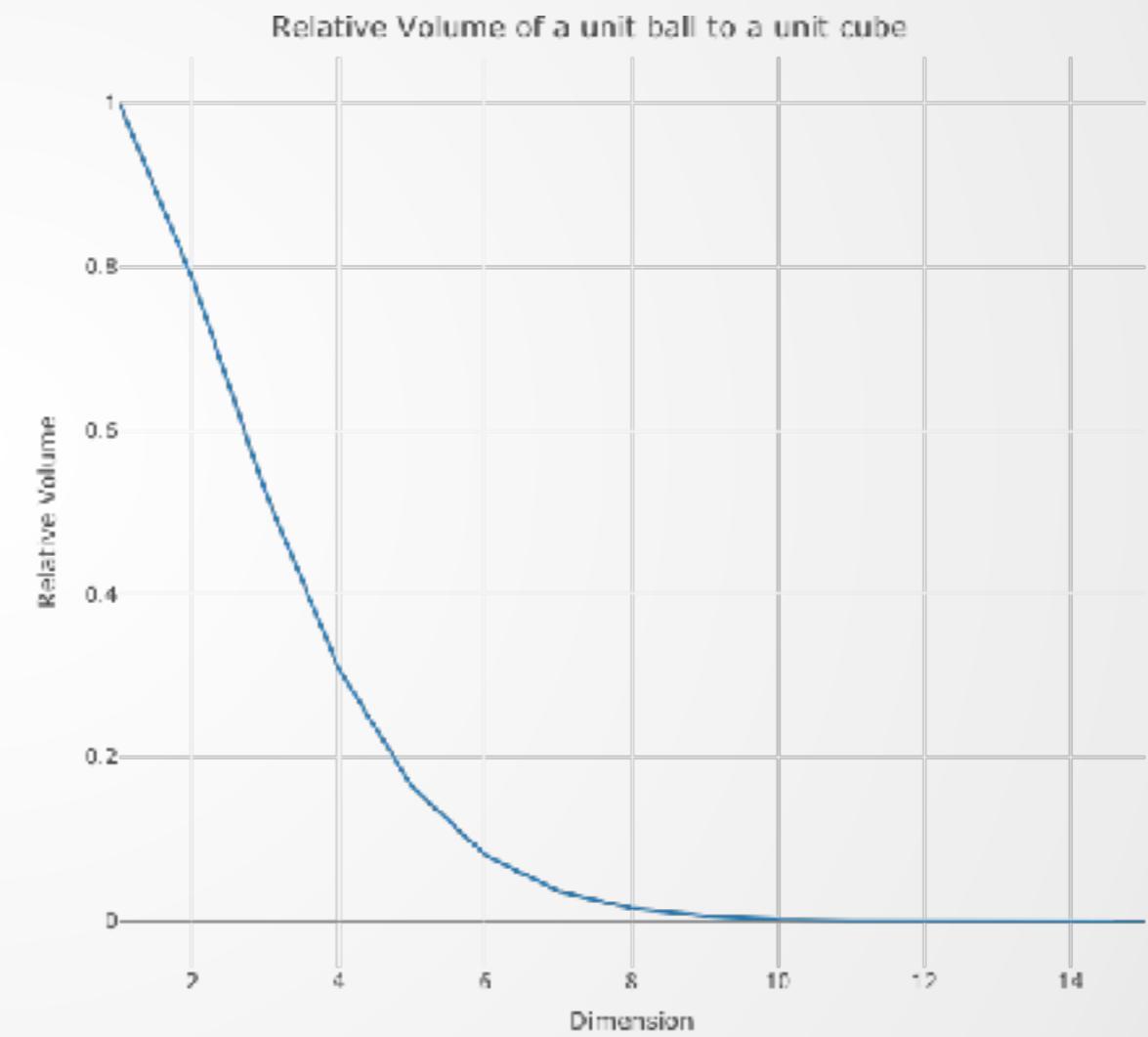
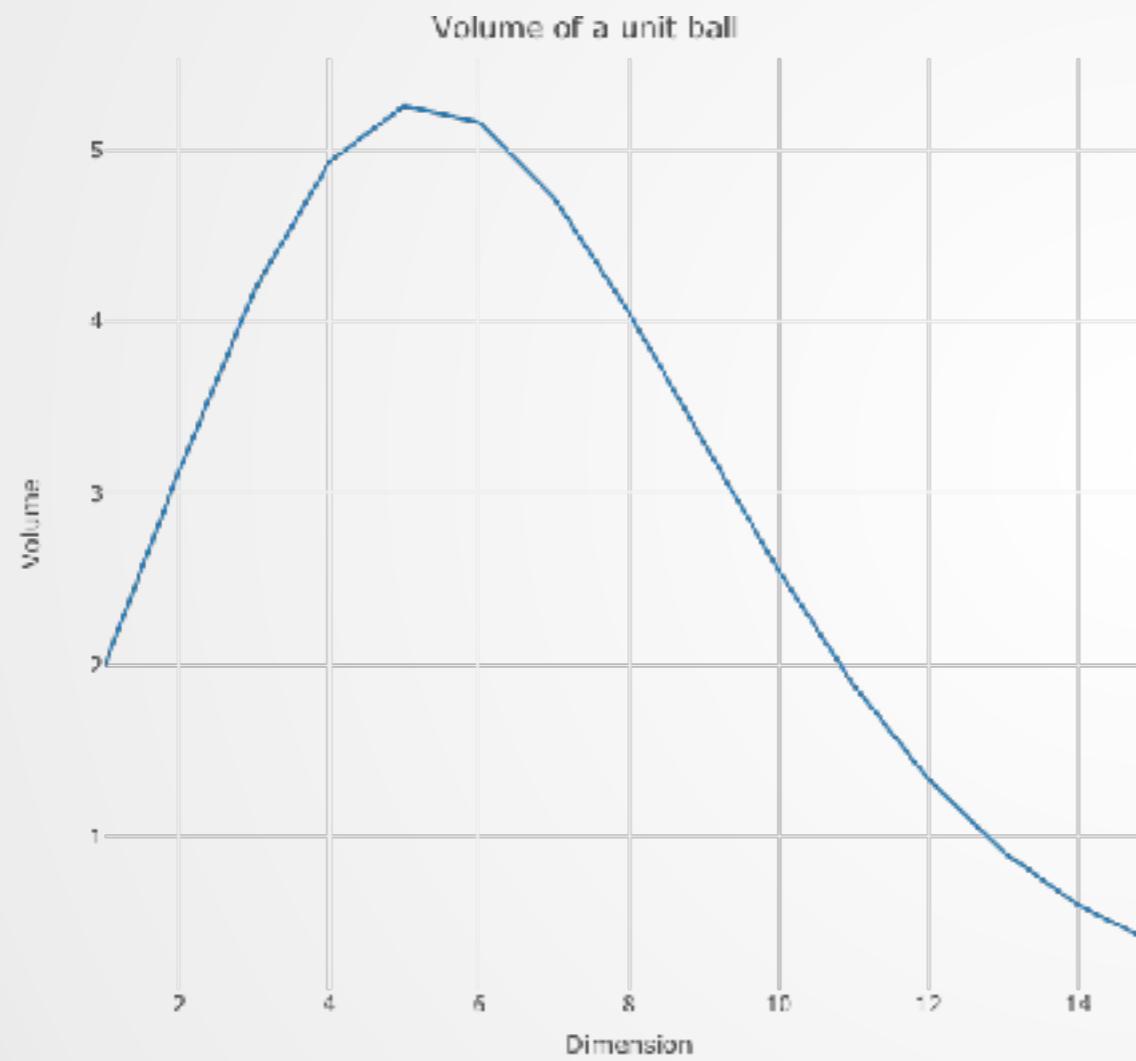
# Clustering in High Dimensions: 4 problems



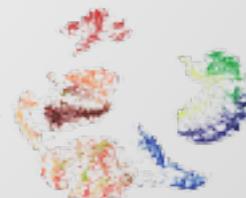
Volume of a  $d$ -dimensional Unit Ball:  $V_d = \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2} + 1)}$



# Clustering in High Dimensions: 4 problems



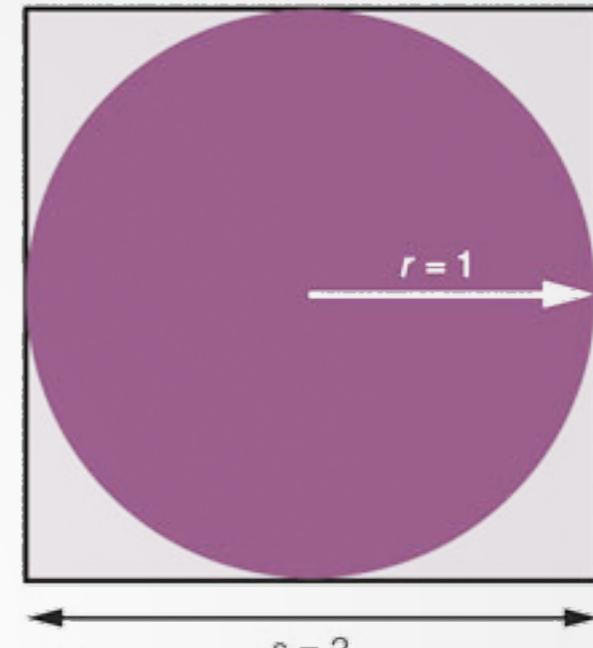
Volume of a  $d$ -dimensional Unit Cube (side length = 2):  $V_d = 2^d$



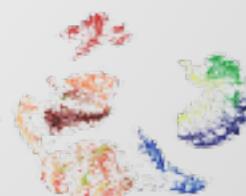
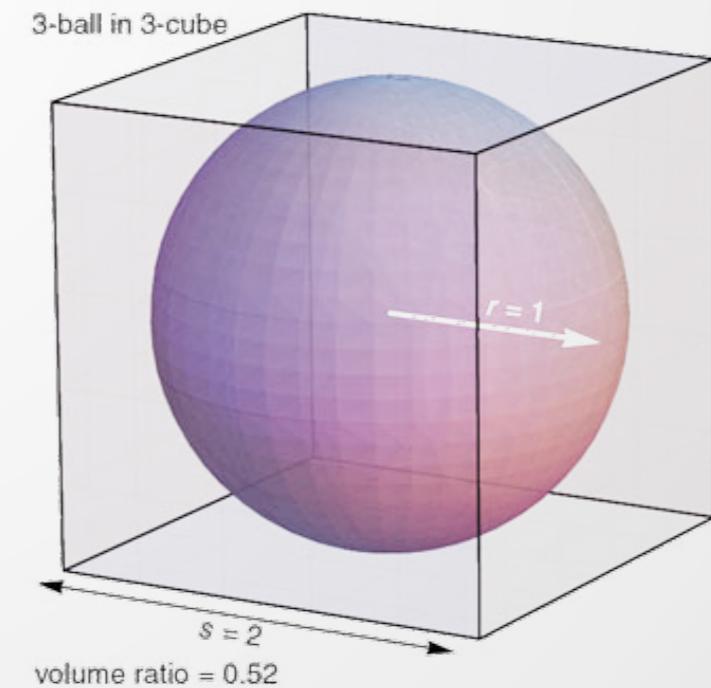
## Clustering in High Dimensions: 4 problems

- Assume  $n = 100$  data points uniformly distributed in unit cube
- Consider unit ball around middle point
- 2 dim.: 79 points inside ball
- 5 dim.: 16 points
- 15 dim.: need 100000 data points to get 1 inside

2-ball in 2-cube



3-ball in 3-cube

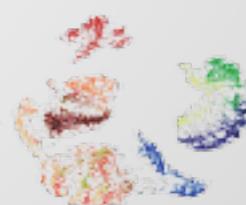


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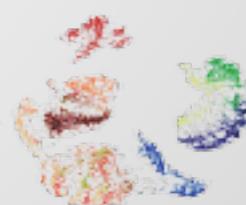
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Dim reduction increases  
accuracy. VizTech to the  
rescue!



# Outline

1. Motivation
2.  $t$ -distributed Stochastic Neighbor Embedding ( $t$ -SNE)
3.  $t$ -SNE example
4. Uniform Manifold Approximation and Projection (UMAP)
5. UMAP example
6.  $t$ -SNE vs. UMAP



## t-SNE VizTech

- t-SNE *t*-distributed stochastic neighbor embedding
- Non-linear VizTech with preservation of local structure
- Embedding: preserve as much *significant structure* of high dim data as *possible* in a low dim

$$X = \{x_1, x_2, \dots, x_n\} \longrightarrow Y = \{y_1, y_2, \dots, y_n\}$$

- $x_i$  in  $\mathbb{R}^k$ ,  $y_i$  in  $\mathbb{R}^l$ ,  $k > l$



t-SNE of Fashion MNIST. Source: [Researchgate](#)

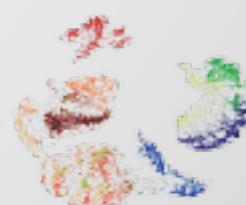


## t-SNE VizTech

- Transform high dim (HD) distances into conditional probabilities:

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

- ▶ shows how close is the point  $x_j$  to the point  $x_i$  with Gaussian distribution around  $x_i$  with deviation  $\sigma_i$



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► shows how close is the point  $x_j$  to the point  $x_i$  with Gaussian distribution around  $x_i$  with deviation  $\sigma_i$

- $\sigma_i$  must be chosen for each data point individually.
  - it is chosen such that points in dense areas are given a smaller variance than points in sparse areas.
  - $\sigma_i$  induces a probability distribution  $P_i$
  - $t$ -SNE performs binary search for the value of  $\sigma_i$  that produces  $P_i$  with fixed perplexity specified by a user

$$Perp(P_i) = 2^{H(P_i)}, \quad H(P_i) = - \sum_j p_{j|i} \log_2 \{p_{j|i}\}$$



## t-SNE VizTech

- Symmetrized version of conditional similarity in HD:

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$$



## t-SNE VizTech

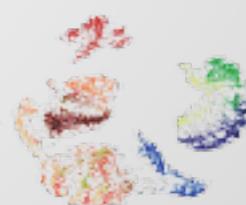
- Symmetrized version of conditional similarity in HD:

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- Similarity in the low dim (LD) space:

► t-student with 1 degree of freedom

$$q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq l} (1 + \|y_k - y_l\|^2)^{-1}}$$



## t-SNE VizTech

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- Minimise Kullback-Leibler divergence using gradient descent

$$C = KL(P || Q) = \sum_i \sum_j p_{ij} \log \left( \frac{p_{ij}}{q_{ij}} \right)$$

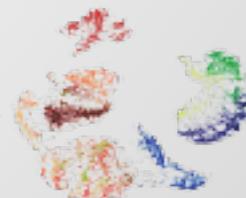
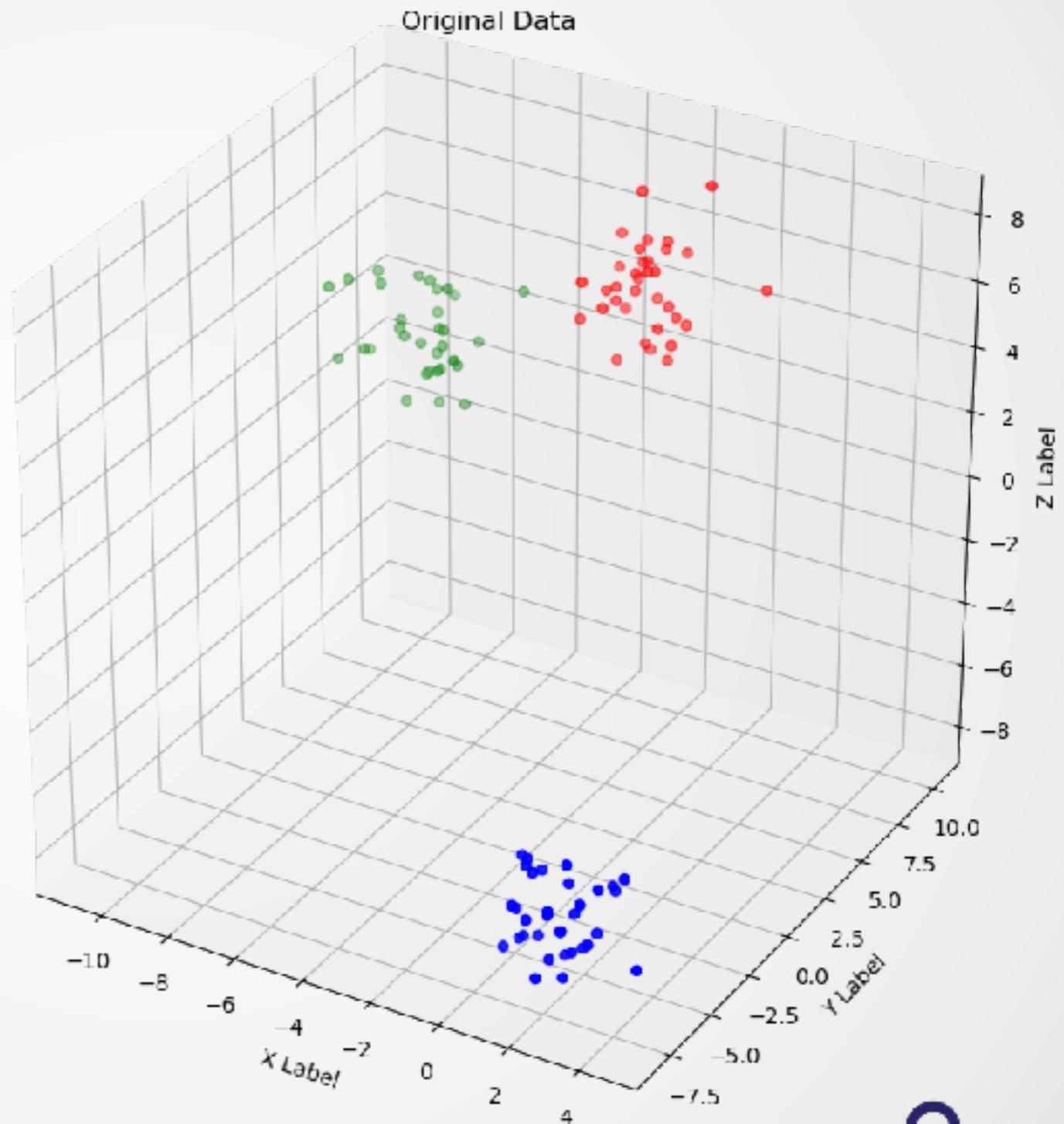


Kullback, Leibler in BBI

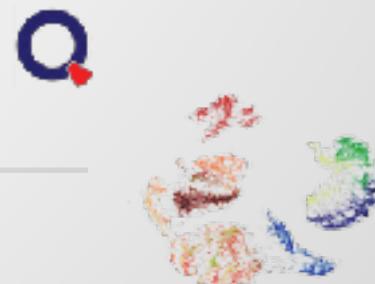
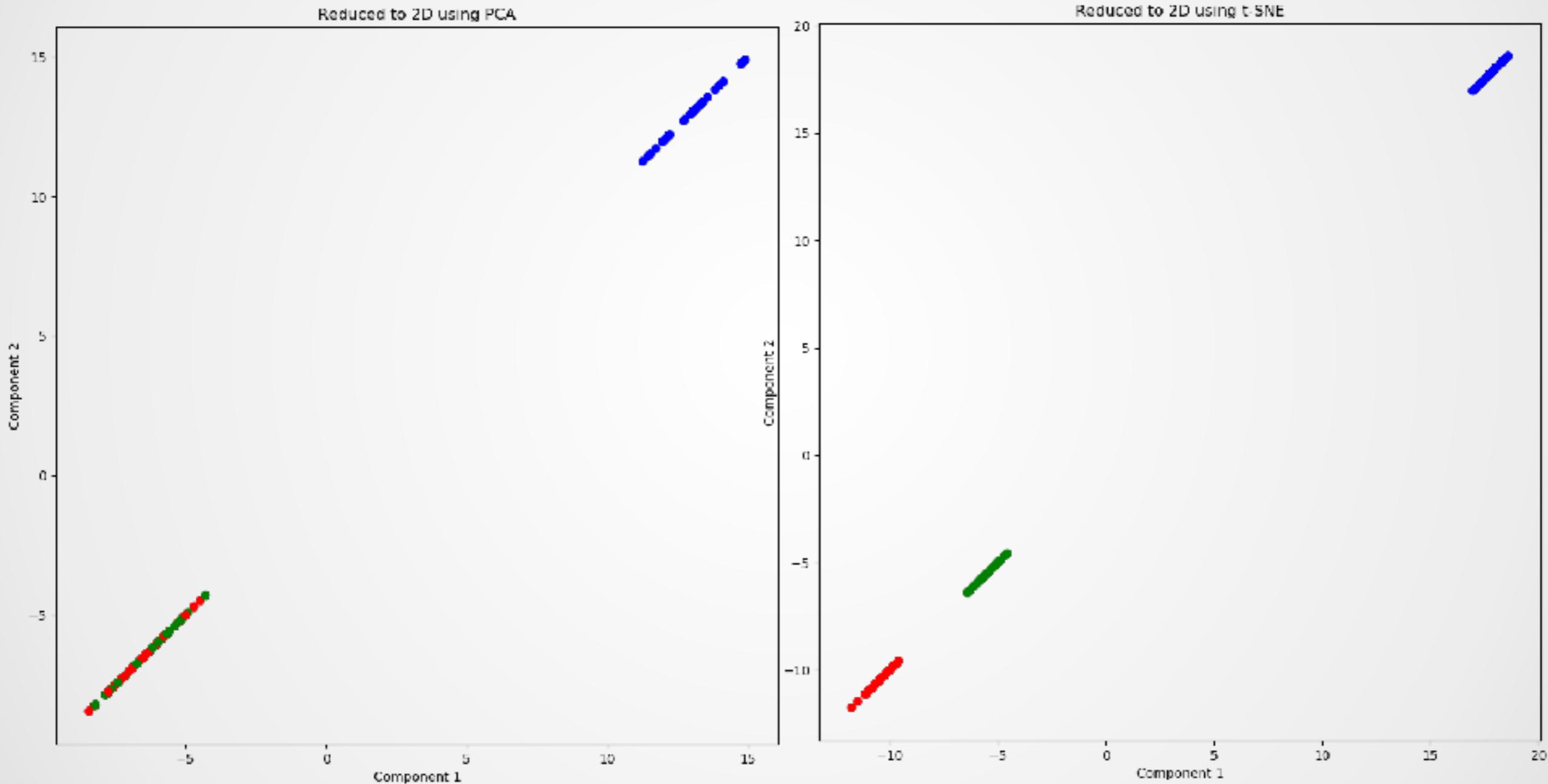


## t-SNE vs PCA

- Original 3D data
  - ▶ 3 clusters
  - ▶ separable in 3D space
  - ▶ t-SNE aims to preserve local structure



## t-SNE vs PCA



## t-SNE algorithm

---

### Algorithm 1: Simple version of t-Distributed Stochastic Neighbor Embedding.

---

**Data:** data set  $\mathcal{X} = \{x_1, x_2, \dots, x_n\}$ ,  
 cost function parameters: perplexity  $Perp$ ,  
 optimization parameters: number of iterations  $T$ , learning rate  $\eta$ , momentum  $\alpha(t)$ .  
**Result:** low-dimensional data representation  $\mathcal{Y}^{(T)} = \{y_1, y_2, \dots, y_n\}$ .

**begin**

compute pairwise affinities  $p_{j|i}$  with perplexity  $Perp$  (using Equation 1)

set  $p_{ij} = \frac{p_{j|i} + p_{i|j}}{2n}$

sample initial solution  $\mathcal{Y}^{(0)} = \{y_1, y_2, \dots, y_n\}$  from  $\mathcal{N}(0, 10^{-4}I)$

**for**  $t=1$  **to**  $T$  **do**

compute low-dimensional affinities  $q_{ij}$  (using Equation 4)

compute gradient  $\frac{\delta C}{\delta \mathcal{Y}}$  (using Equation 5)

set  $\mathcal{Y}^{(t)} = \mathcal{Y}^{(t-1)} + \eta \frac{\delta C}{\delta \mathcal{Y}} + \alpha(t) (\mathcal{Y}^{(t-1)} - \mathcal{Y}^{(t-2)})$

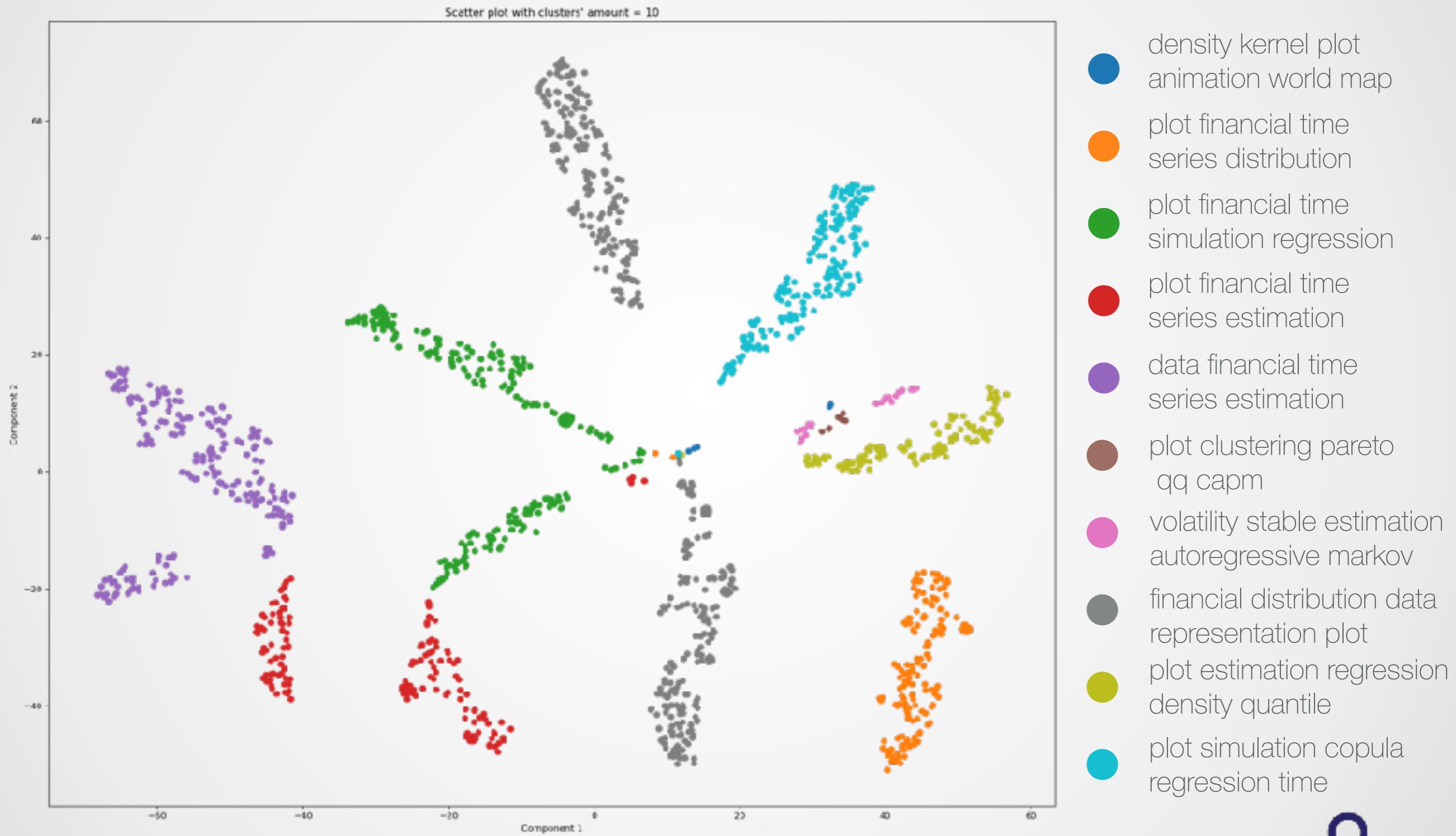
**end**

**end**

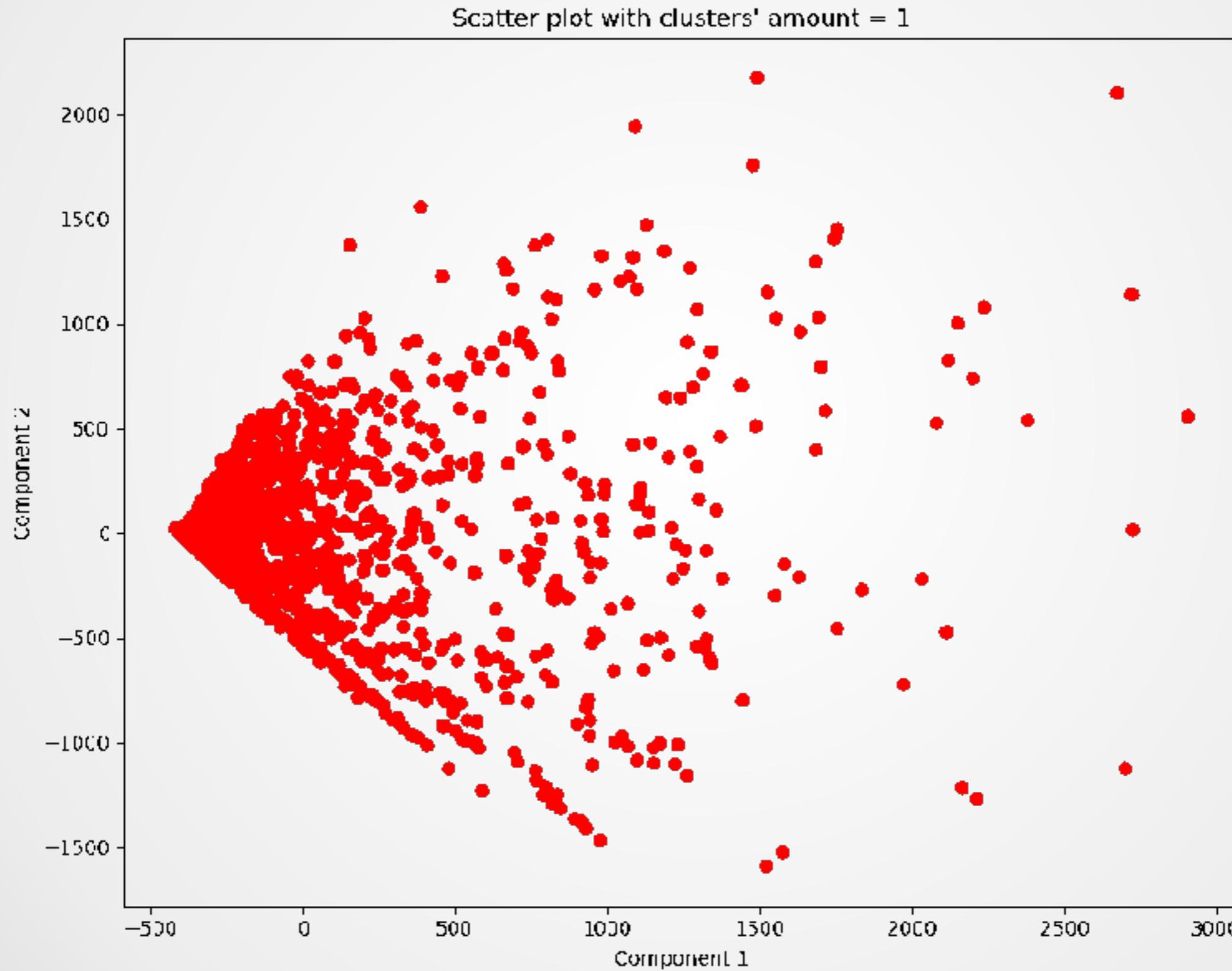
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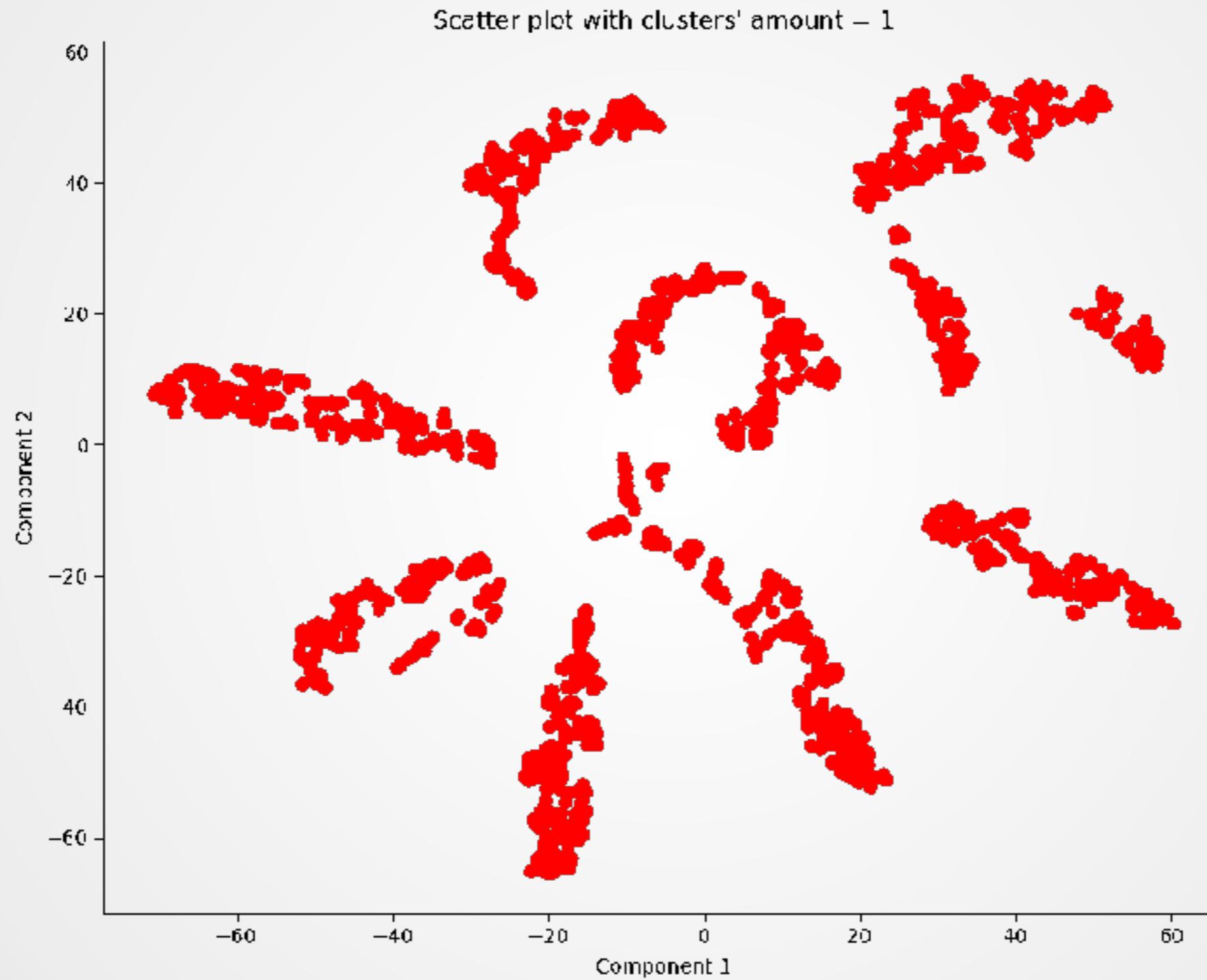
# t-SNE VizTech



## Dynamics of different amount of clusters (PCA)

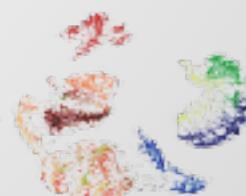


## Dynamics of different amount of clusters (t-SNE)



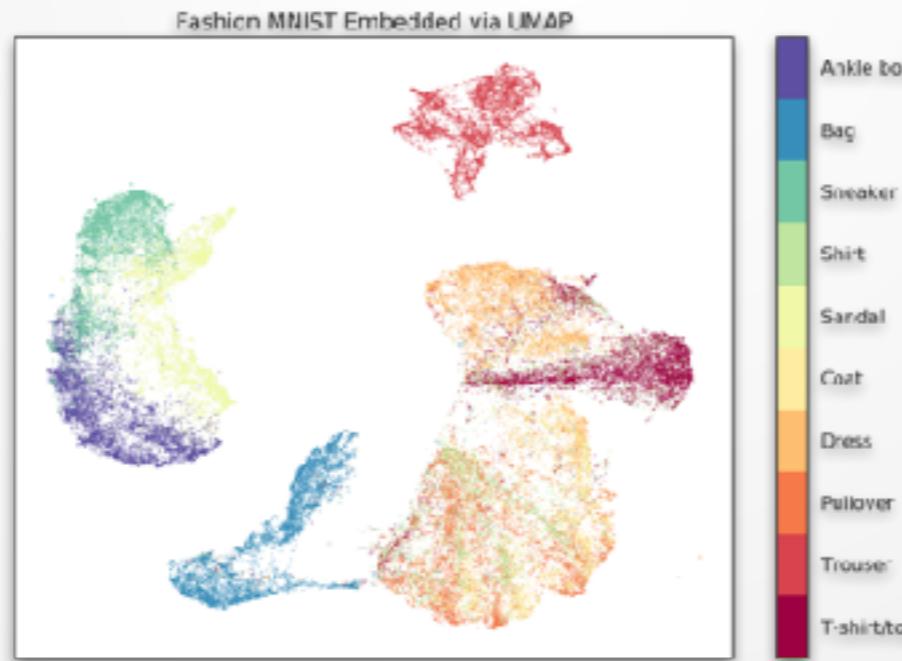
## t-SNE bottomline

- Useful if the underlying application has a taxonomy.
- Agglomerative hierarchical clustering algorithms are expensive in terms of their computational and storage requirements.
- Merges are final and cannot be undone later, preventing global optimisation and causing trouble for noisy, high-dimensional data.



## UMAP VizTech

- UMAP Uniform Manifold Approximation & Projection
- Preserves HD local structure as does *t*-SNE
- Often better at displaying global structure than *t*-SNE
- Constructs a topological representation of HD data
- For some LD representation, layout is optimized to minimize cross-entropy between HD & LD topological representations



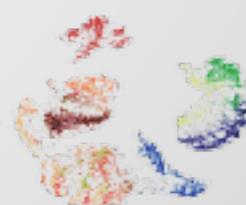
Source: [UMAP documentation](#)



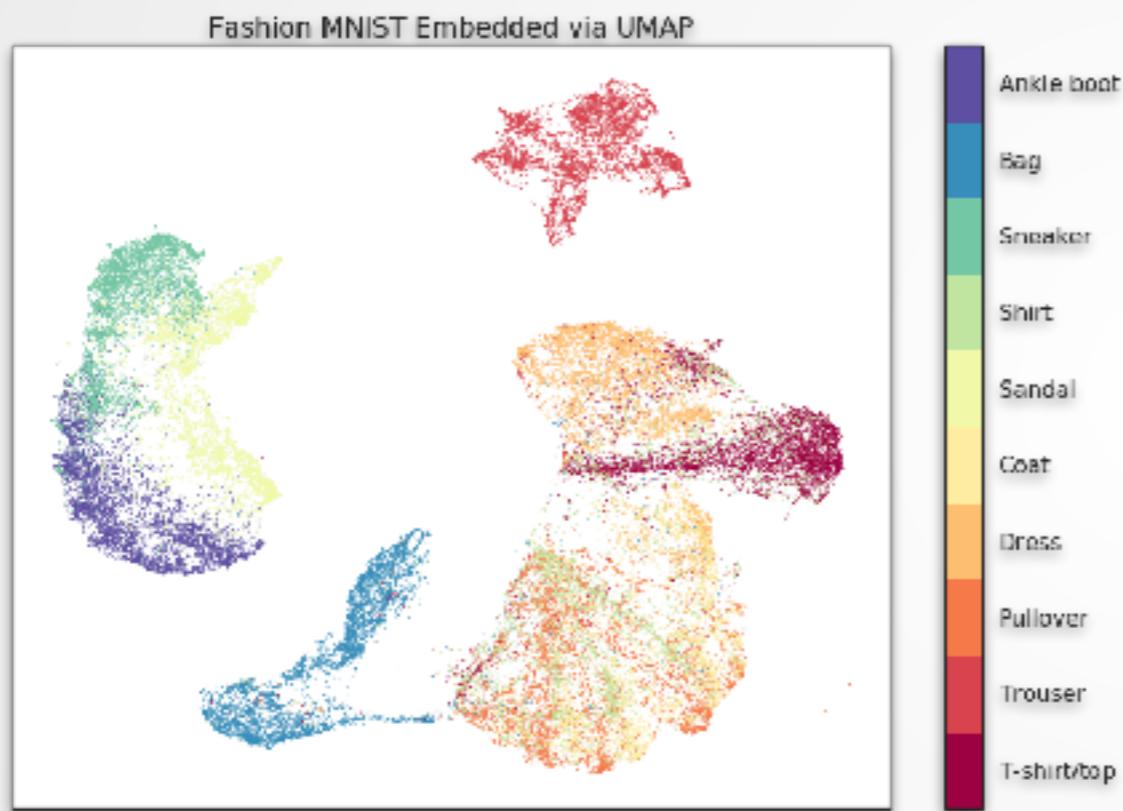
## UMAP VizTech



Source: [UMAP documentation](#)



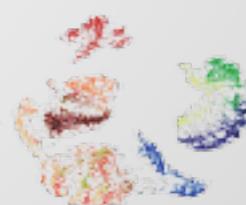
# UMAP VizTech



Source: [UMAP documentation](#)



t-SNE of Fashion MNIST. Source: [Researchgate](#)



## UMAP intuition

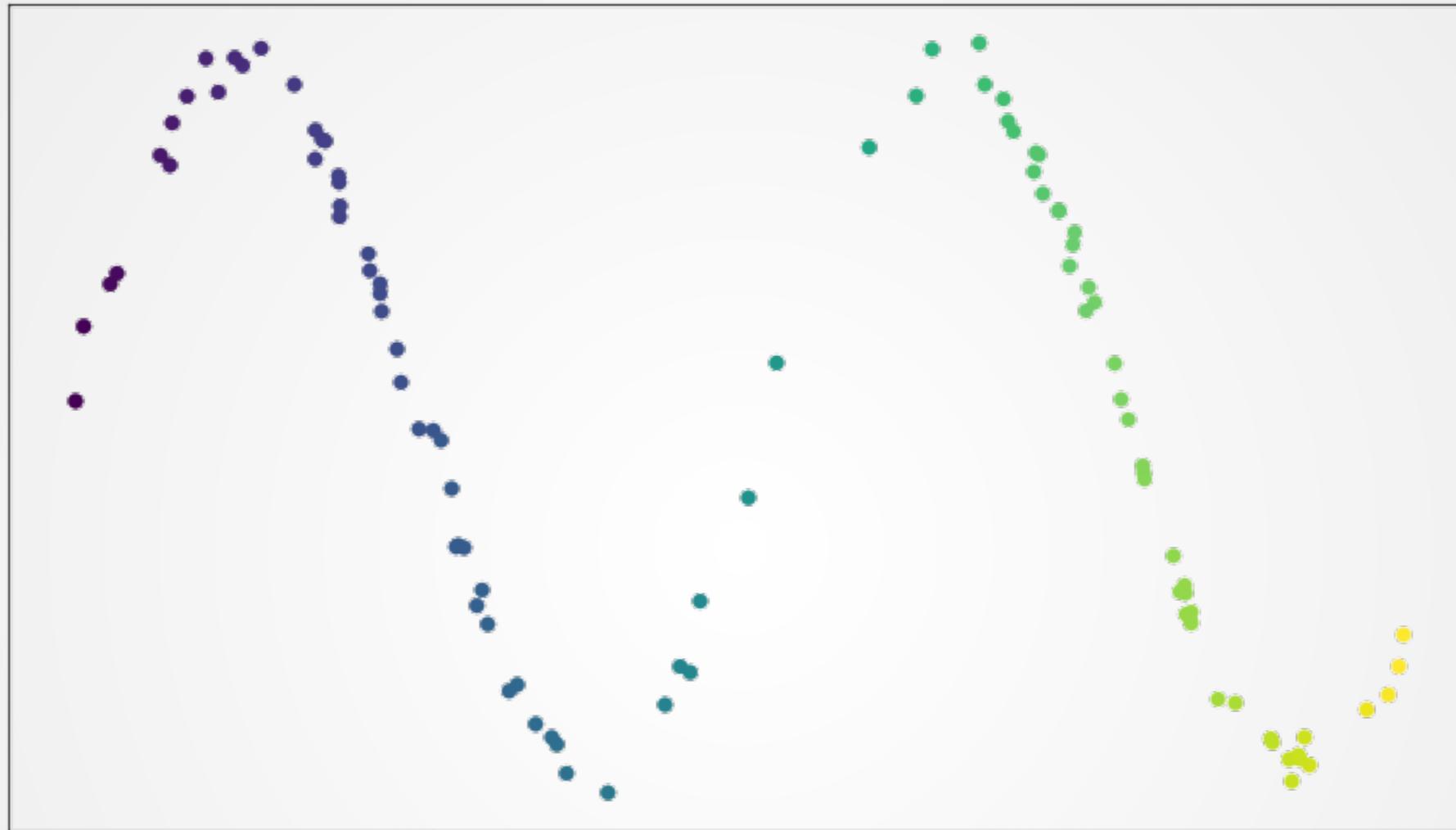
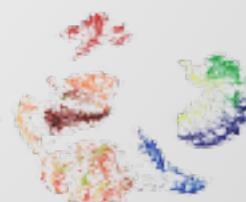


Image Source: [UMAP documentation](#)

Let us look at a nice sine curve.

Note that mesh points are not uniformly distributed



## UMAP intuition

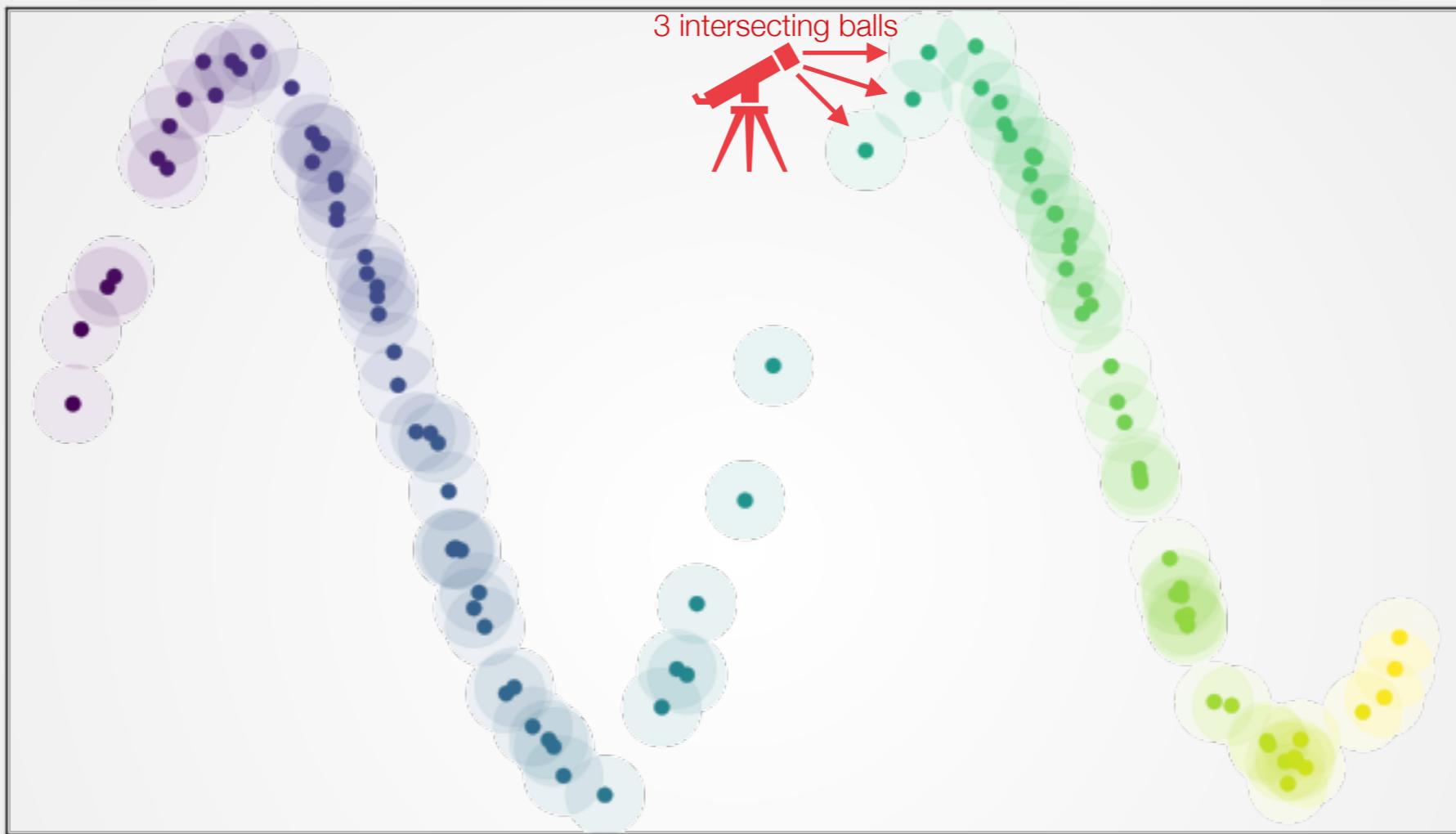


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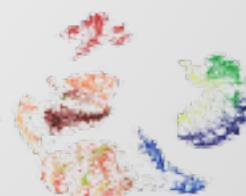
- Generate an open cover
- Way to approximate open cover: balls of fixed radius around data



## UMAP intuition



Look, how we convert balls into simplices!



## UMAP intuition

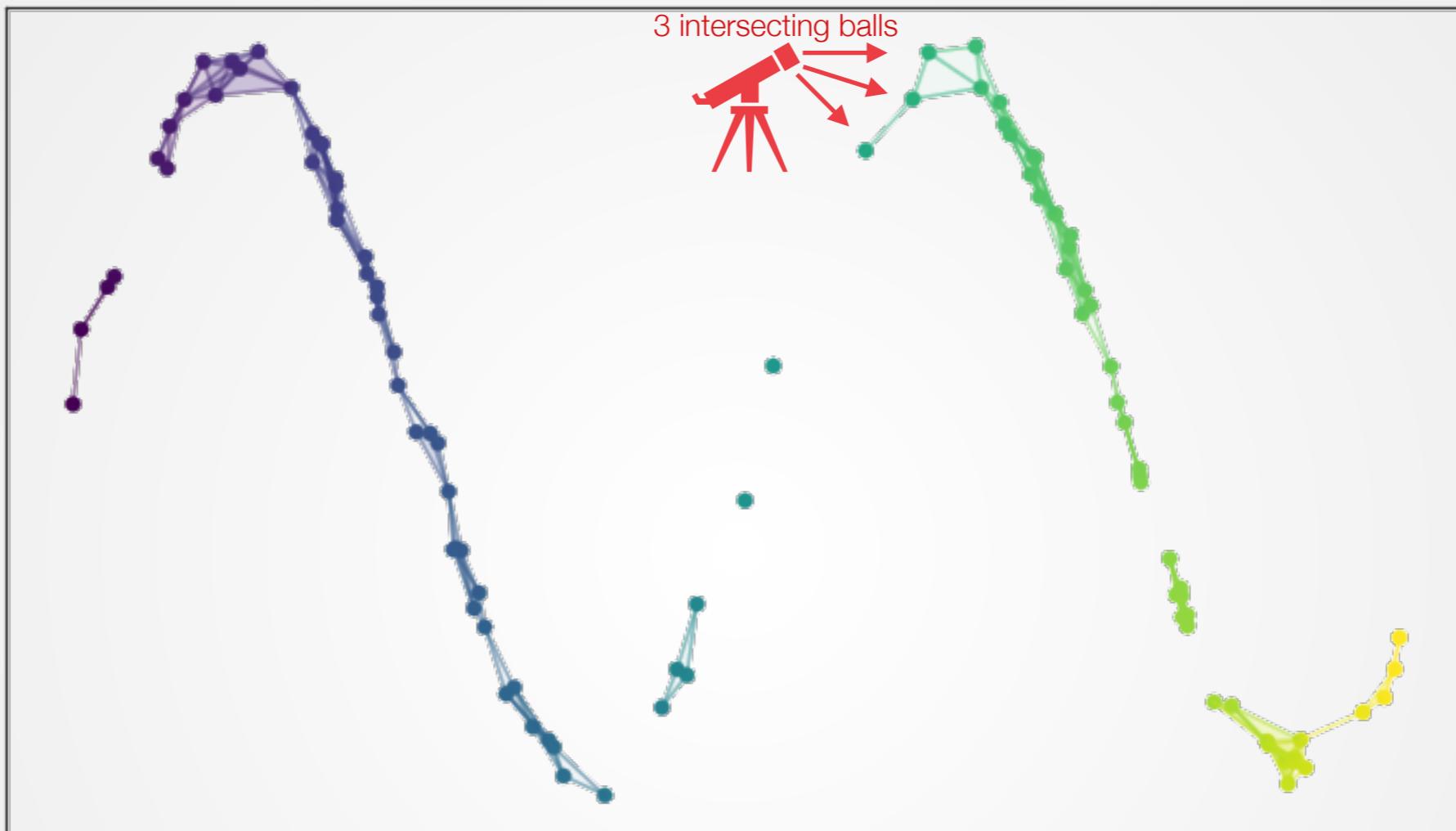


Image Source: [UMAP documentation](#)

Build simplicial complex of 0-, 1- and 2-simplices by connecting overlapping balls



## UMAP intuition



Image Source: [UMAP documentation](#)

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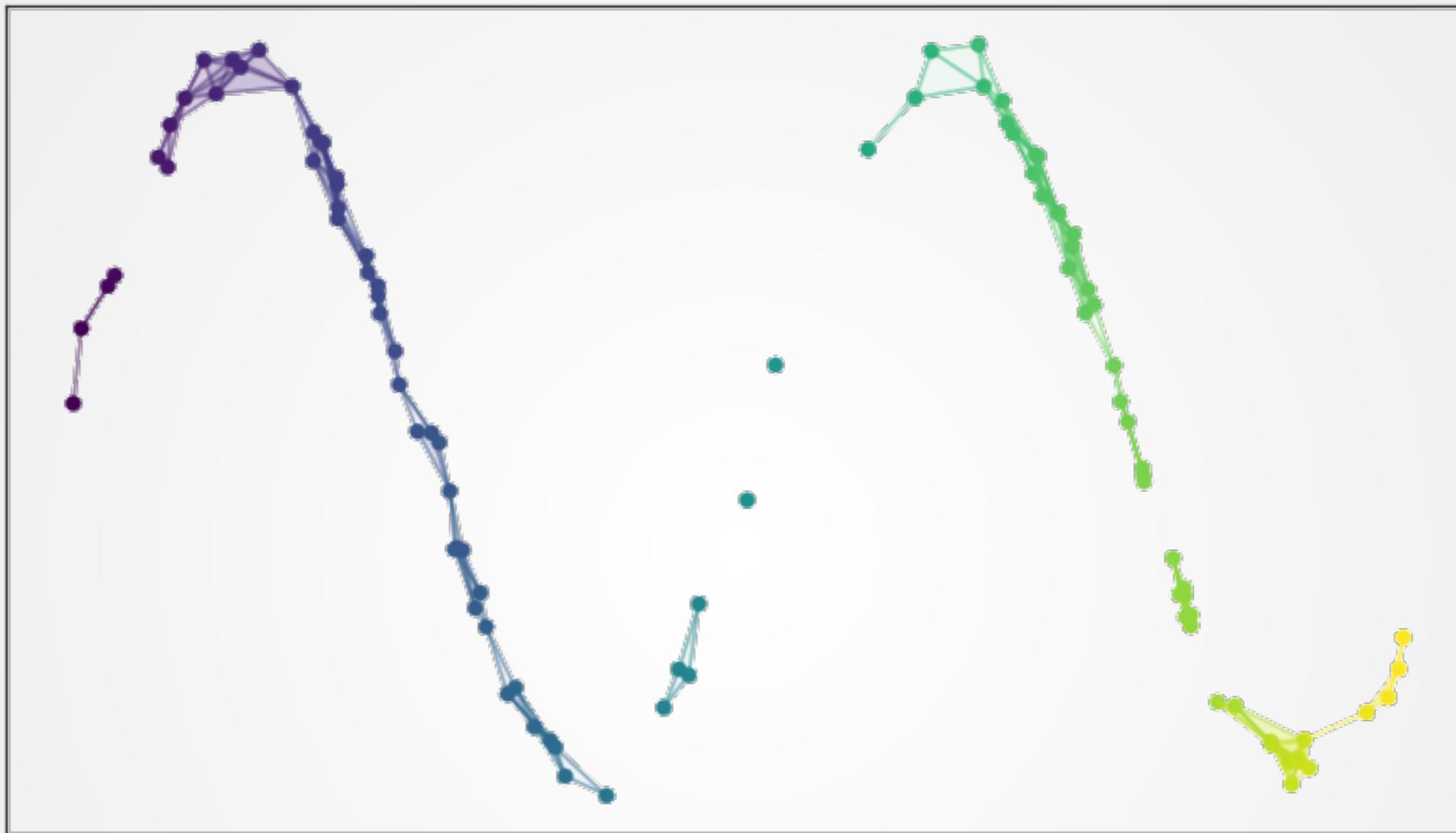


Image Source: [UMAP documentation](#)

- Build simplicial complex of 0-, 1- and 2-simplices
- Does a reasonable job of capturing fundamental topology



## UMAP intuition

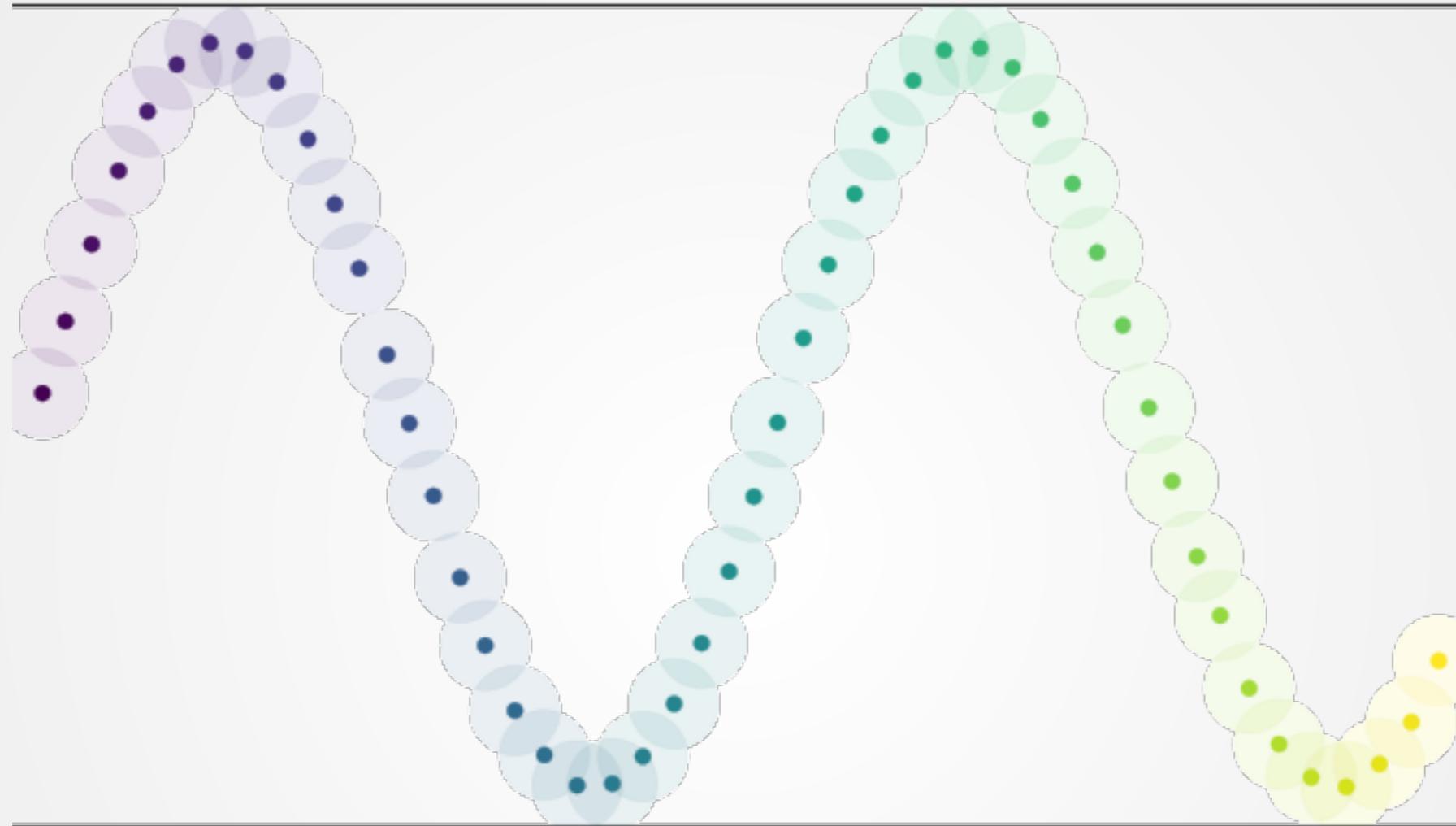
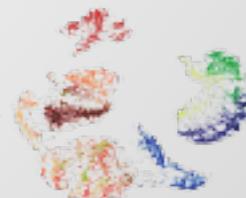


Image Source: [UMAP documentation](#)

- ◻ If data is uniformly distributed, open balls with the same radius work well
- ◻ But not in general!



## UMAP intuition

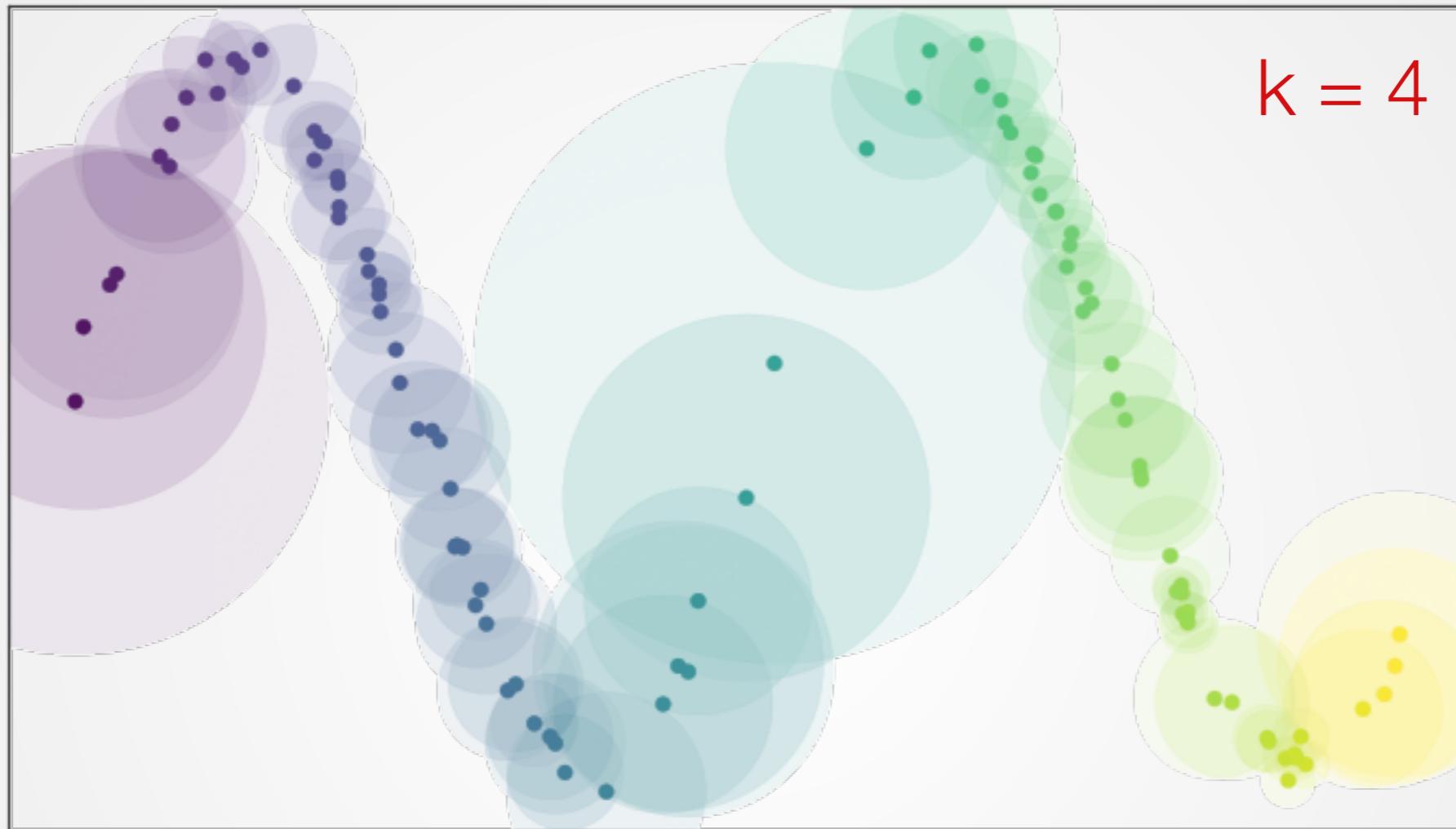


Image Source: [UMAP documentation](#)

- Let the „metric“ vary locally
- Still open balls with radius 1, but with varying metric
- Metric is chosen s.t. a ball of radius 1 touches  $k$  nearest neighbors



## UMAP intuition

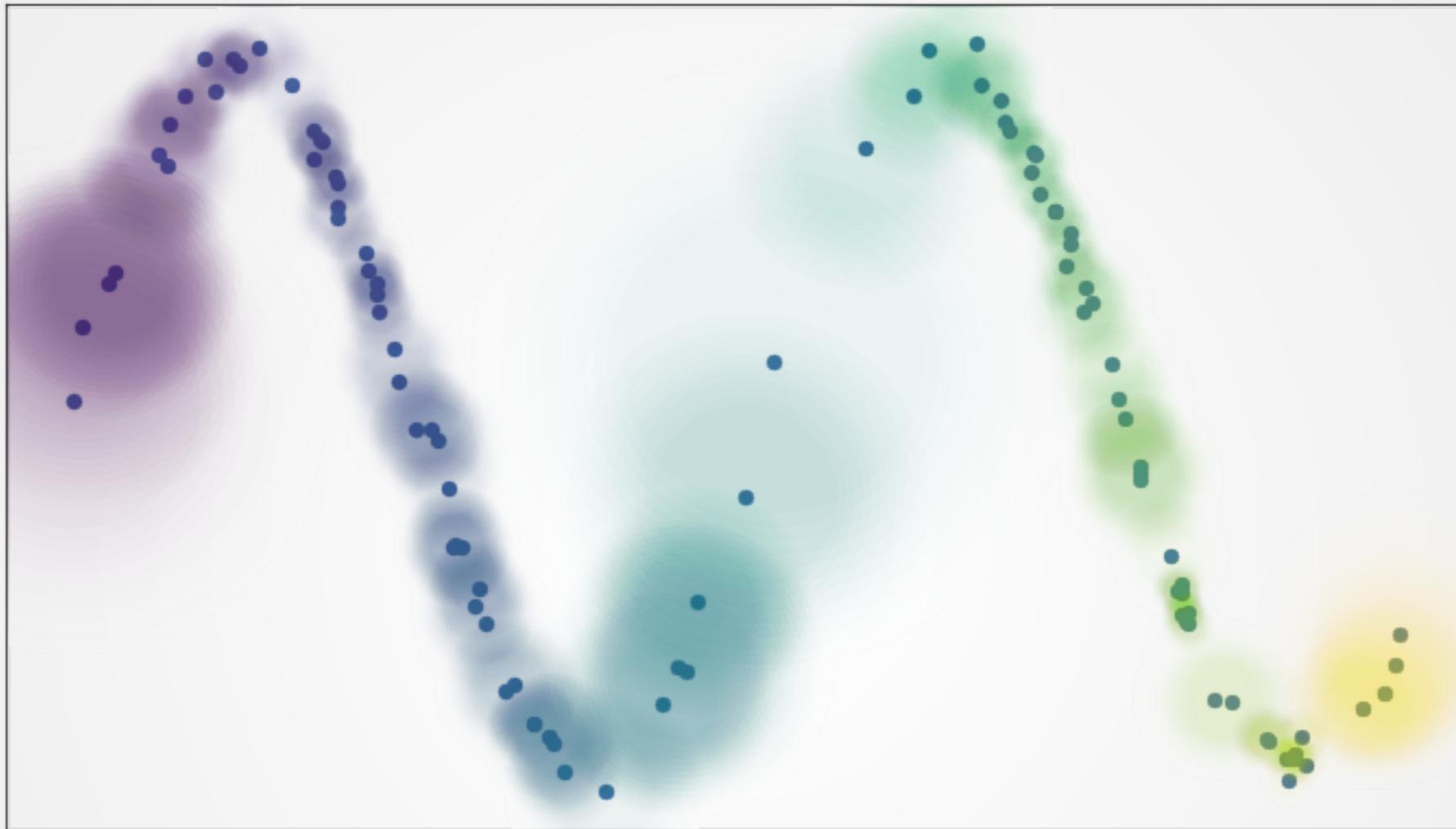


Image Source: [UMAP documentation](#)

- ☐ Refine to a fuzzy cover
- ☐ Interpret weights as probabilities of being connected



## UMAP intuition

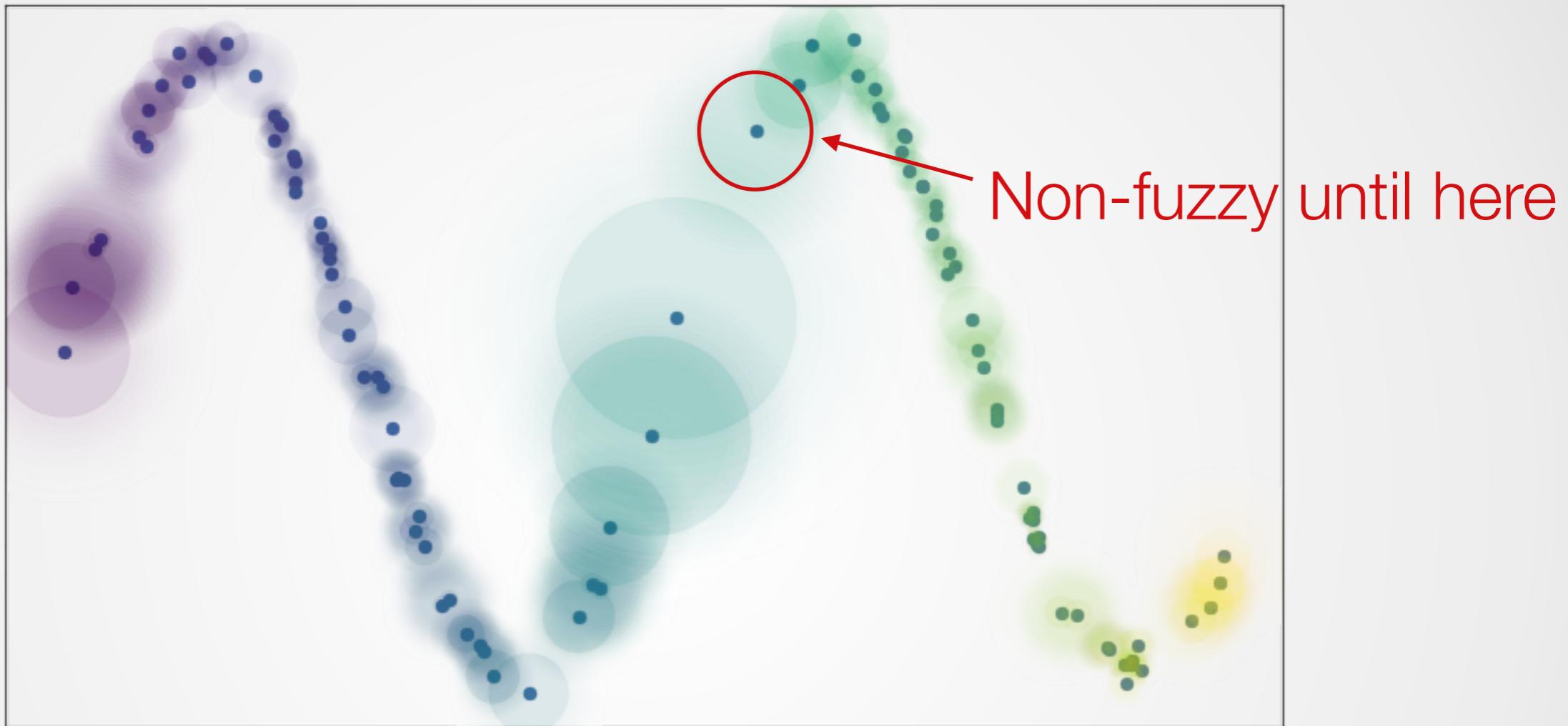
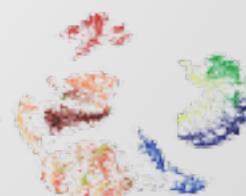


Image Source: [UMAP documentation](#)

- ☐ Leave no one (point) behind!
- ☐ To make sure no point is completely isolated, let fuzzy distance decay only after reaching the nearest neighbor



## UMAP intuition

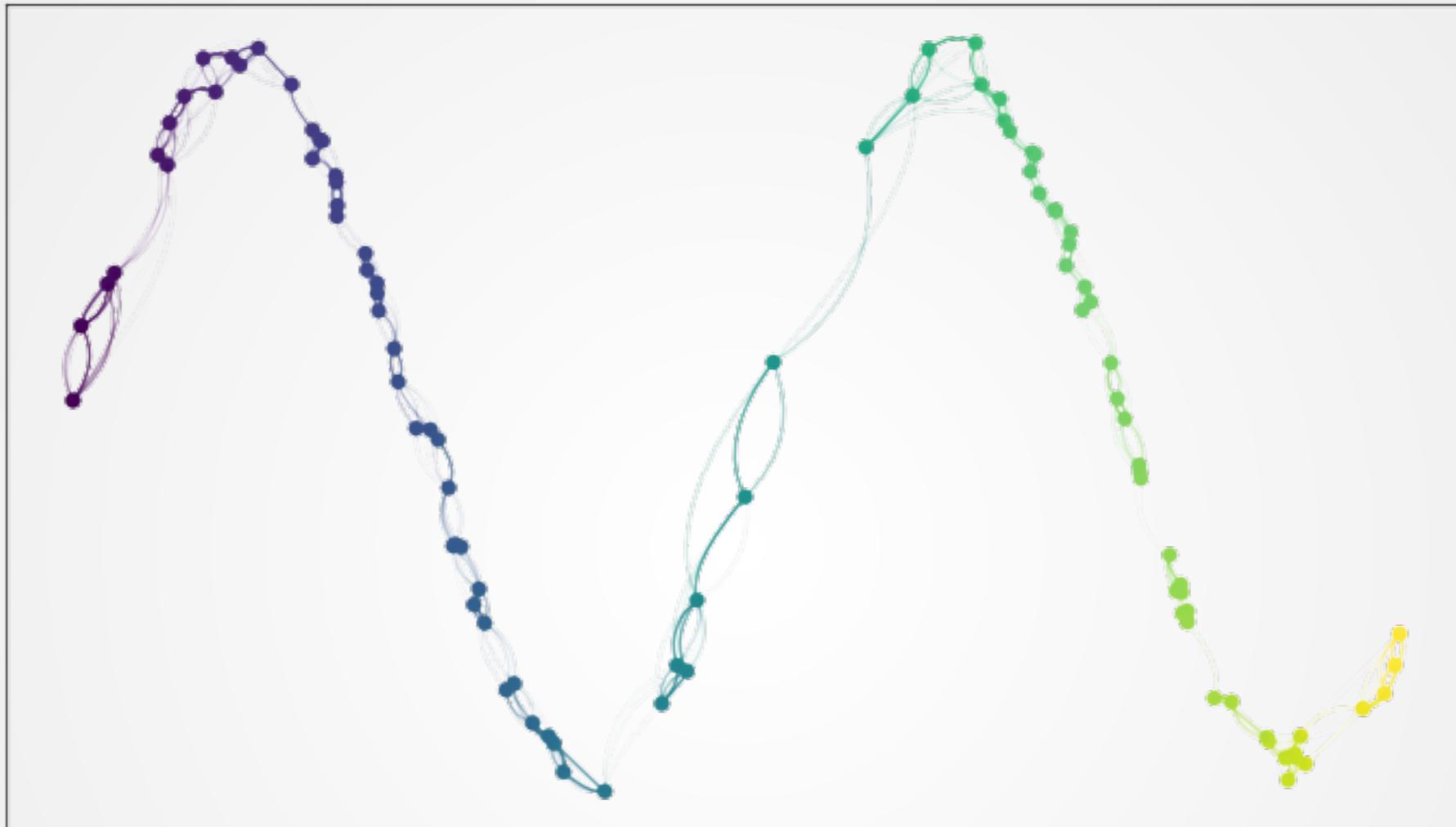
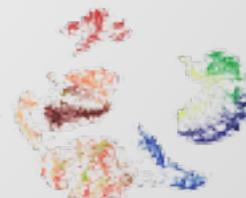


Image Source: [UMAP documentation](#)

- Problem: local metrics are incompatible. Edges can have different weights depending on metrics of endpoints
- Merge disagreeing two edges  $a$  and  $b$



## UMAP intuition

Edges with different weights

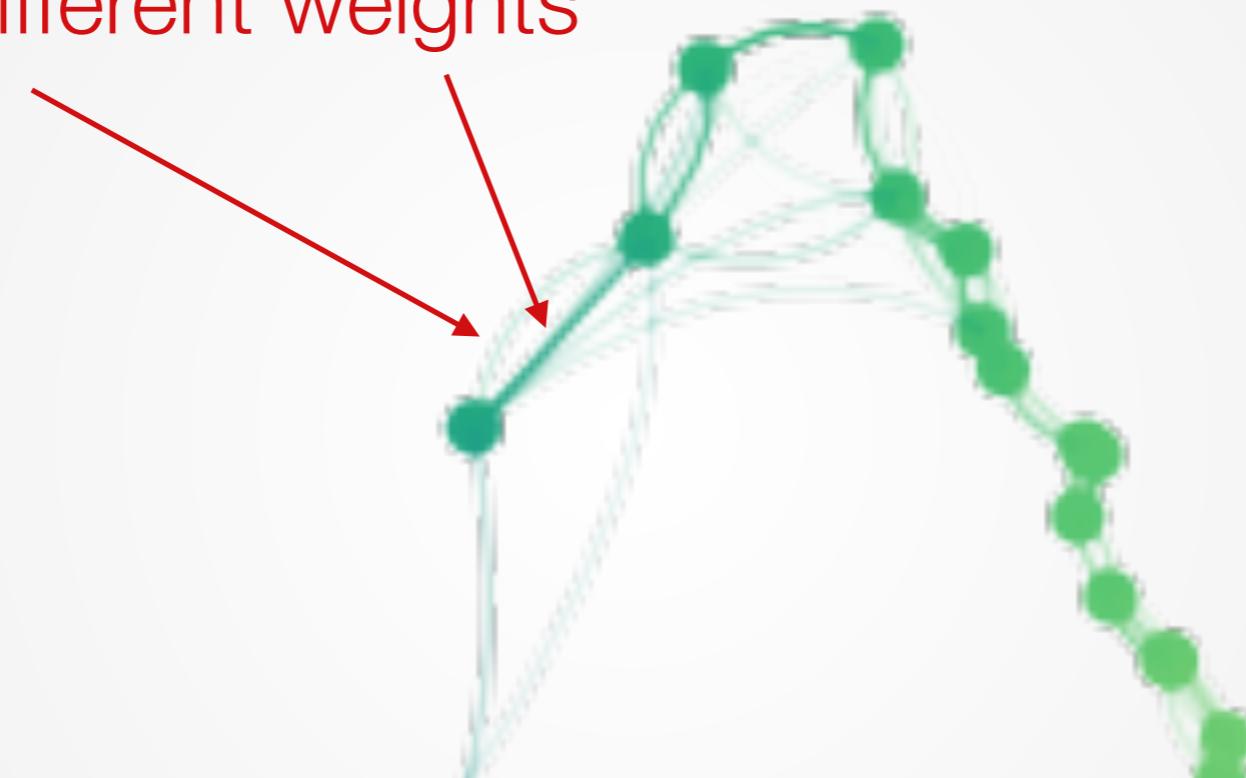
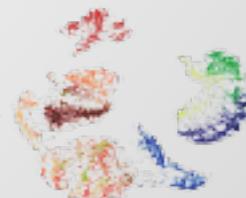


Image Source: [UMAP documentation](#)

- Problem: local metrics are incompatible. Edges can have different weights depending on metrics of endpoints
- Merge disagreeing two edges  $a$  and  $b$



## UMAP intuition

Extreme case: there can even be only one edge

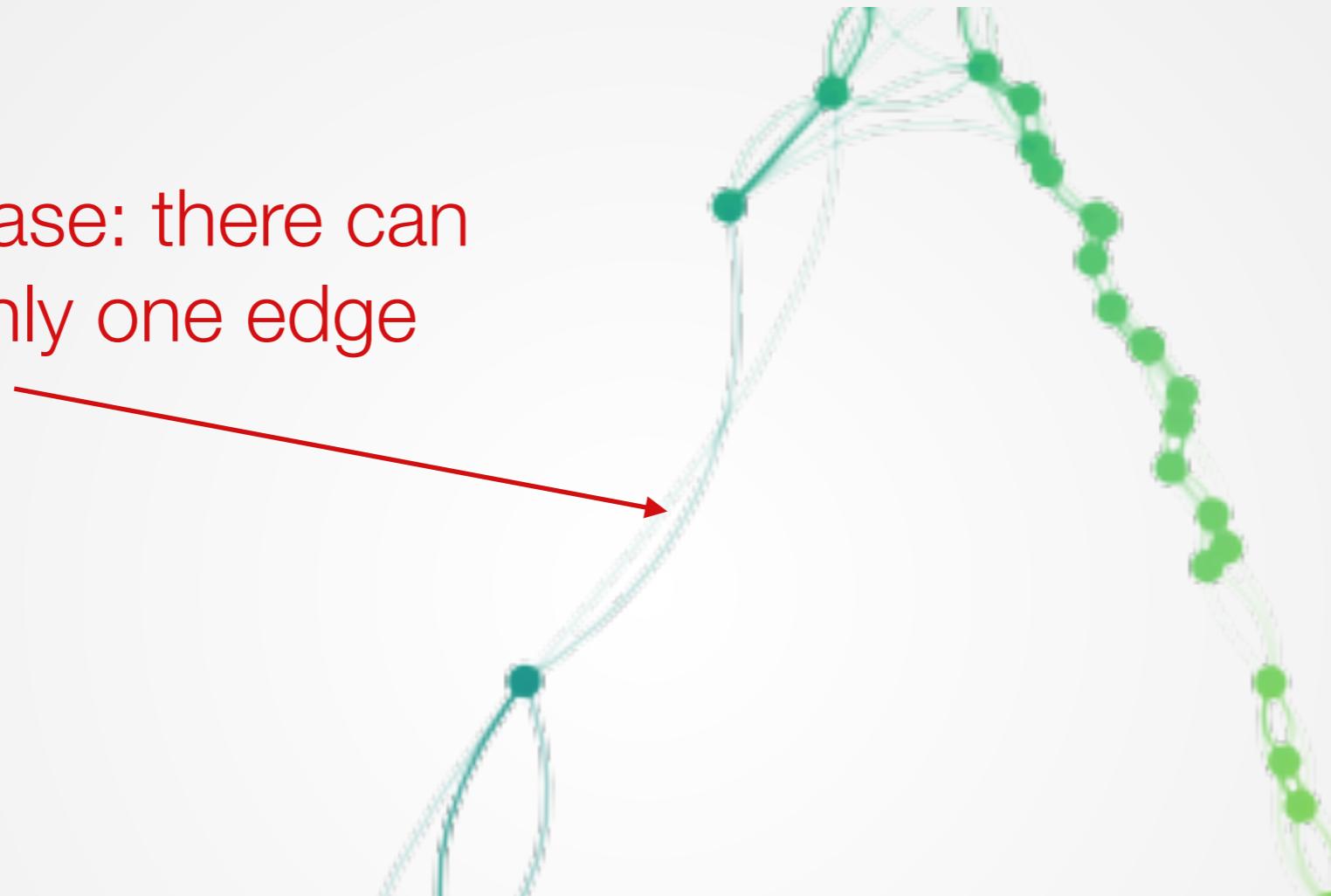
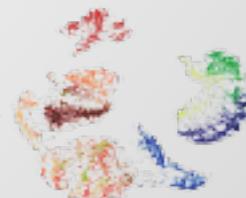


Image Source: [UMAP documentation](#)

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- Merge disagreeing two edges  $a$  and  $b$



## UMAP intuition

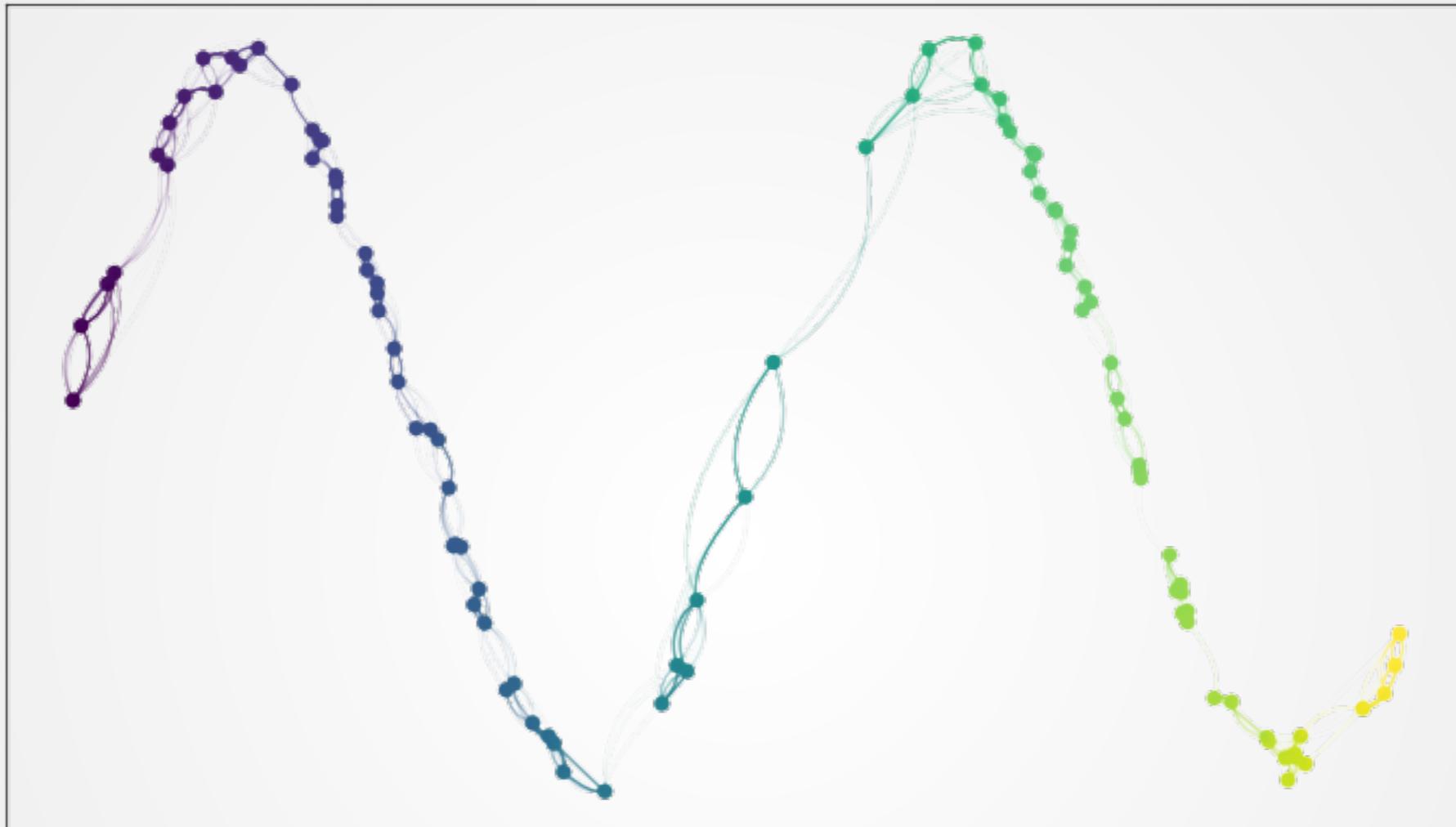
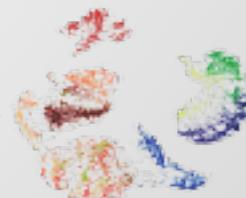


Image Source: [UMAP documentation](#)

- Merge disagreeing two edges  $a$  and  $b$
- Combined weight:  $a + b - ab$
- Interpretation: probability that at least one of the edges exists



## UMAP intuition

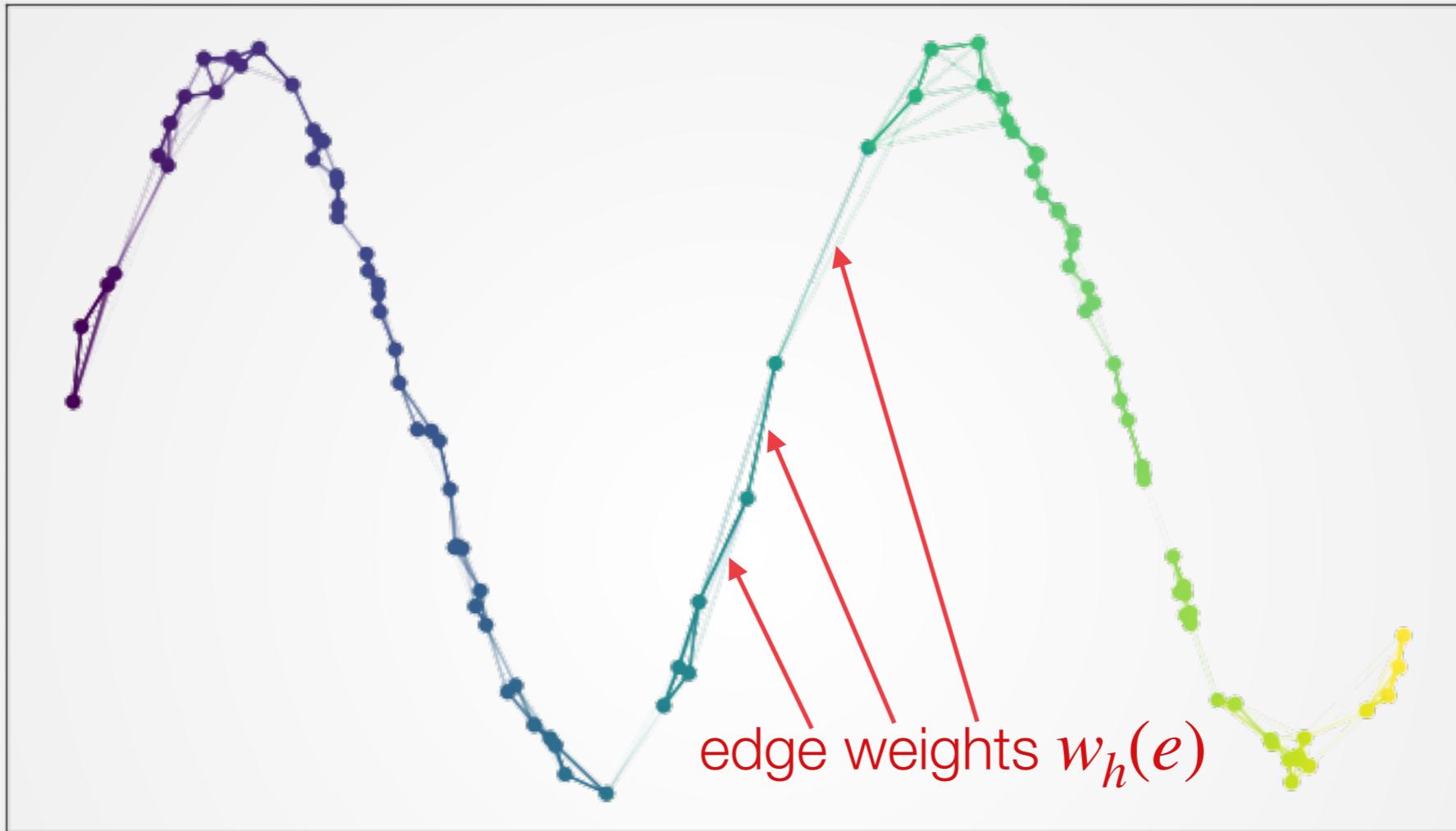
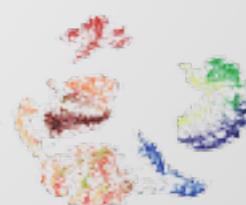


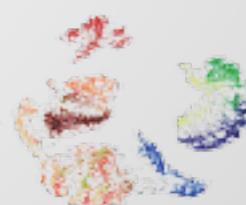
Image Source: [UMAP documentation](#)

- Graph with combined edge weights



## UMAP intuition

- Main step: find representation in low dim. that is „close“ to high dim.
- How to measure closeness?
  - ▶ Compare vectors of 1-simplices = probabilities = edge weights between 0-simplices (data points)
  - ▶ These are Bernoulli random variables, edge either exists or not
  - ▶ Cross-entropy is an appropriate measure
- Minimize cross-entropy leads to maximum „closeness“



## UMAP intuition

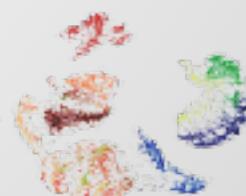
- Cross-entropy:

$$\sum_{e \in E} w_h(e) * \log \left\{ \frac{w_h(e)}{w_l(e)} \right\} + \{1 - w_h(e)\} * \log \left\{ \frac{1 - w_h(e)}{1 - w_l(e)} \right\}$$

$E$ : set of edges

$w_h(e)$ : edge weight in high dimension

$w_l(e)$ : edge weight in low dimension



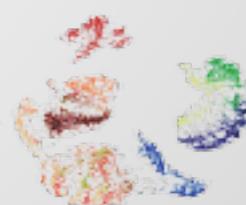
## UMAP intuition

- Cross-entropy:

$$\sum_{e \in E} \left[ w_h(e) * \log \left\{ \frac{w_h(e)}{w_l(e)} \right\} + \{1 - w_h(e)\} * \log \left\{ \frac{1 - w_h(e)}{1 - w_l(e)} \right\} \right]$$

Attractive force: Minimized when  $w_l(e)$  is as large as possible.

Large weights = small distances



## UMAP intuition

- Cross-entropy:

$$\sum_{e \in E} w_h(e) * \log \left\{ \frac{w_h(e)}{w_l(e)} \right\} + \{1 - w_h(e)\} * \log \left\{ \frac{1 - w_h(e)}{1 - w_l(e)} \right\}$$

Repulsive force: Minimized when  $w_l(e)$  is as small as possible

Remember: Small weights = large distances

Attractive force: Minimized when  $w_h(e)$  is as large as possible

Remember: Large weights = small distances



## UMAP intuition

- Cross-entropy:

$$\sum_{e \in E} w_h(e) * \log \left\{ \frac{w_h(e)}{w_l(e)} \right\} + \{1 - w_h(e)\} * \log \left\{ \frac{1 - w_h(e)}{1 - w_l(e)} \right\}$$

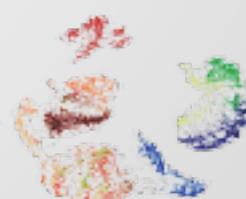
Balance of pull and push lets low dimensional representation settle into accurate representation of high dimensional topology

Repulsive force: Minimized when  $w_h(e)$  is as small as possible

Remember: Small weights = large distances

Attractive force: Minimized when  $w_h(e)$  is as large as possible

Remember: Large weights = small distances



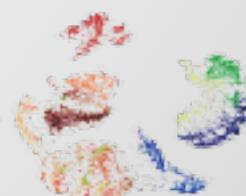
# UMAP Hyperparameters

- Number of neighbors
  - ▶ How many neighbors are considered for open balls?
  - ▶ Controls local vs. global
- Minimal distance
  - ▶ How tight can points in lower dimensional space be?
- Number components
  - ▶ How many dimensions should lower dimensional space have?
- Metric
  - ▶ What metric is used?
  - ▶ e.g. Euclidean, Manhattan, Mahalanobis, etc.

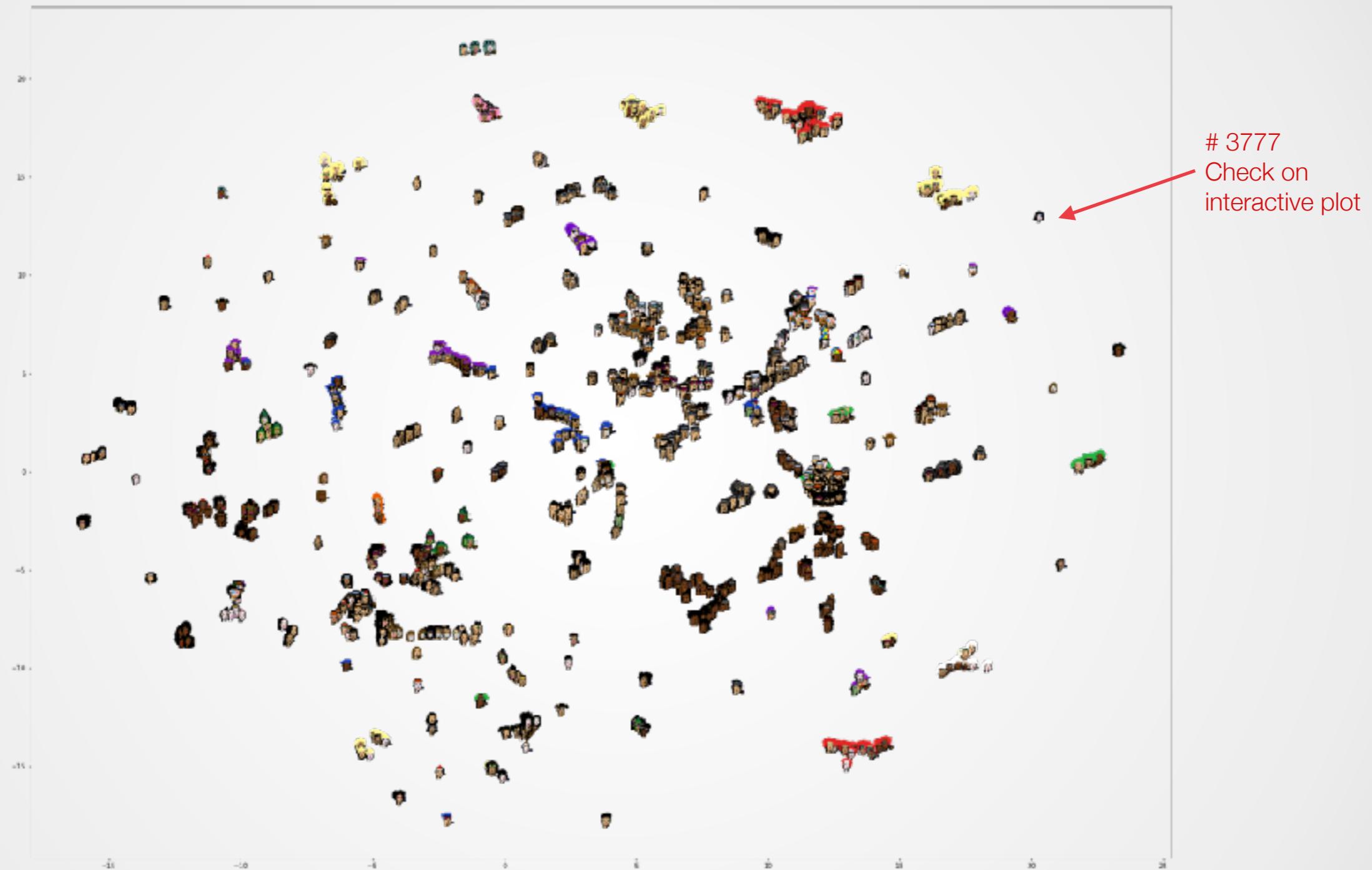


## Image data: CryptoPunks

- 10000 images, each  $24 \times 24$  pixels, RGB colour space
- Image data are high-dimensional
- Flatten the data by converting each image to an array
- Remove noninformative pixels (pixels that are black in every image)
- Hyperparameter settings in the following examples
  - ▶ `n_neighbors = 10`
  - ▶ `min_dist = 0.1`
  - ▶ `n_components = 2`
  - ▶ `metric = euclidean`

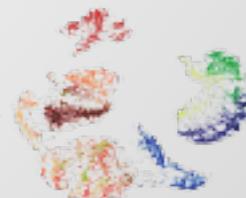


# Image data: CryptoPunks

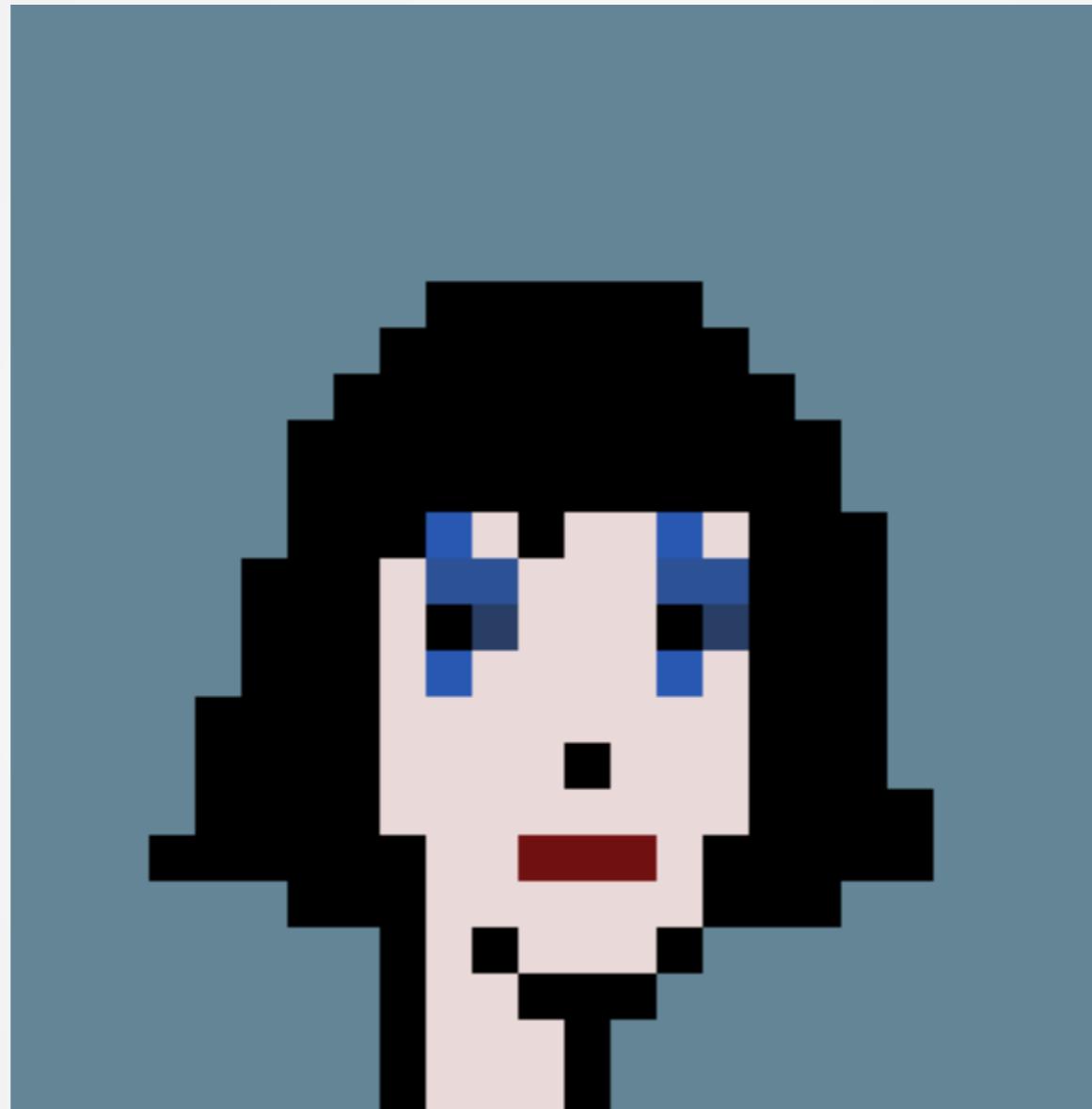


Click here for interactive plot

 UMAP

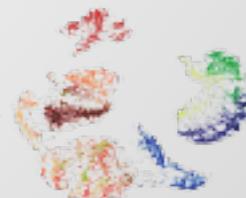


## Image data: CryptoPunks



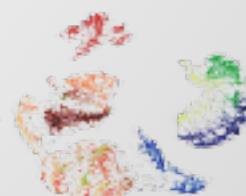
an isolated Punk?!

Click here for interactive plot



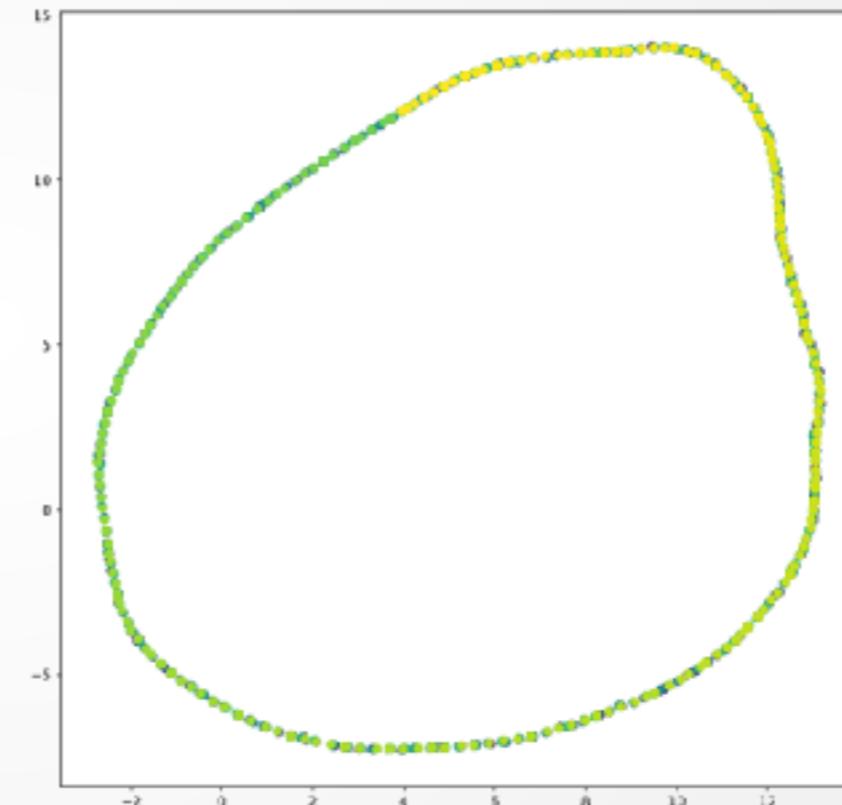
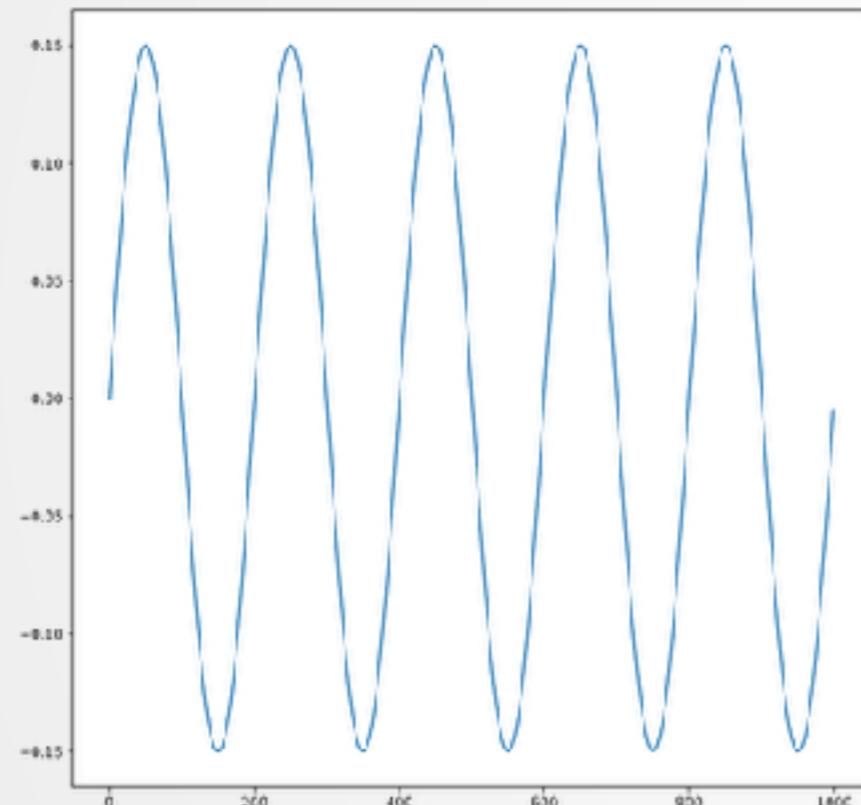
## Illustrative examples

- Challenge are time series!
- Univariate here, multivariate time series later
- Time series transformed in a sequence of rolling windows
- Window at time  $t$ : data point  $x_t$
- Window width  $w > \mathbb{R}^w$  dimensional data points
- Default hyperparameter settings in the following examples
  - ▶ `n_neighbors = 15`
  - ▶ `min_dist = 0.1`
  - ▶ `n_components = 2`
  - ▶ `metric = euclidean`



## Illustrative examples with simulated data

- Example 1: Simple Sine curve, period = 200, n = 1000
- Window = lag size:  $d=5$

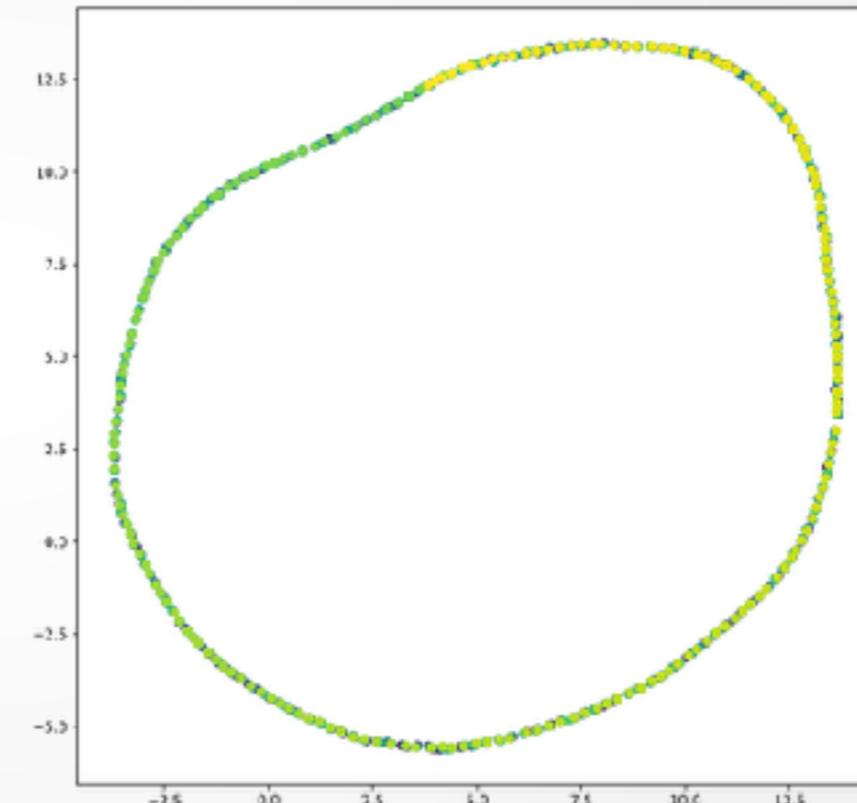
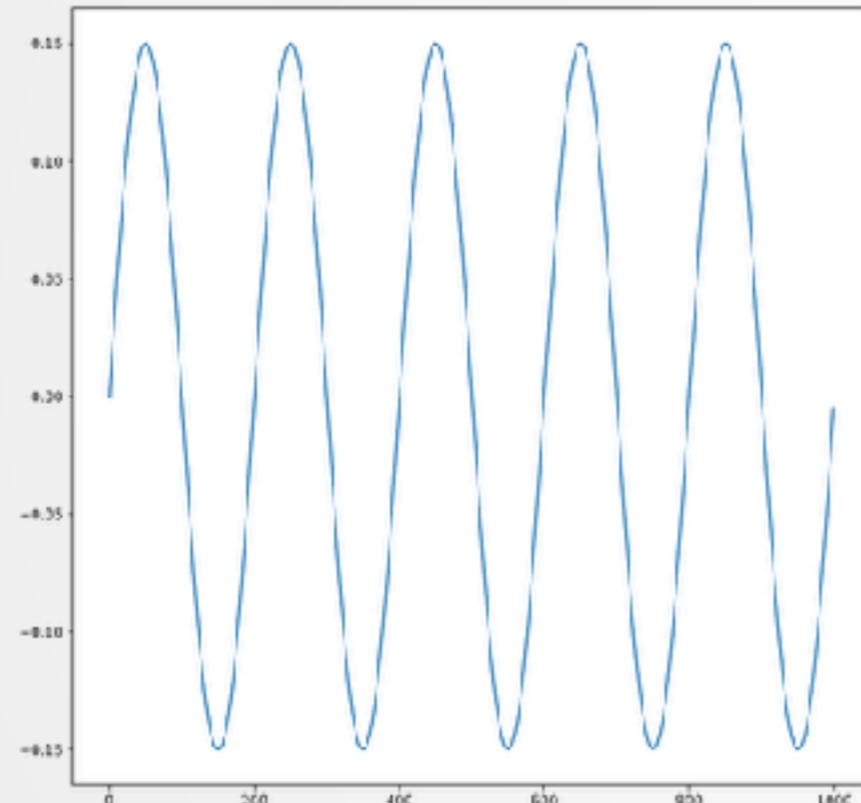


- UMAP recovers periodic structure well
- Interpretation: „data goes in circles“



## Illustrative examples with simulated data

- Example 1: Simple Sine curve, period = 200, n = 1000
- Window = lag size:  $d=30$

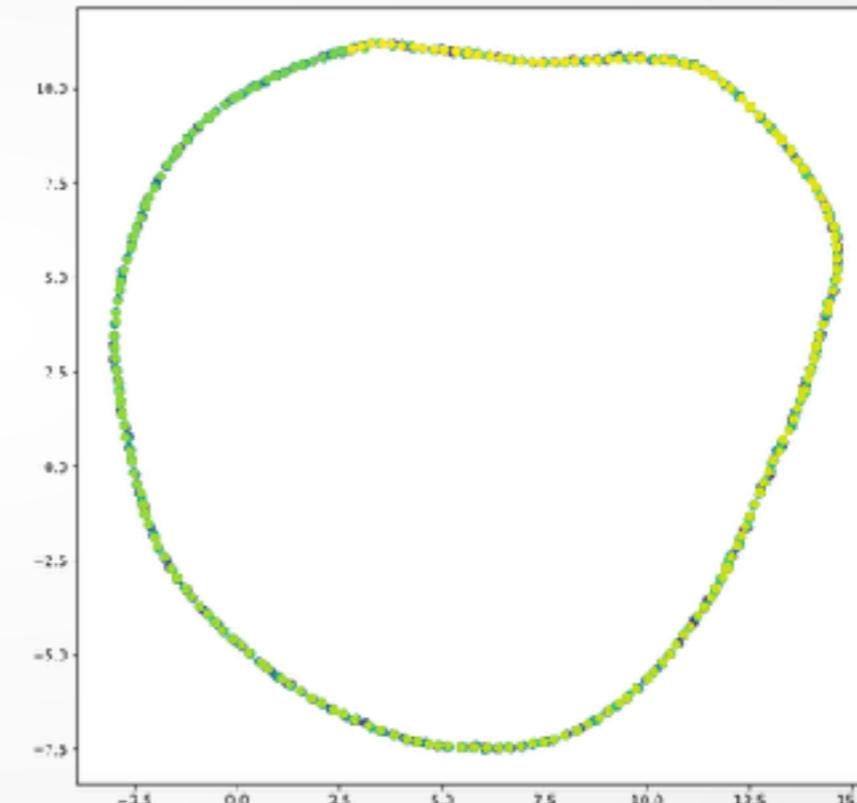
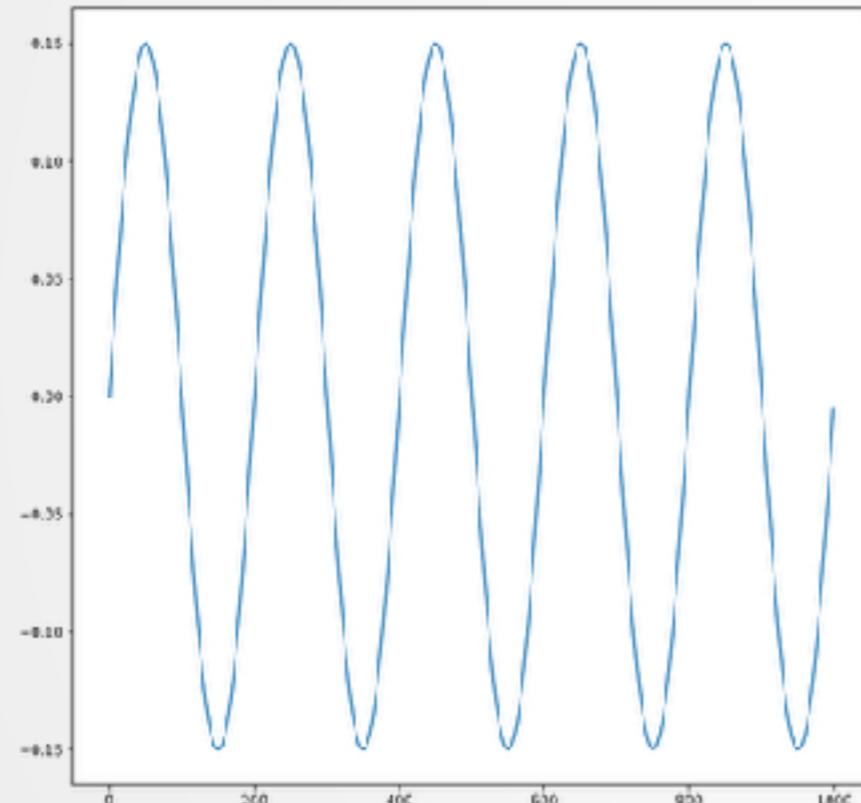


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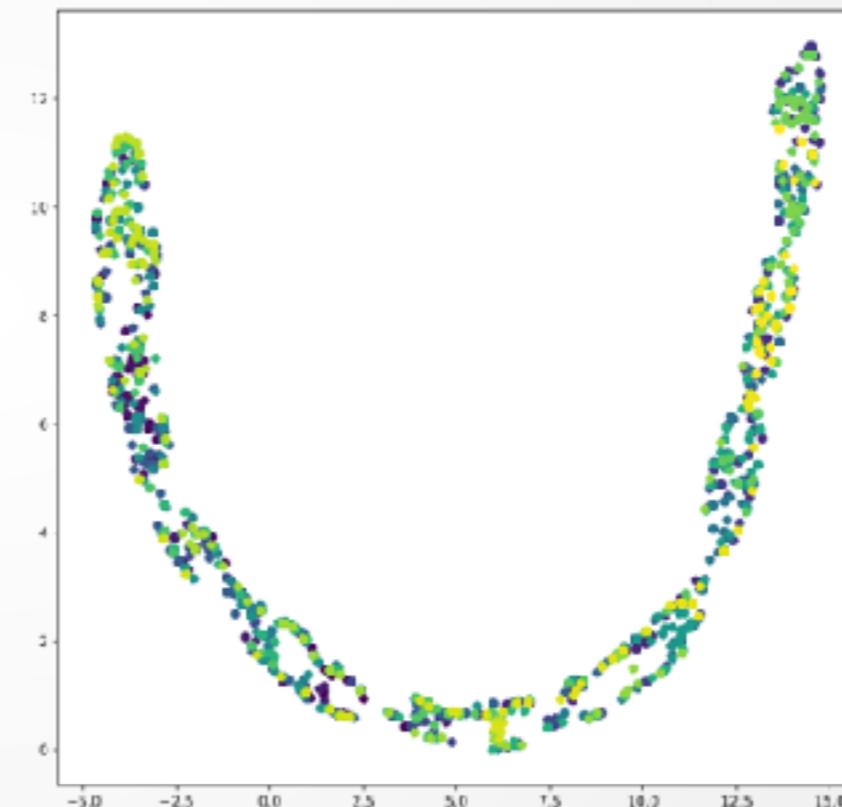
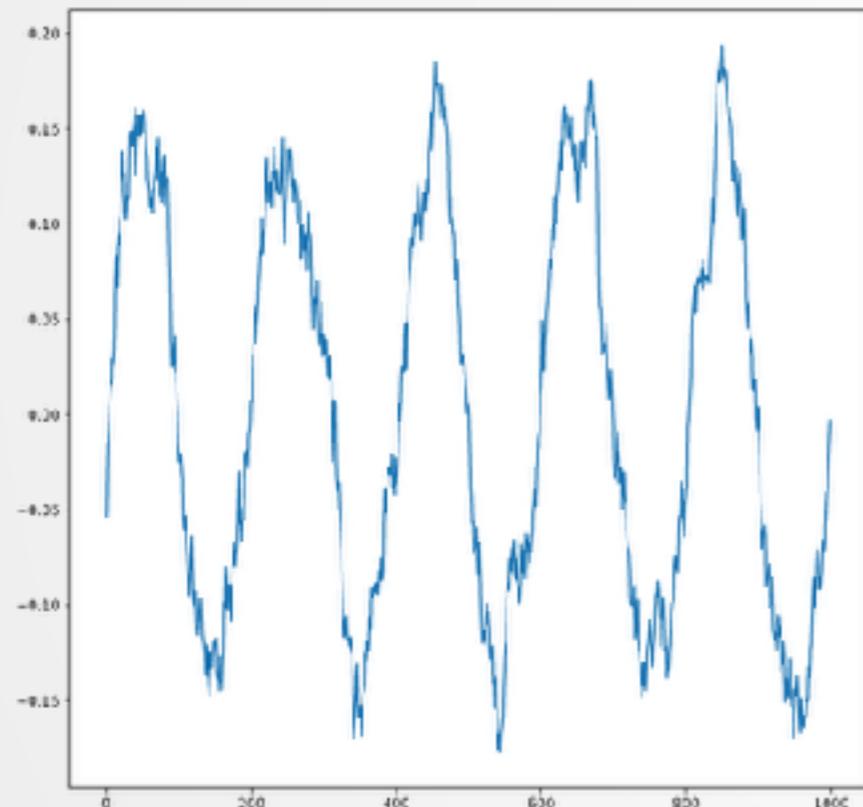


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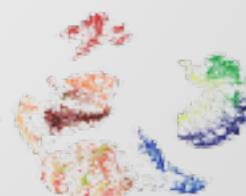


## Illustrative examples with simulated data

- Example 2: Sine curve from example 1 with added AR(1) process
- Autoregressive parameter: 0.9, Error sd: 0.1
- Window = lag size:  $d=5$

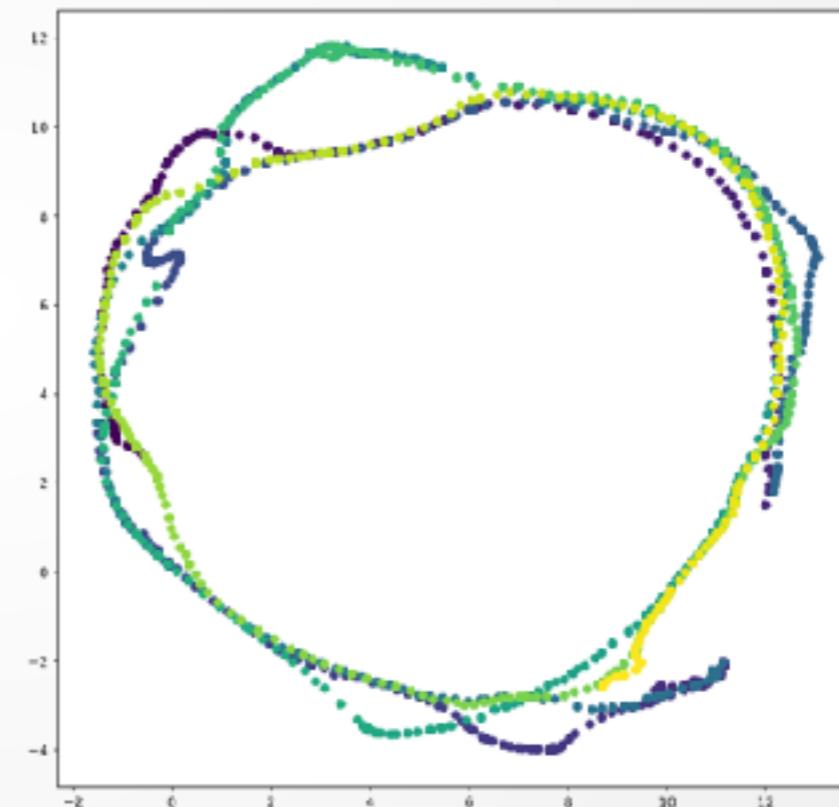
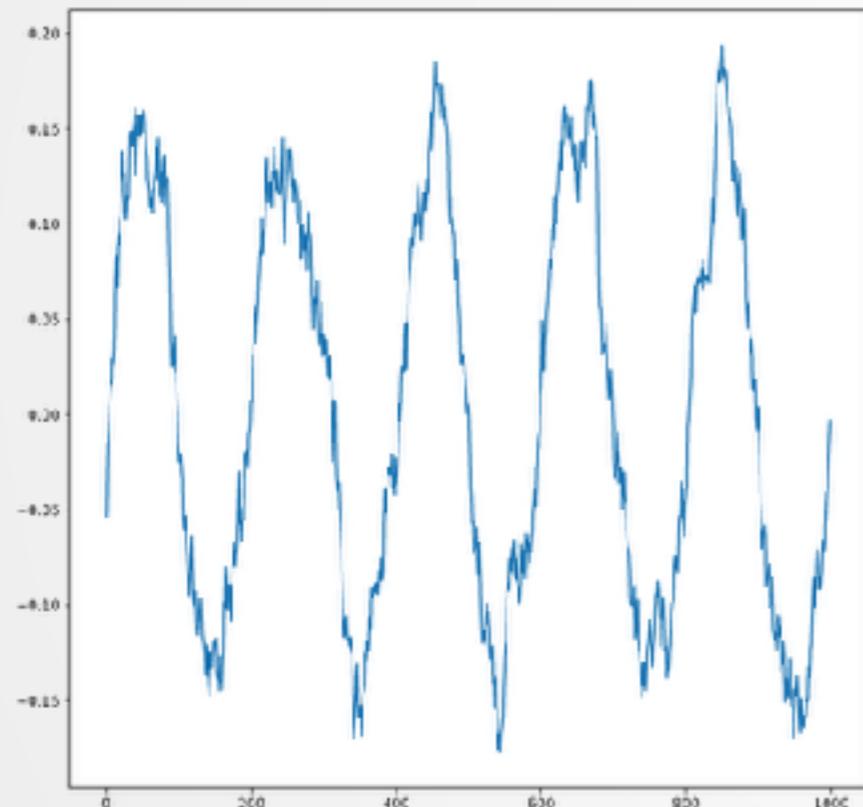


- UMAP still recovers periodicity
- Even though the structure of the data is more irregular



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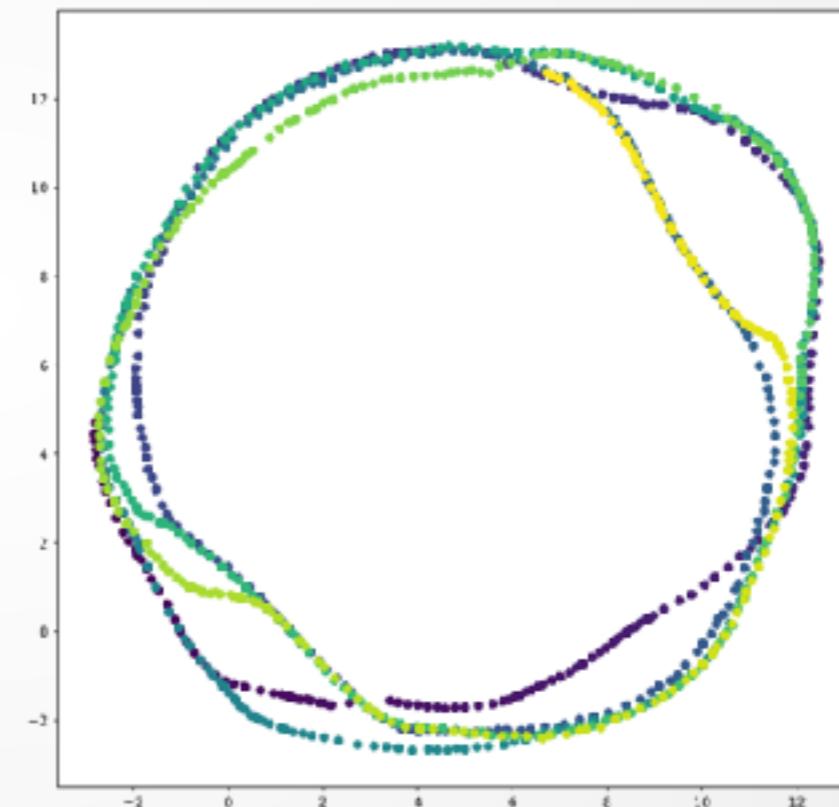
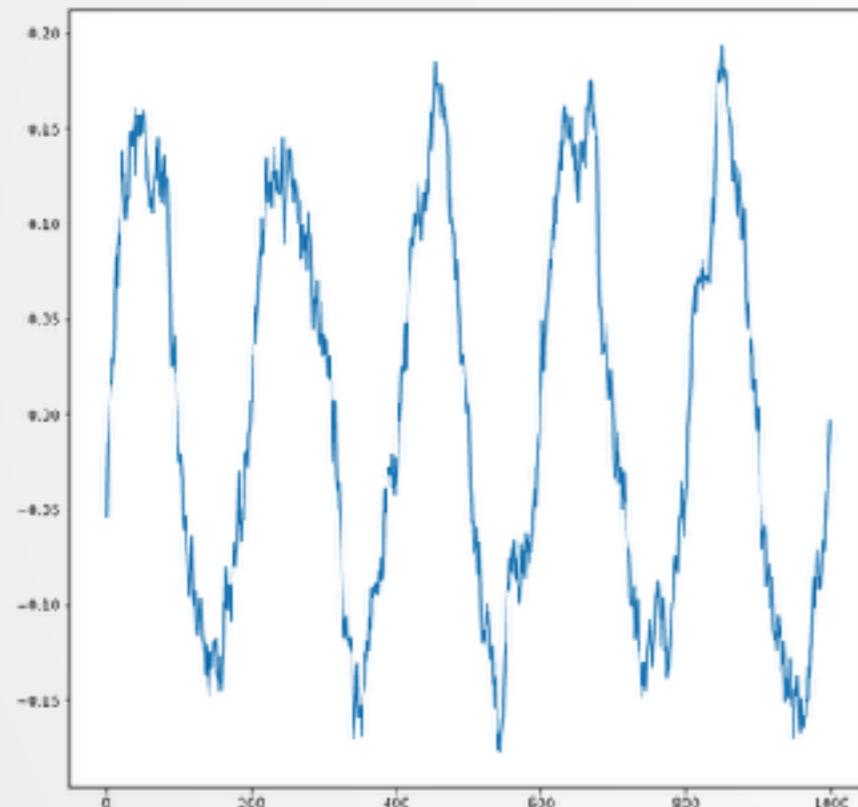


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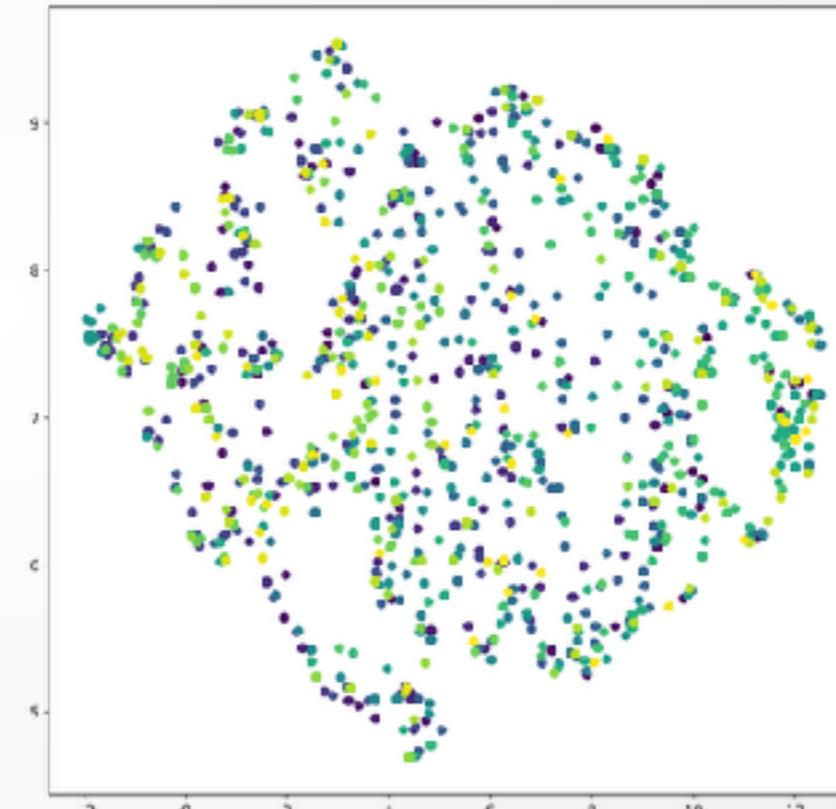
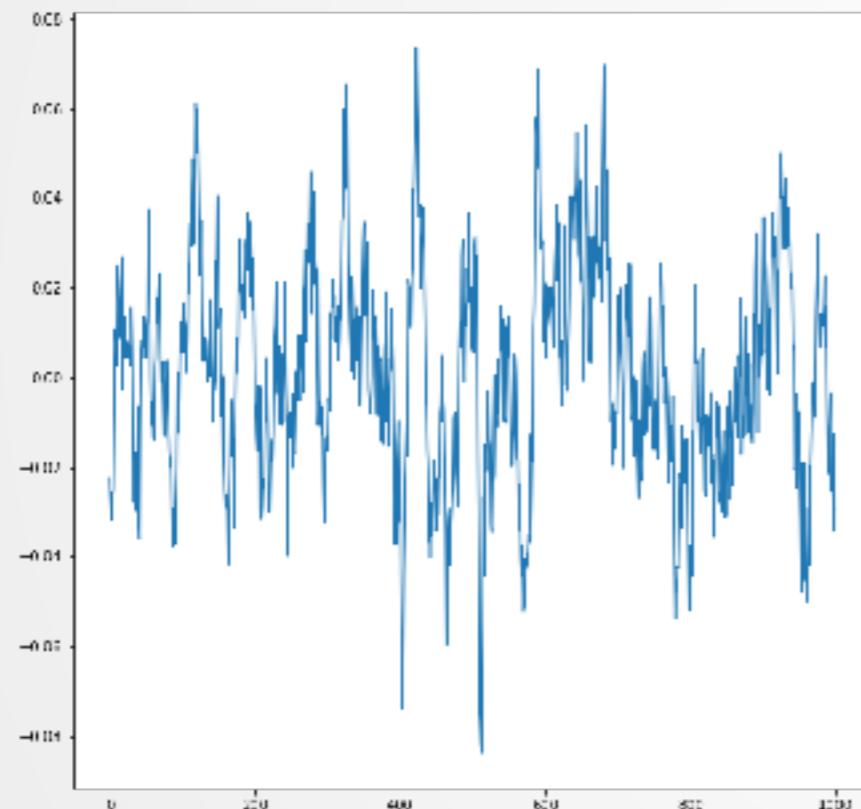


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## Illustrative examples with simulated data

- Example 3: Only AR(1) process
- Autoregressive parameter: 0.9 Error sd: 0.1
- Window = lag size:  $d=5$

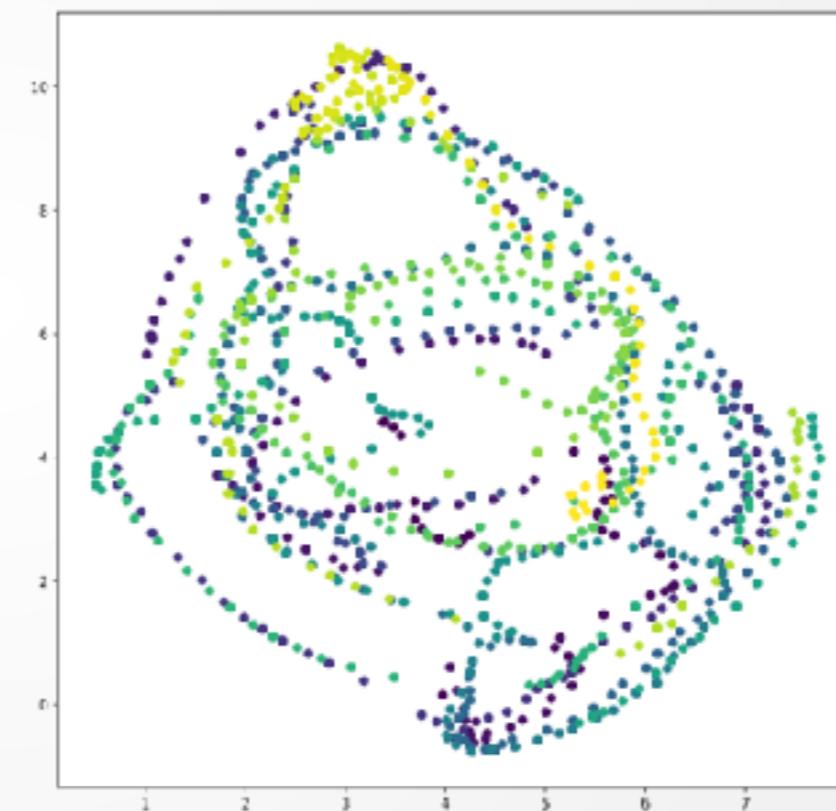
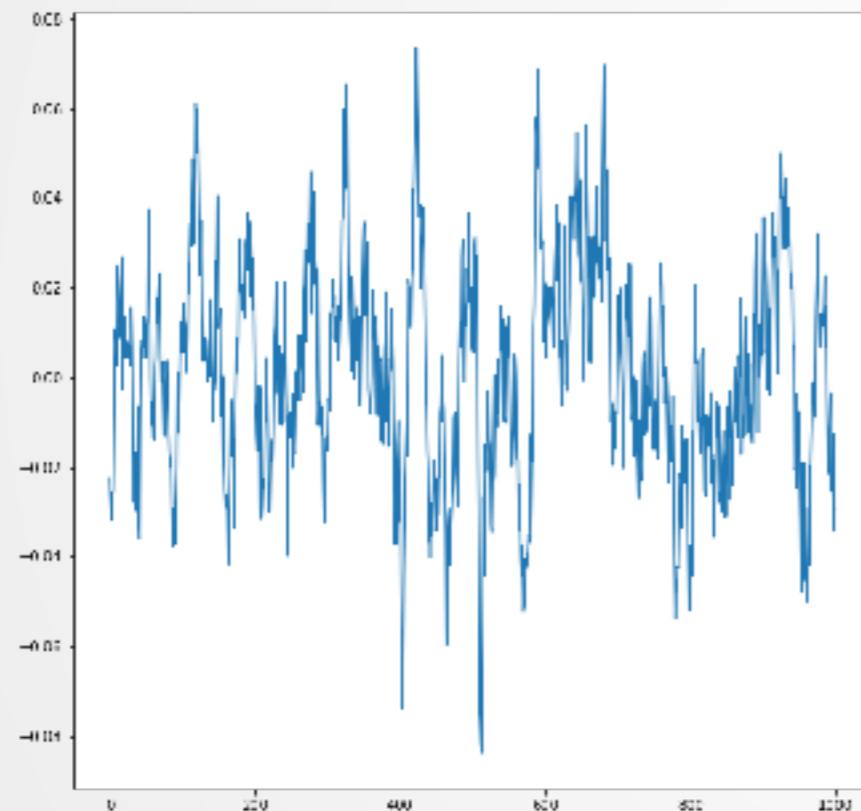


- UMAP recovers local structure for sufficient window size



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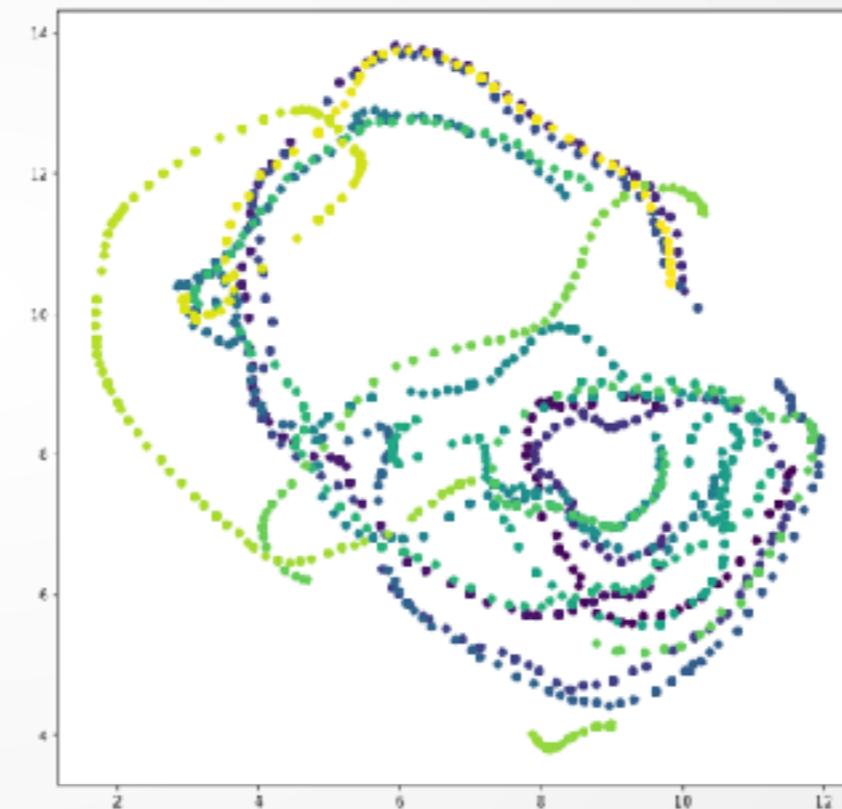
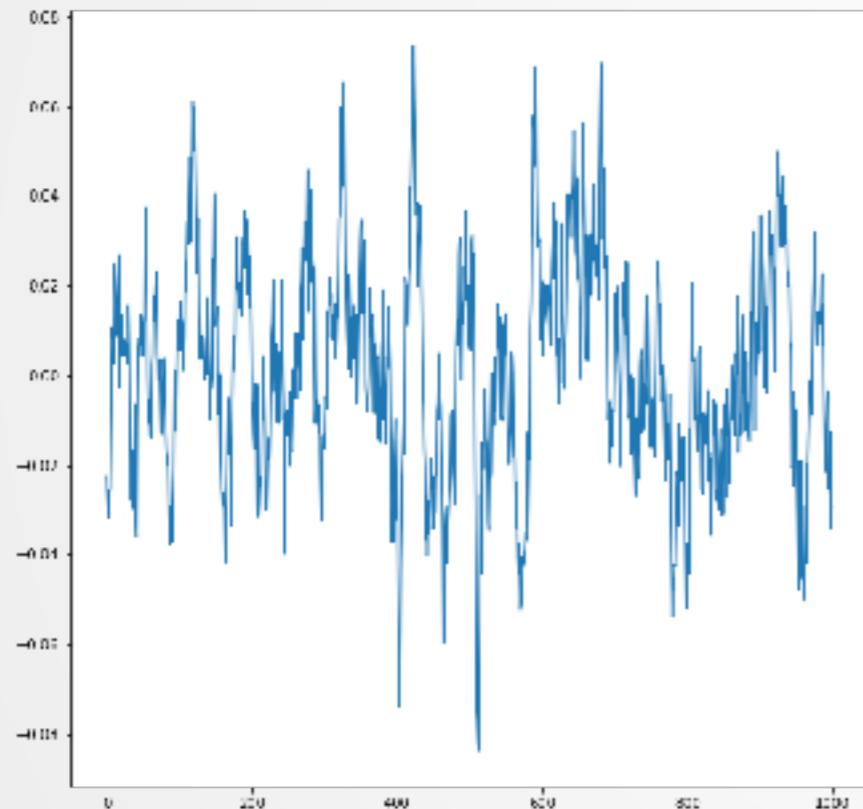


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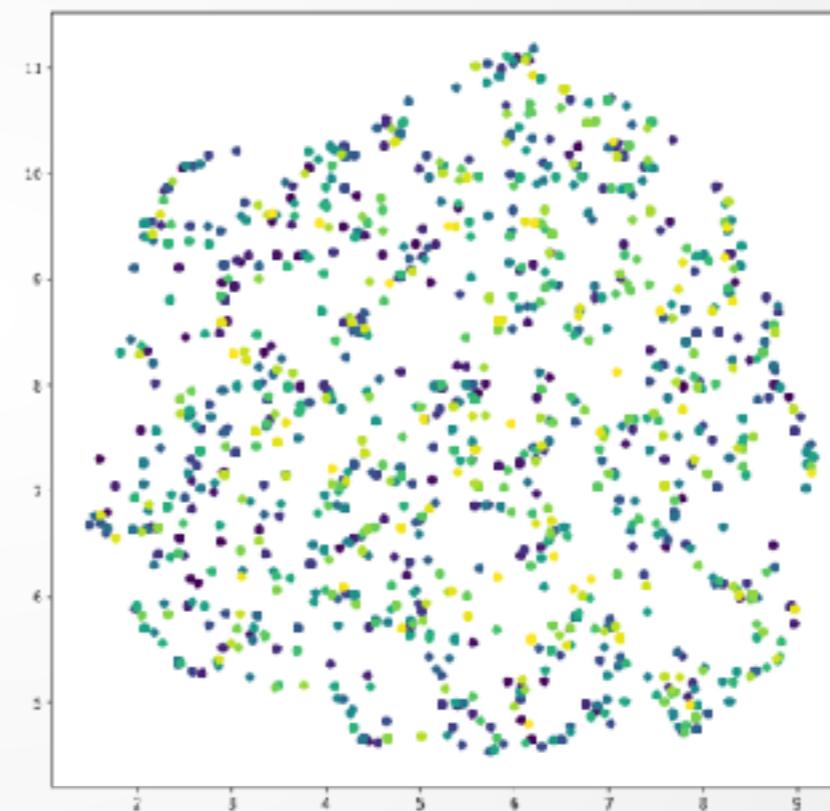
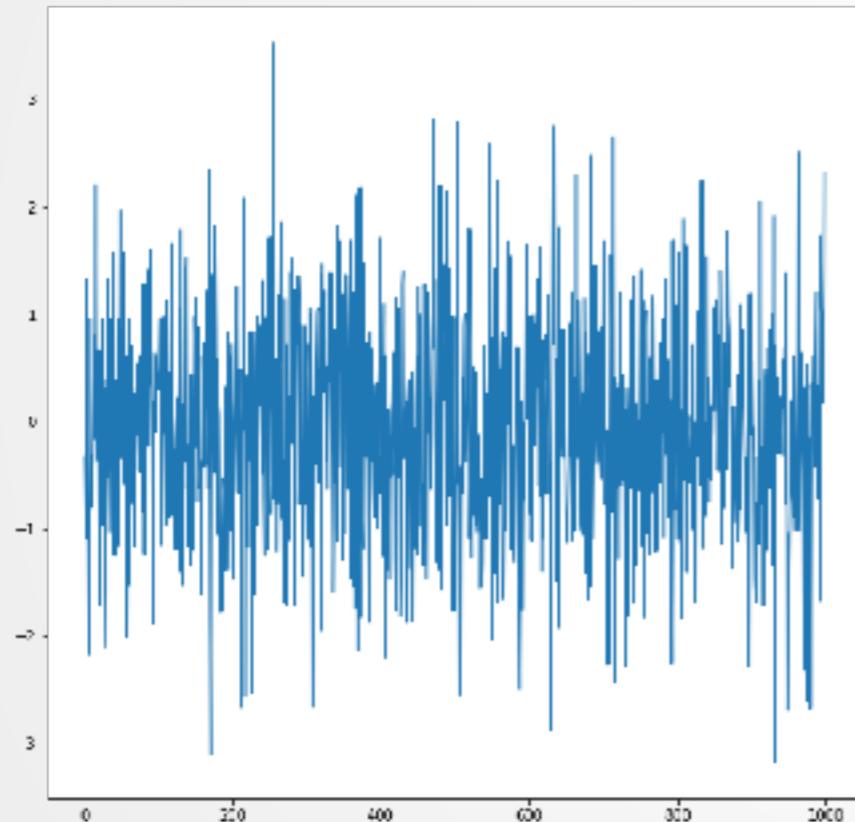


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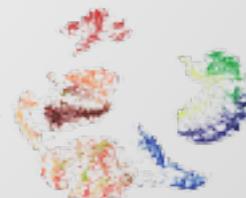


## Illustrative examples with simulated data

- Example 4: White Noise
- Gaussian White Noise:  $Sd = 1$ , Mean = 0
- Window = lag size:  $d=5$

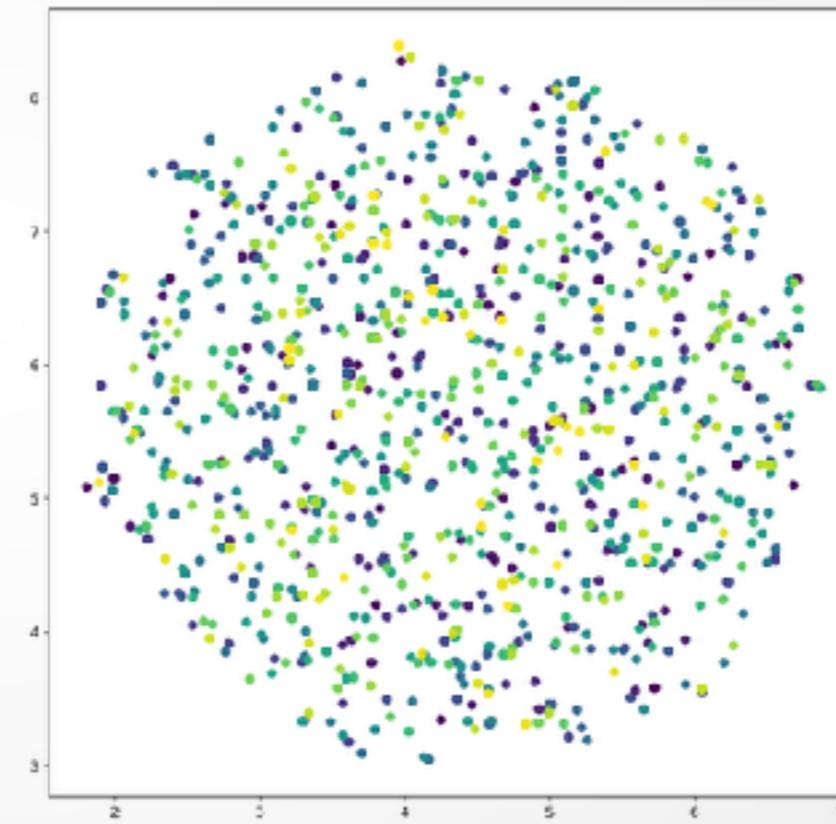
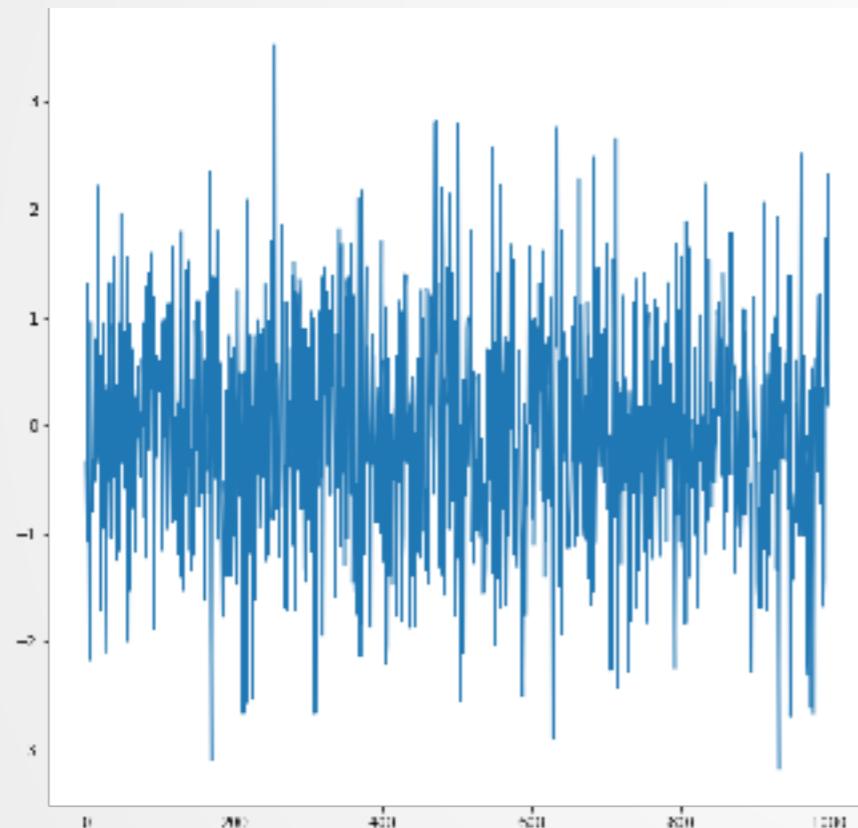


- UMAP recovers no structure



## Illustrative examples with simulated data

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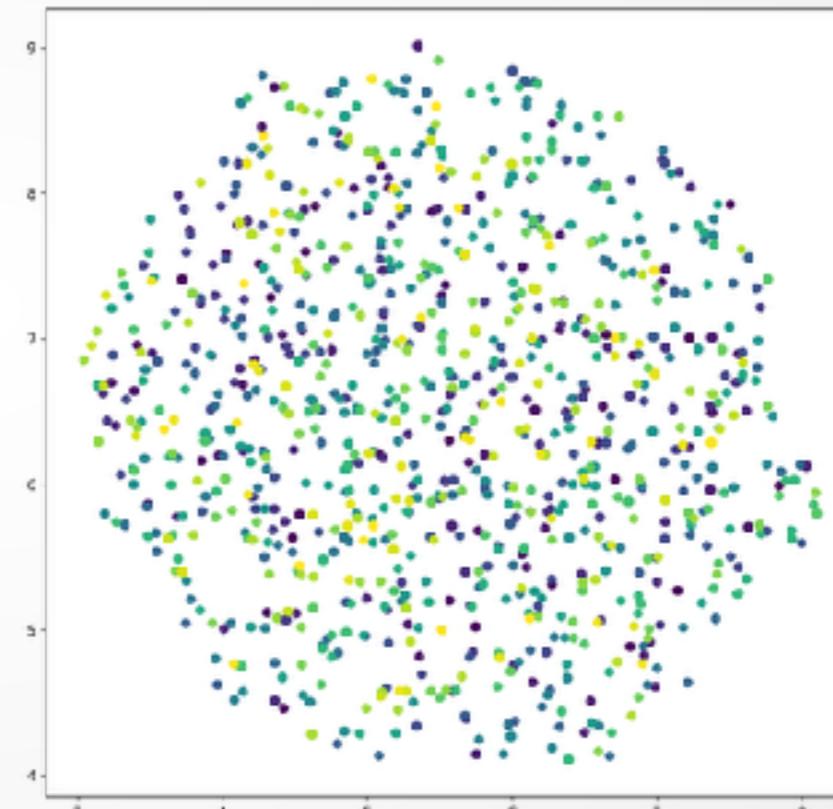
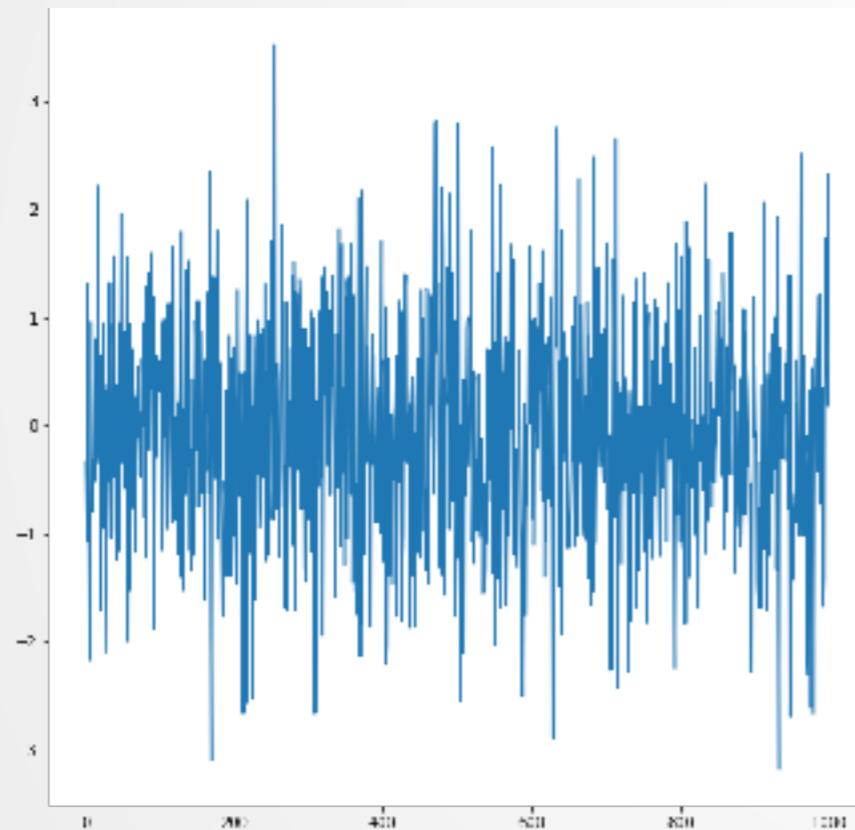


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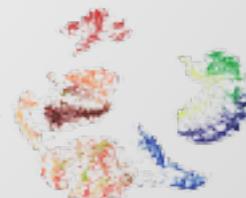


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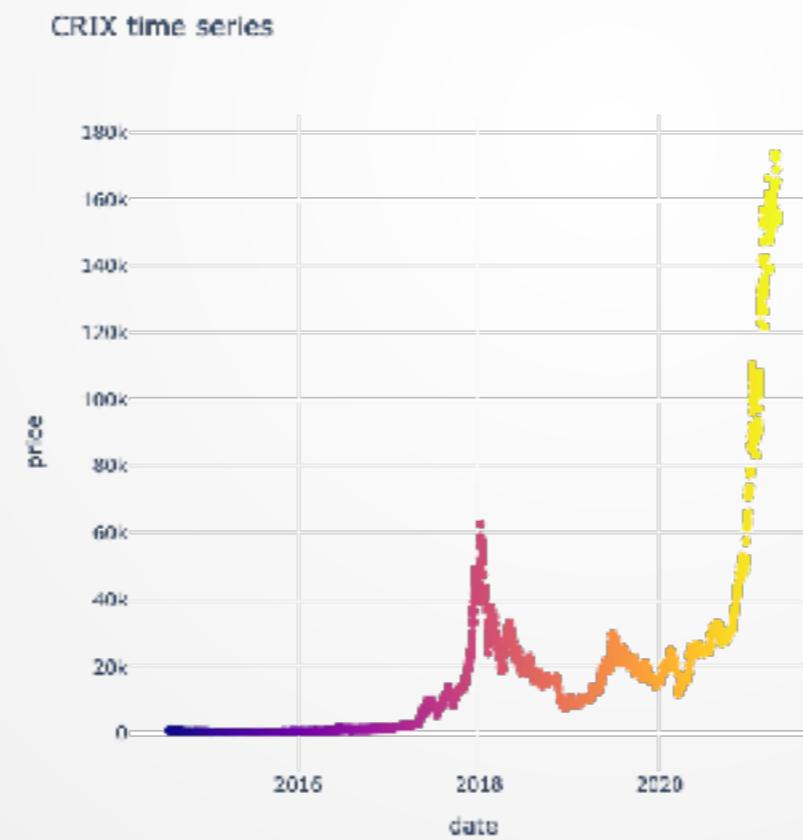


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## Time Series Example: CRIX

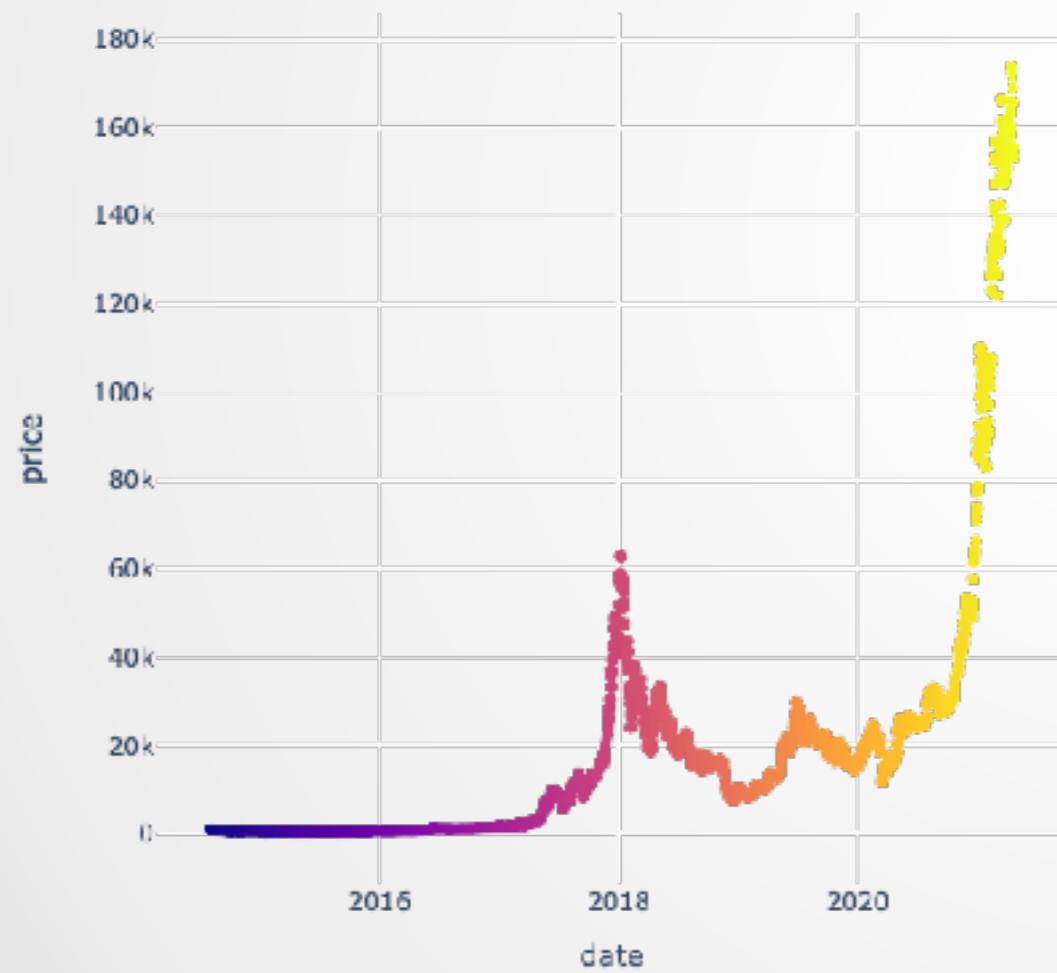
- CRIX is a market index for cryptocurrencies
- Constructed from cryptocurrencies with high market capitalization
- Captures dynamics of the cryptocurrencies market



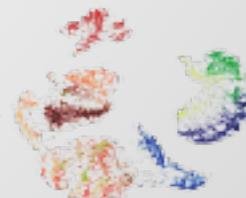
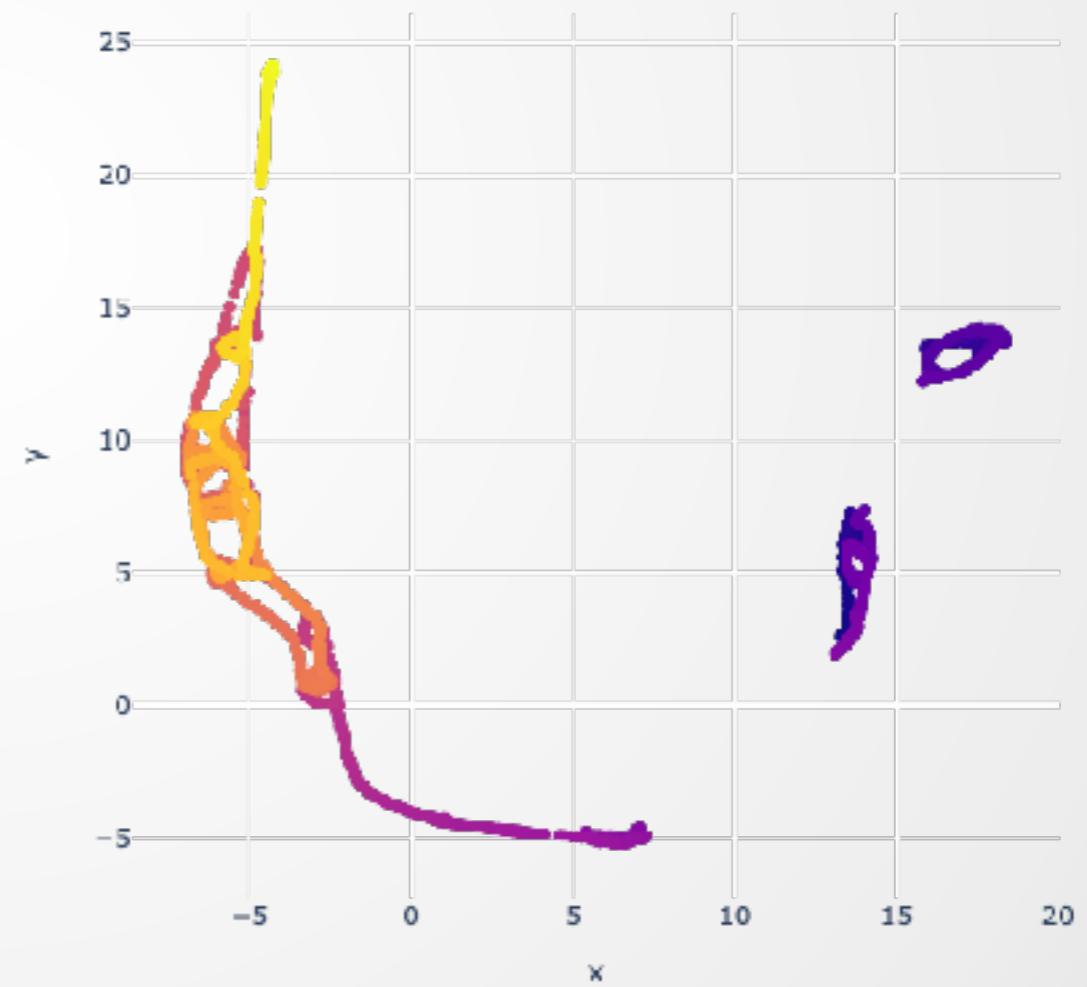
## Time Series Example: CRIX

- Window size = 30, n\_neighbors = 60

CRIX time series



UMAP CRIX

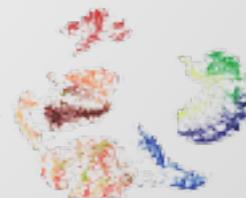
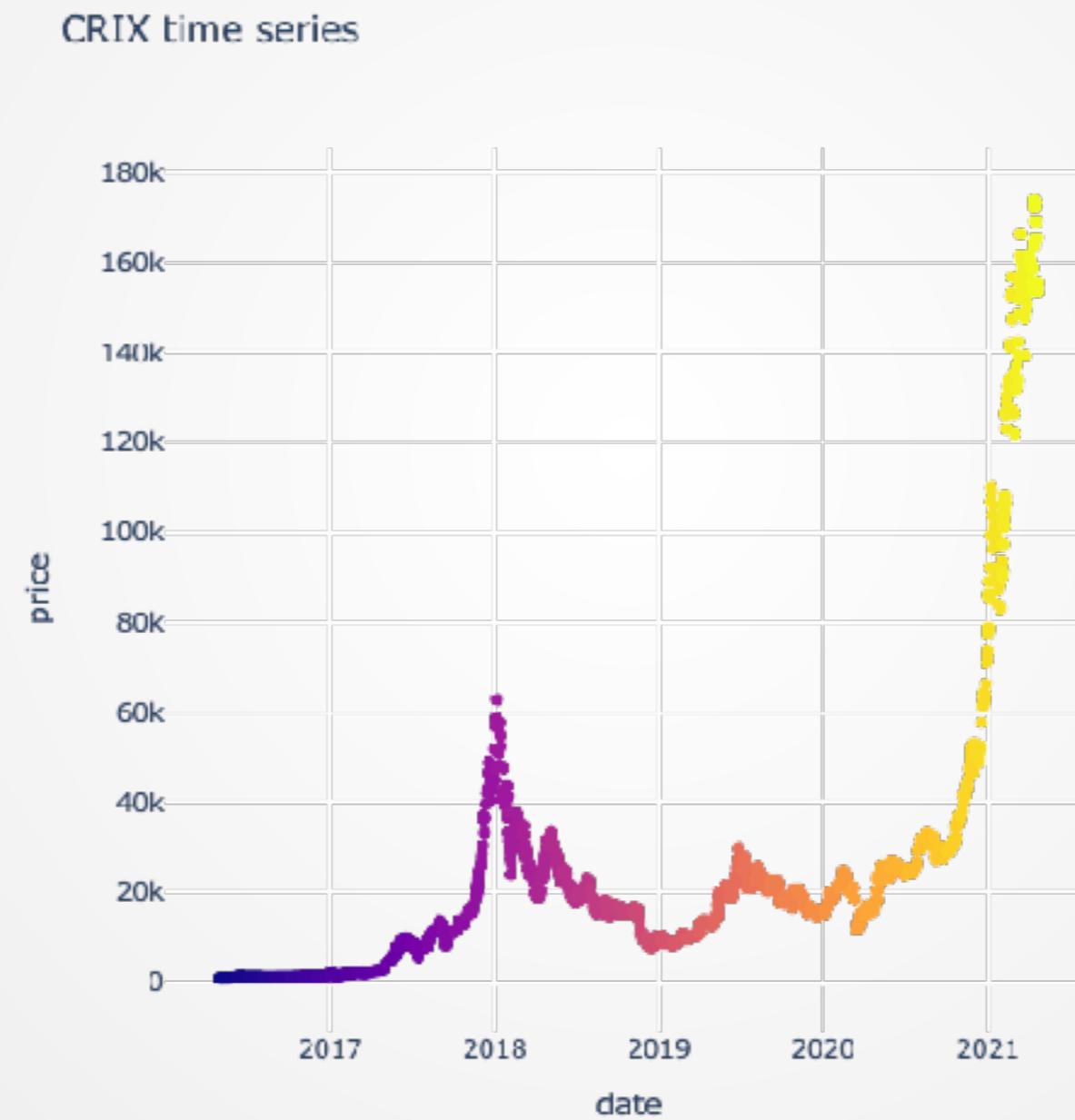


## Time Series Example: CRIX

- Alternative method: look at constituents of CRIX instead of at CRIX time series
- Weights of CRIX constituents are a high-dimensional time series



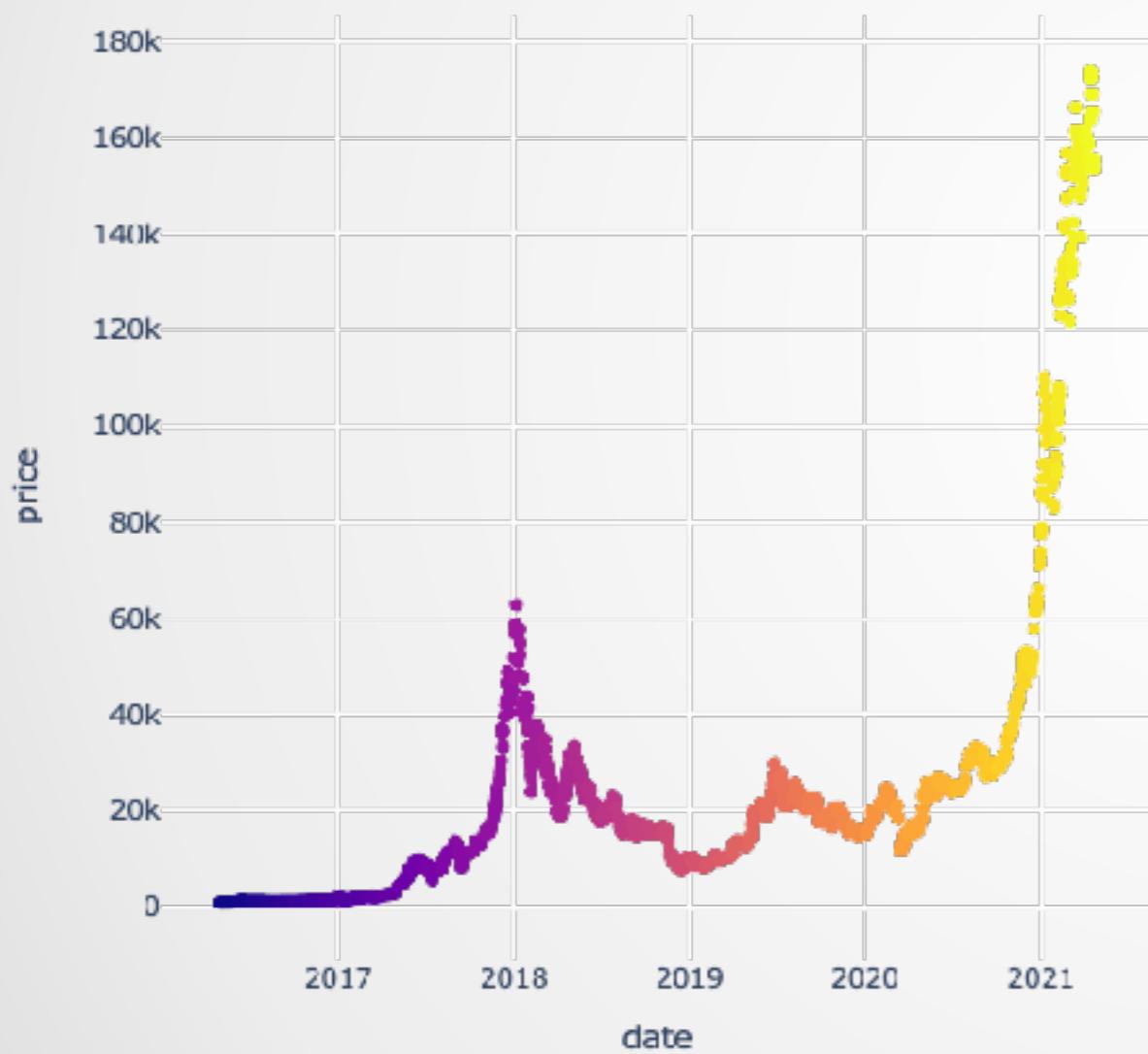
# Time Series Example: CRIX



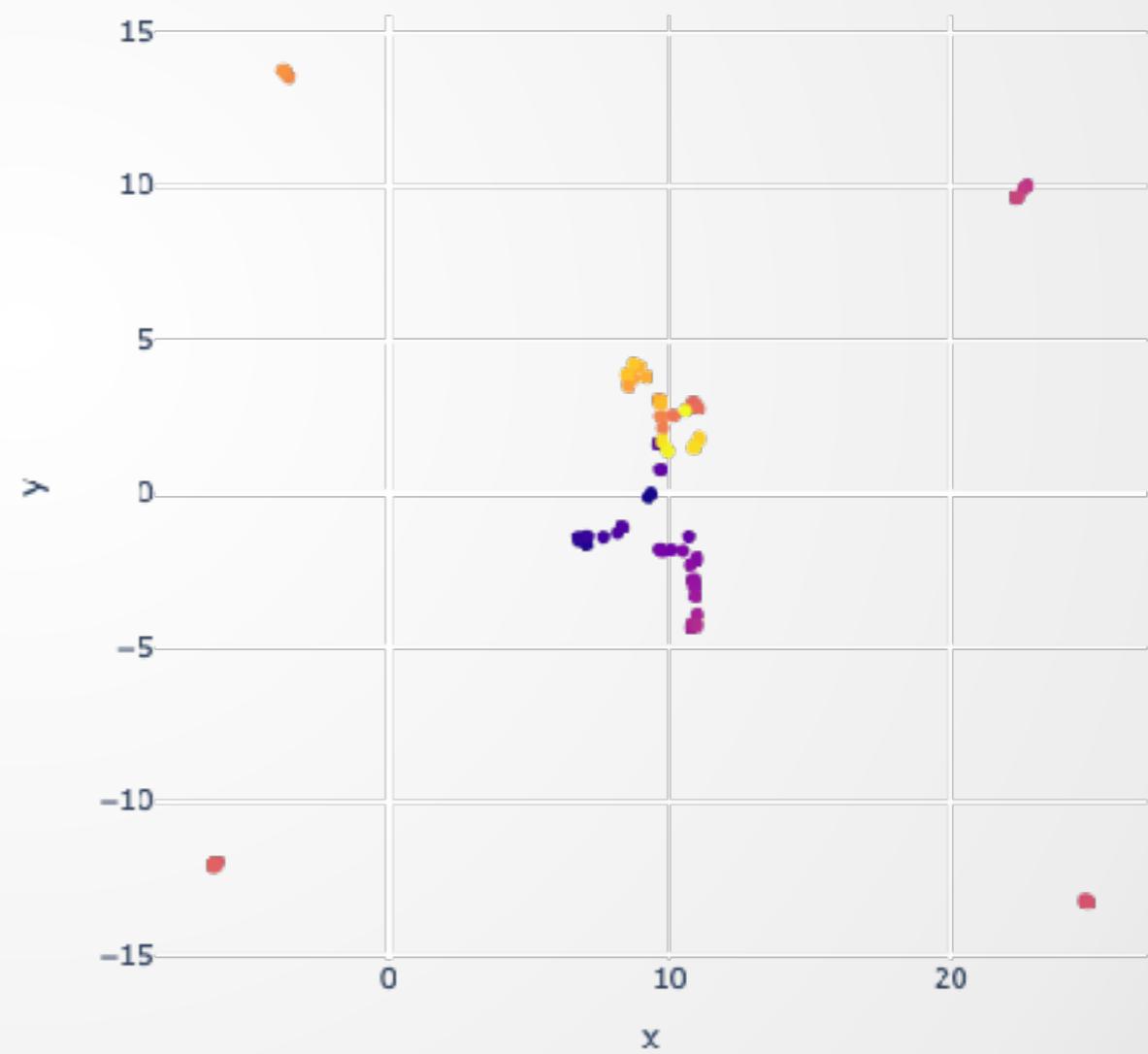
## Time Series Example: CRIX

- n\_neighbors = 3

CRIX time series



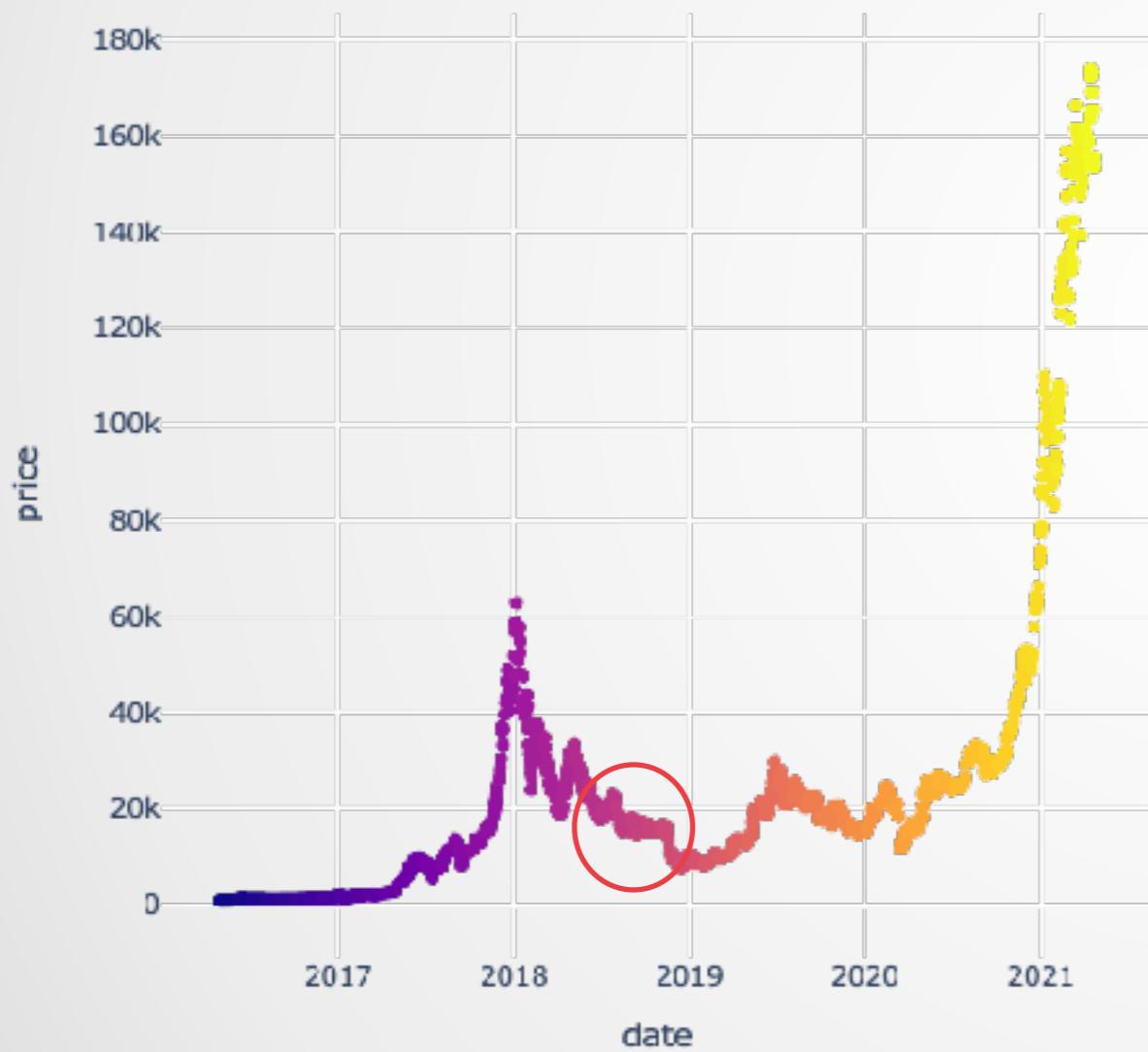
UMAP CRIX



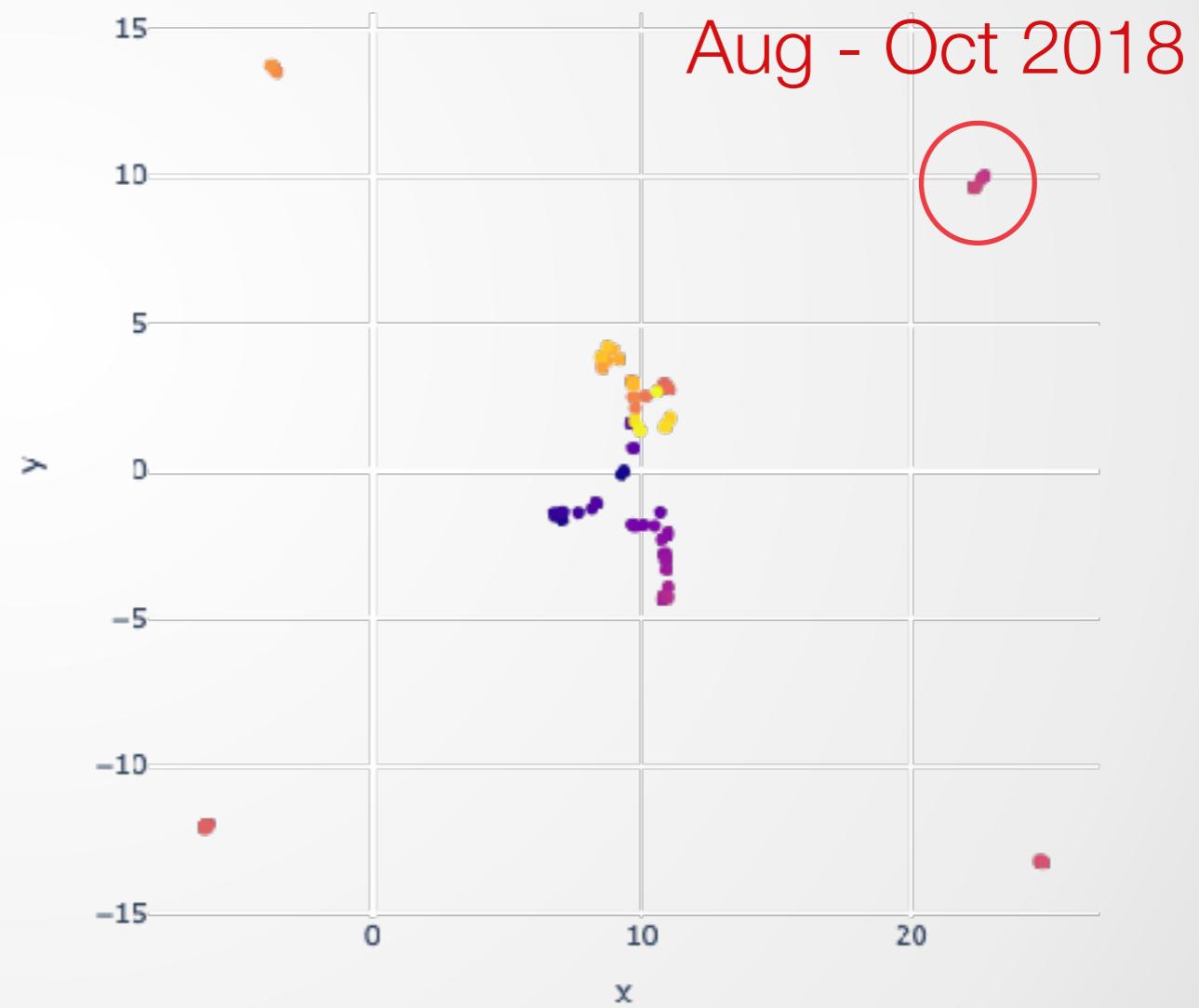
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CRIX time series



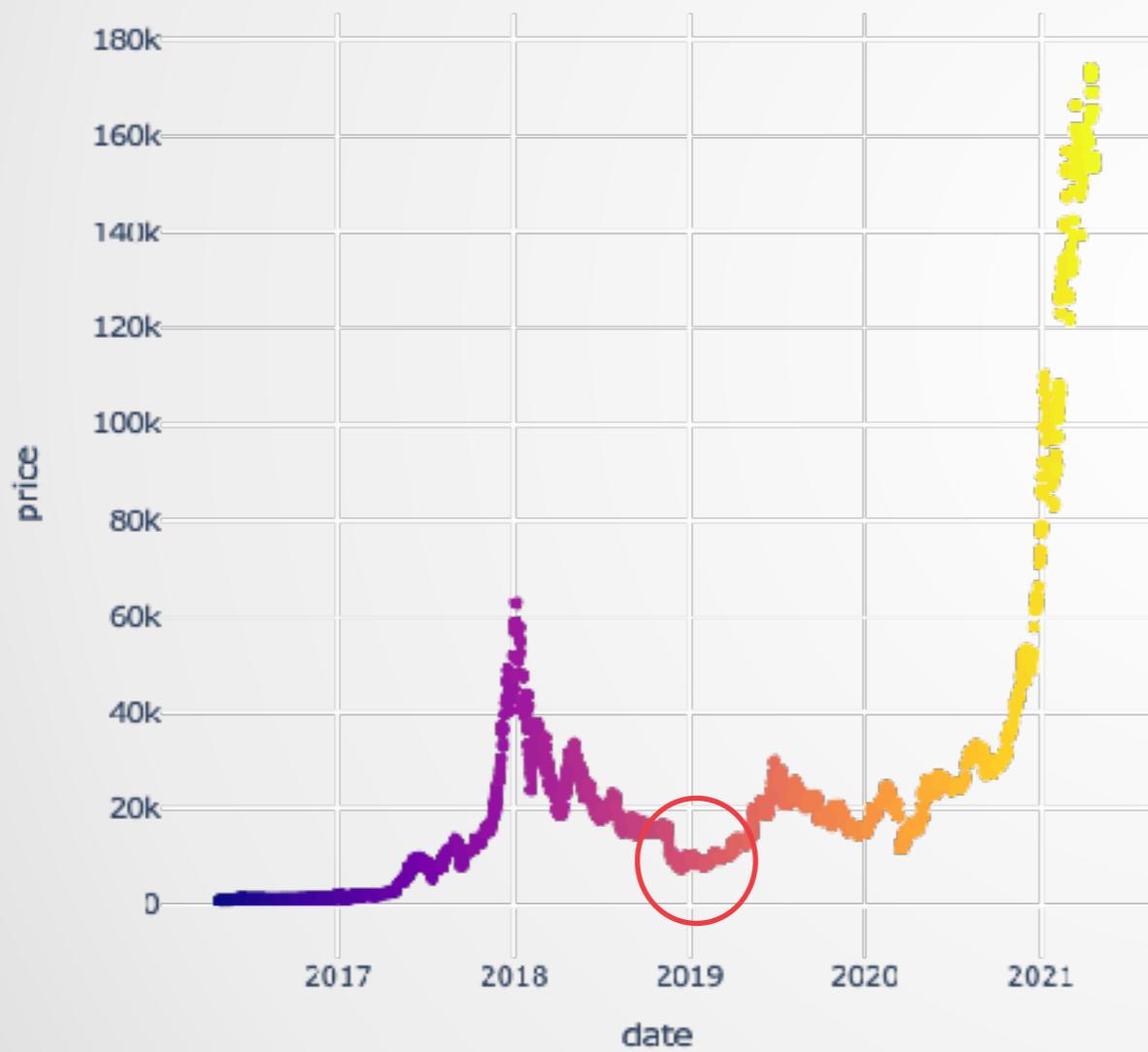
UMAP CRIX



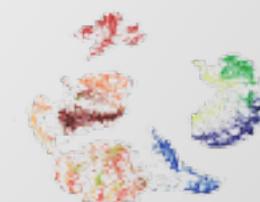
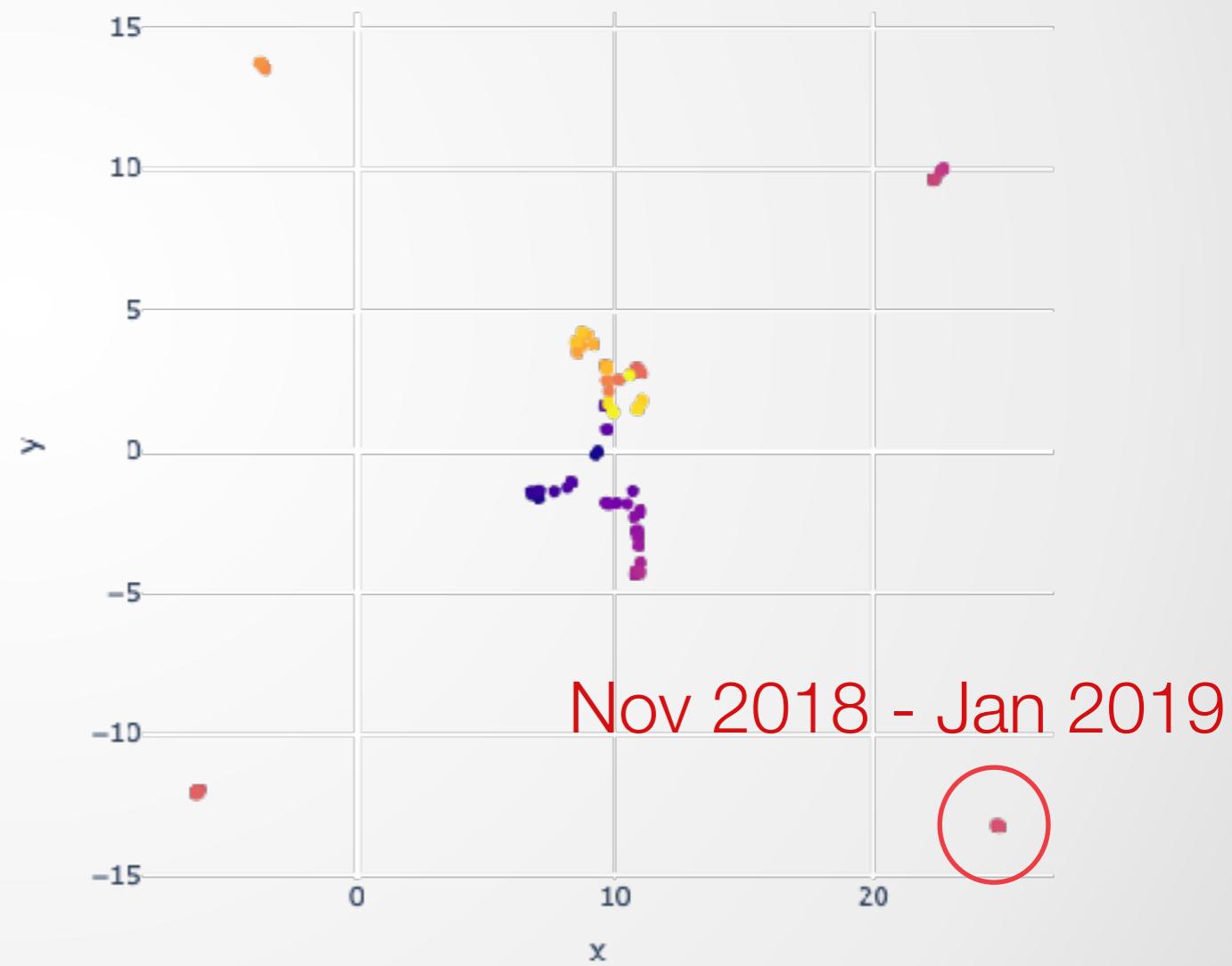
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CRIX time series



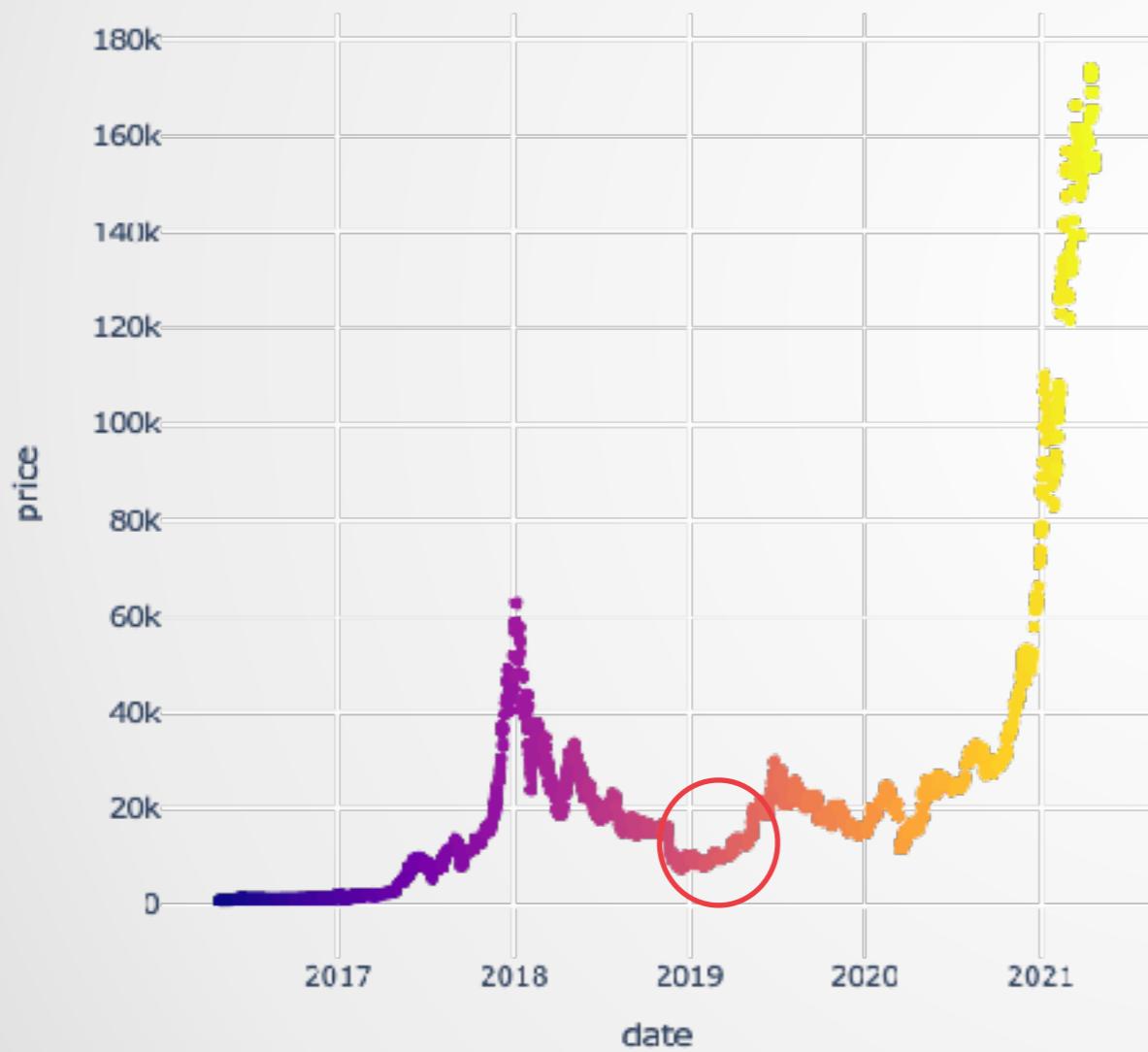
UMAP CRIX



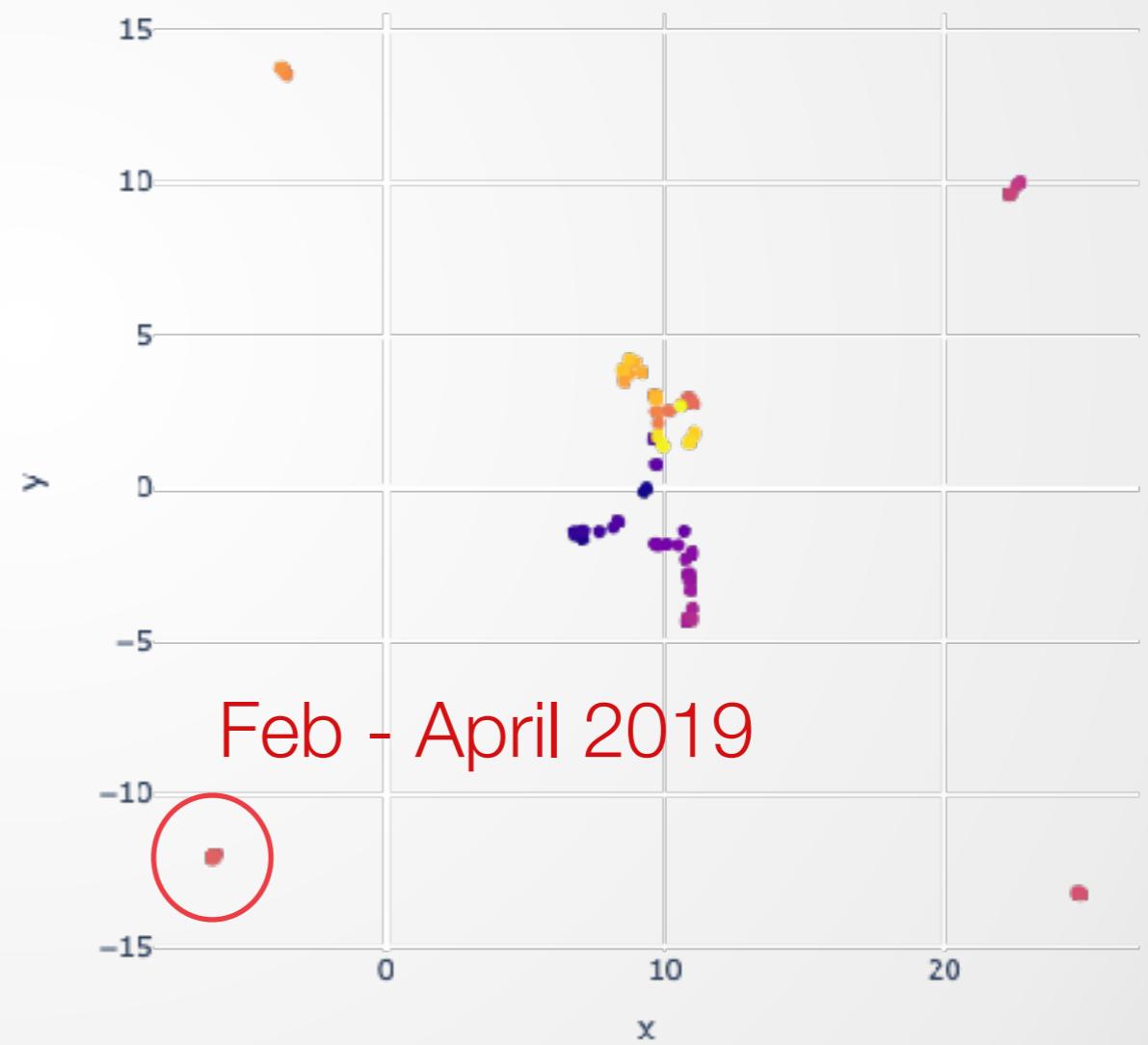
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CRIX time series



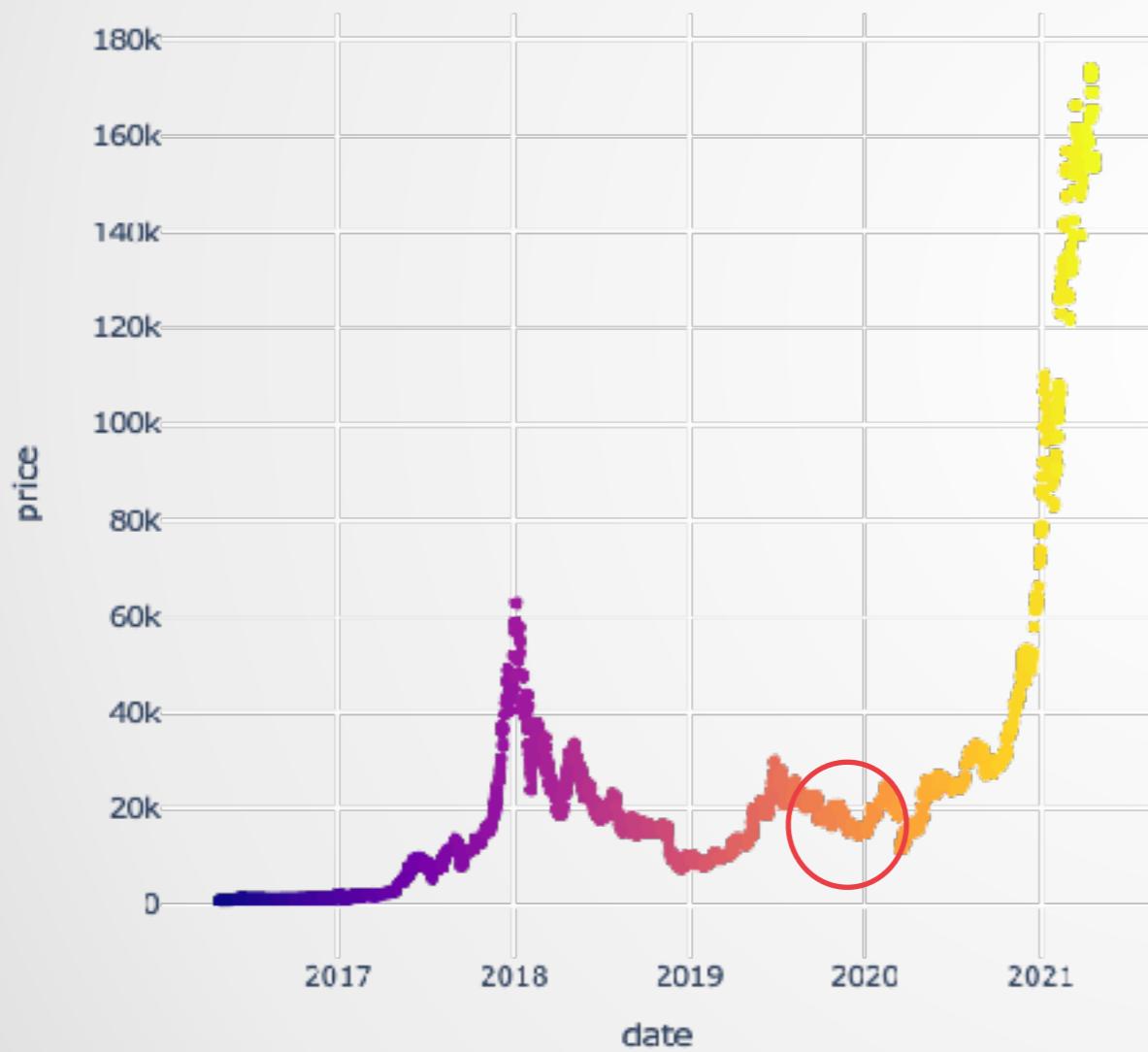
UMAP CRIX



## Time Series Example: CRIX

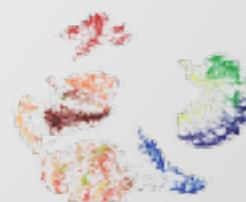
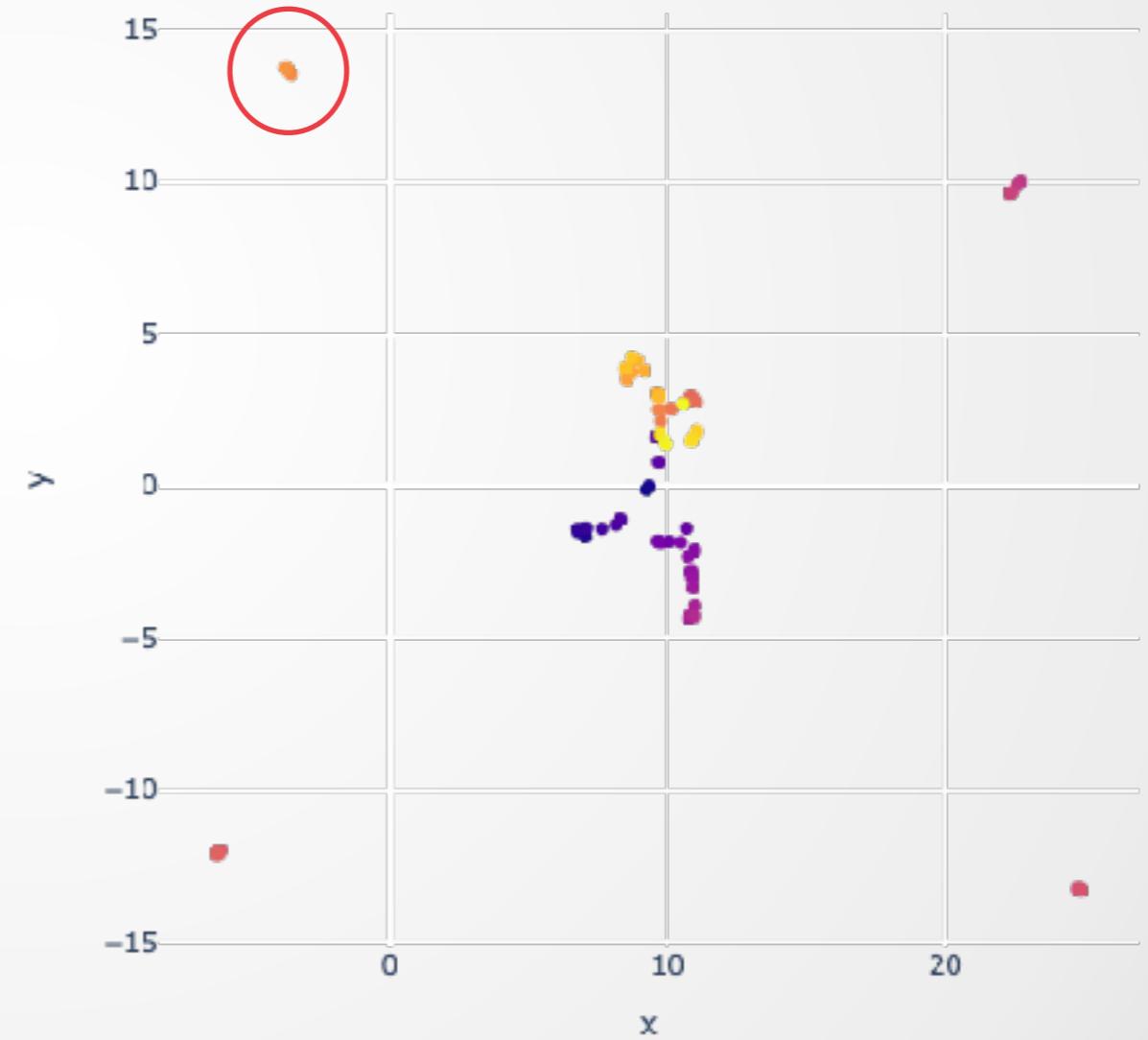
- n\_neighbors = 3

CRIX time series



UMAP CRIX

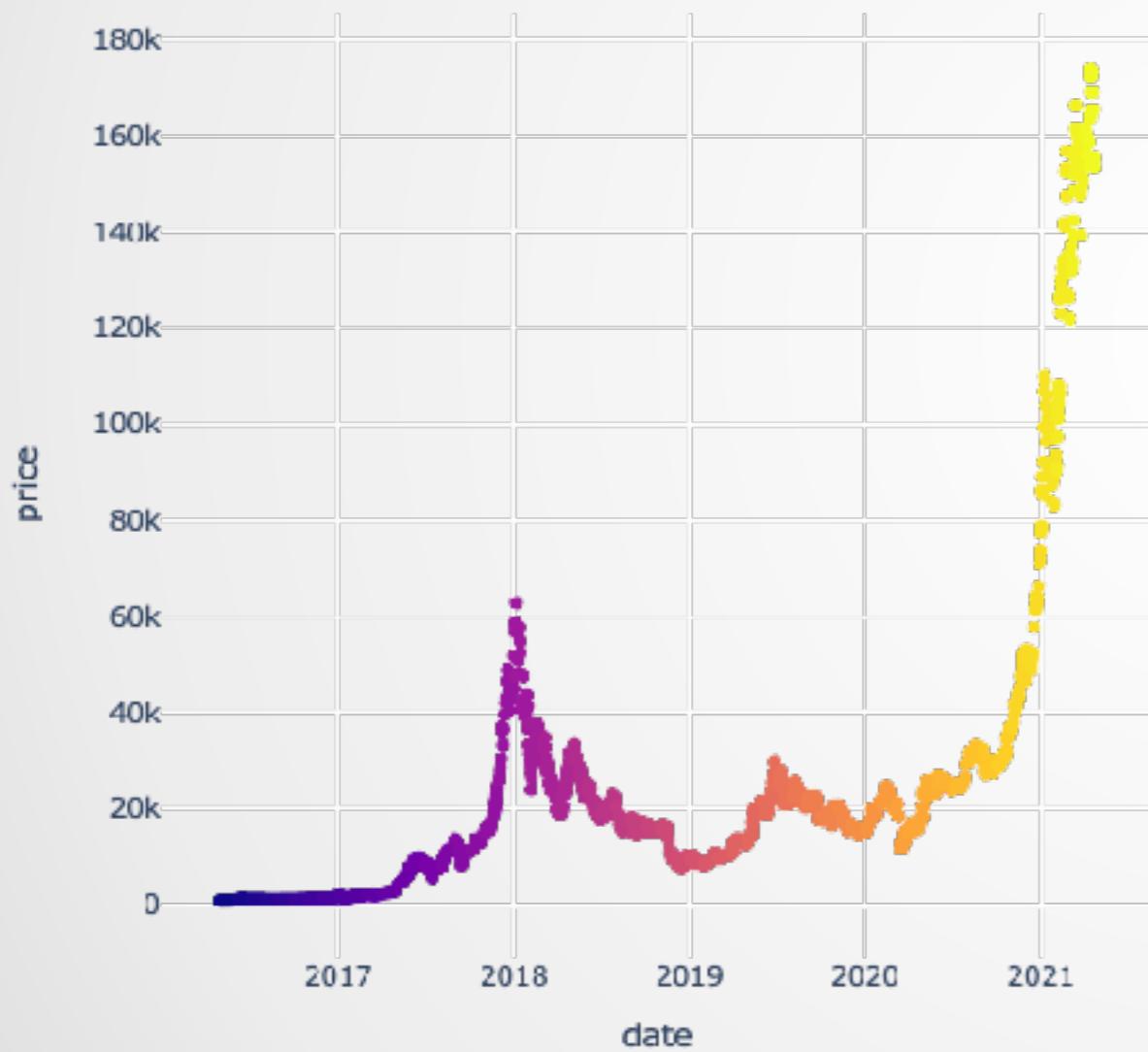
Nov 2019 - Jan 2020



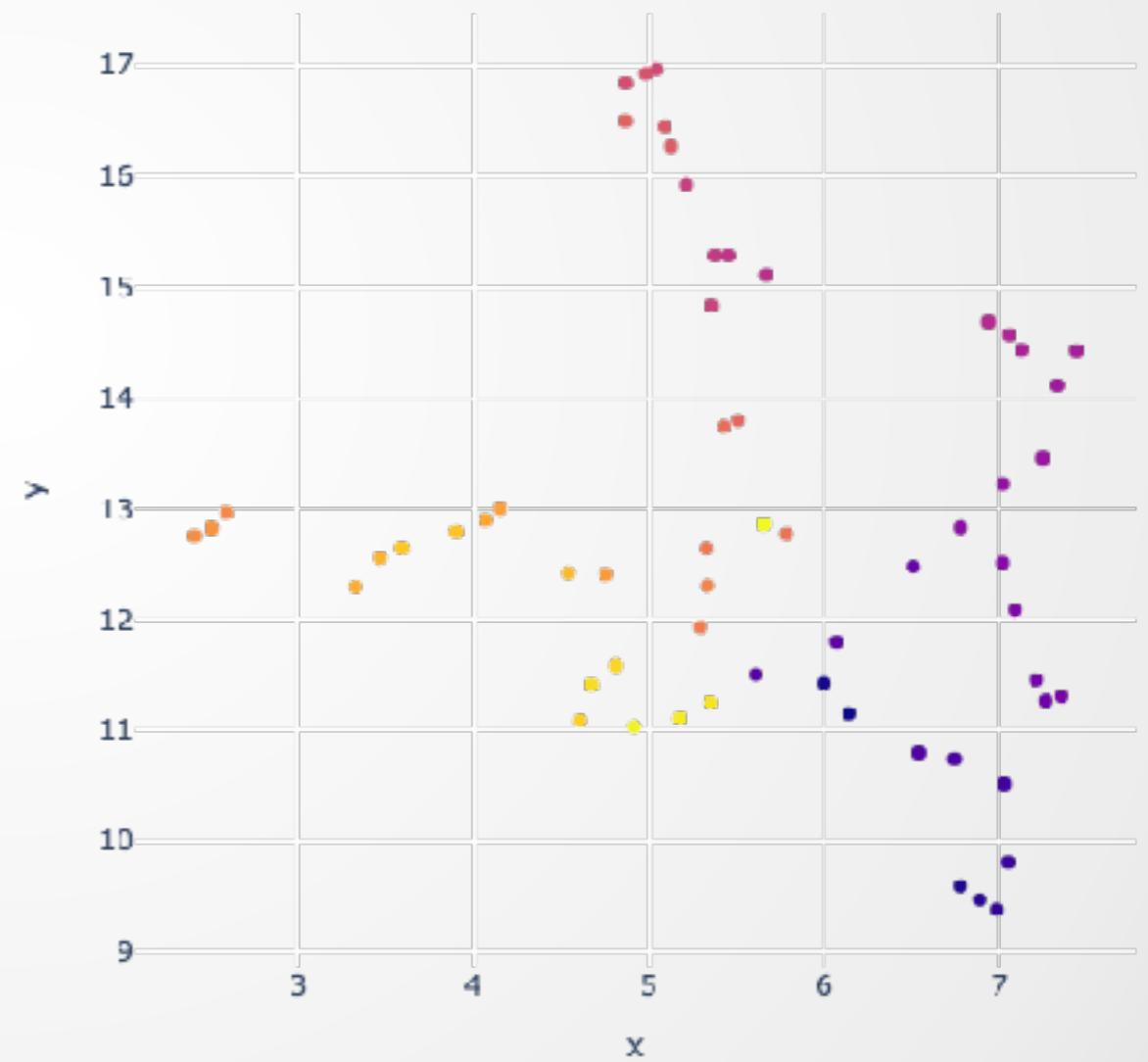
## Time Series Example: CRIX

- $n_{neighbors} = 5$

CRIX time series



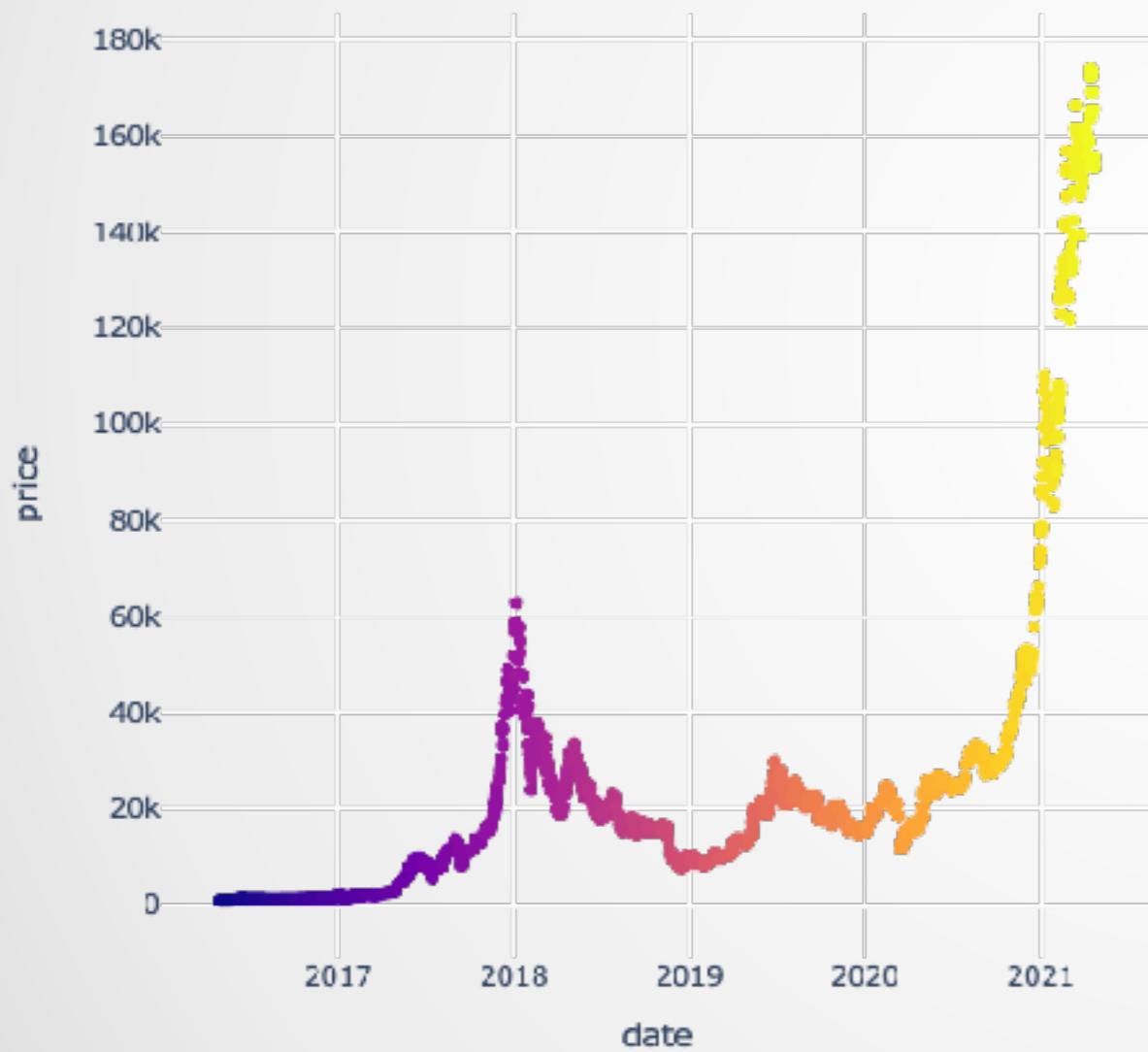
UMAP CRIX



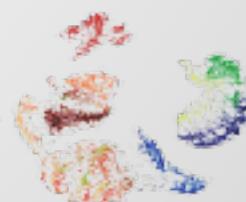
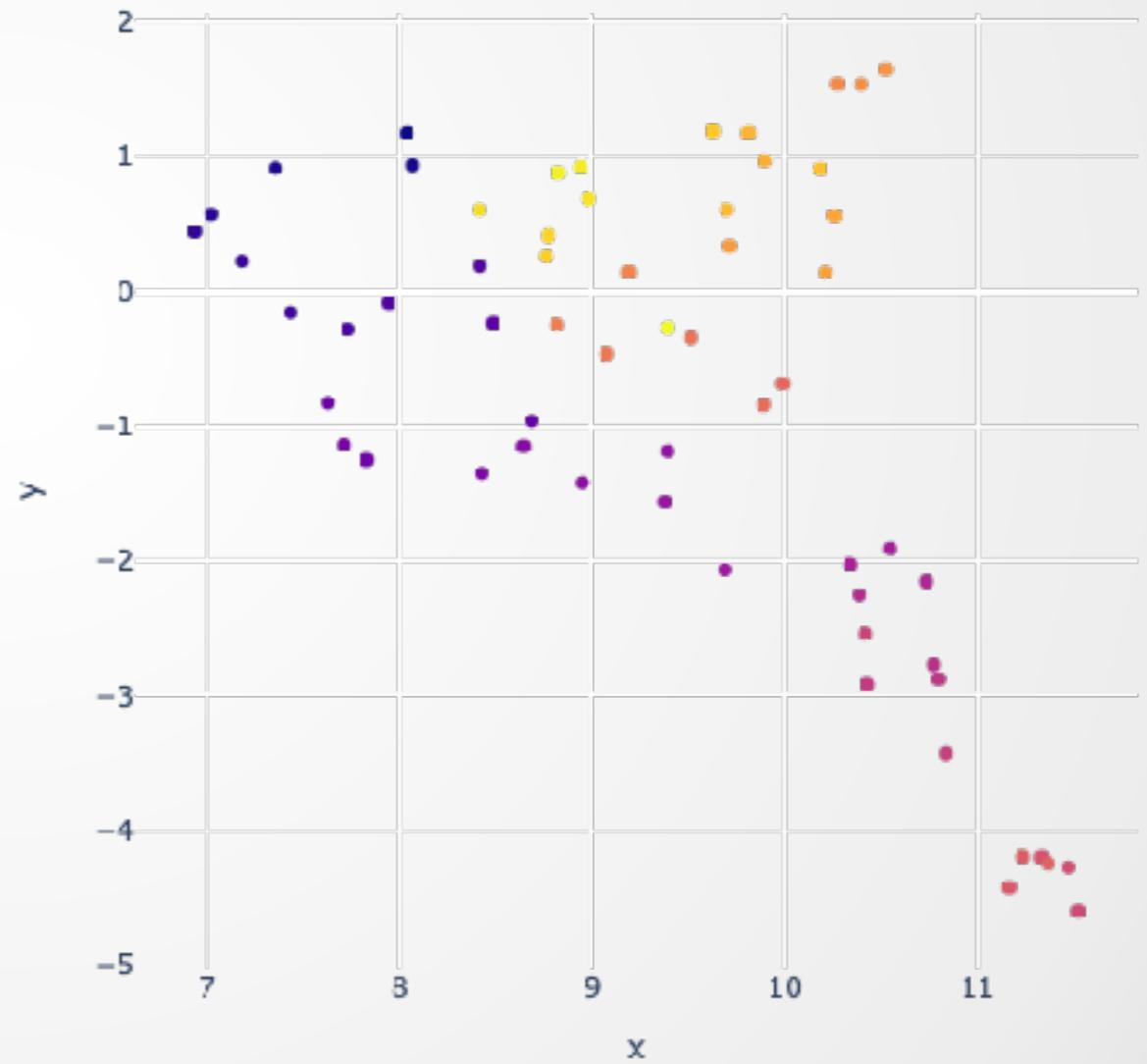
# Time Series Example: CRIX

- ☐  $n_{neighbors} = 12$

CRIX time series

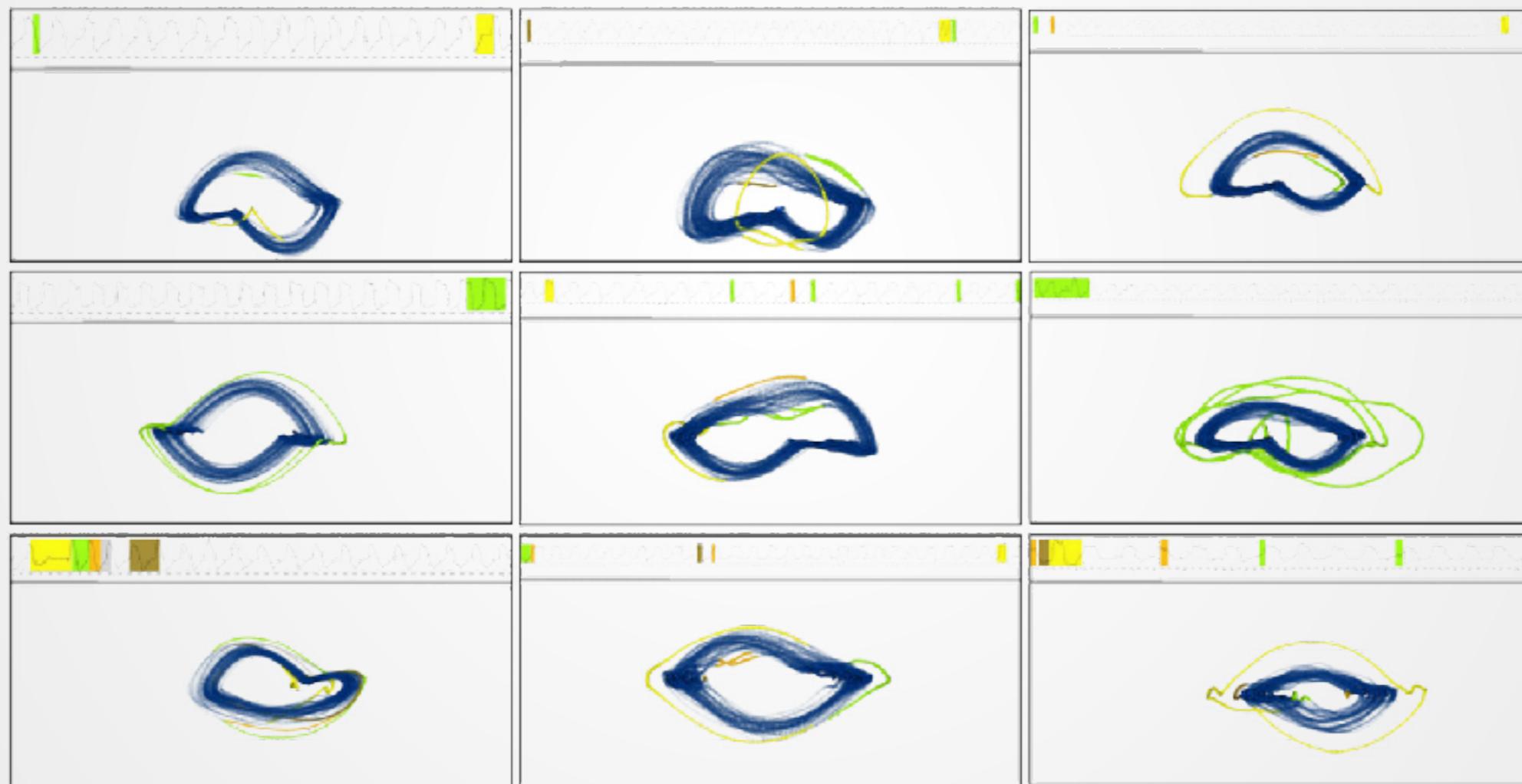


UMAP CRIX



## Real data example: Ali, Jones, Xie et al. (2019)

- UMAP of breathing patterns
- Diagnosis of problematic breathing patterns possible (Fig. 6)

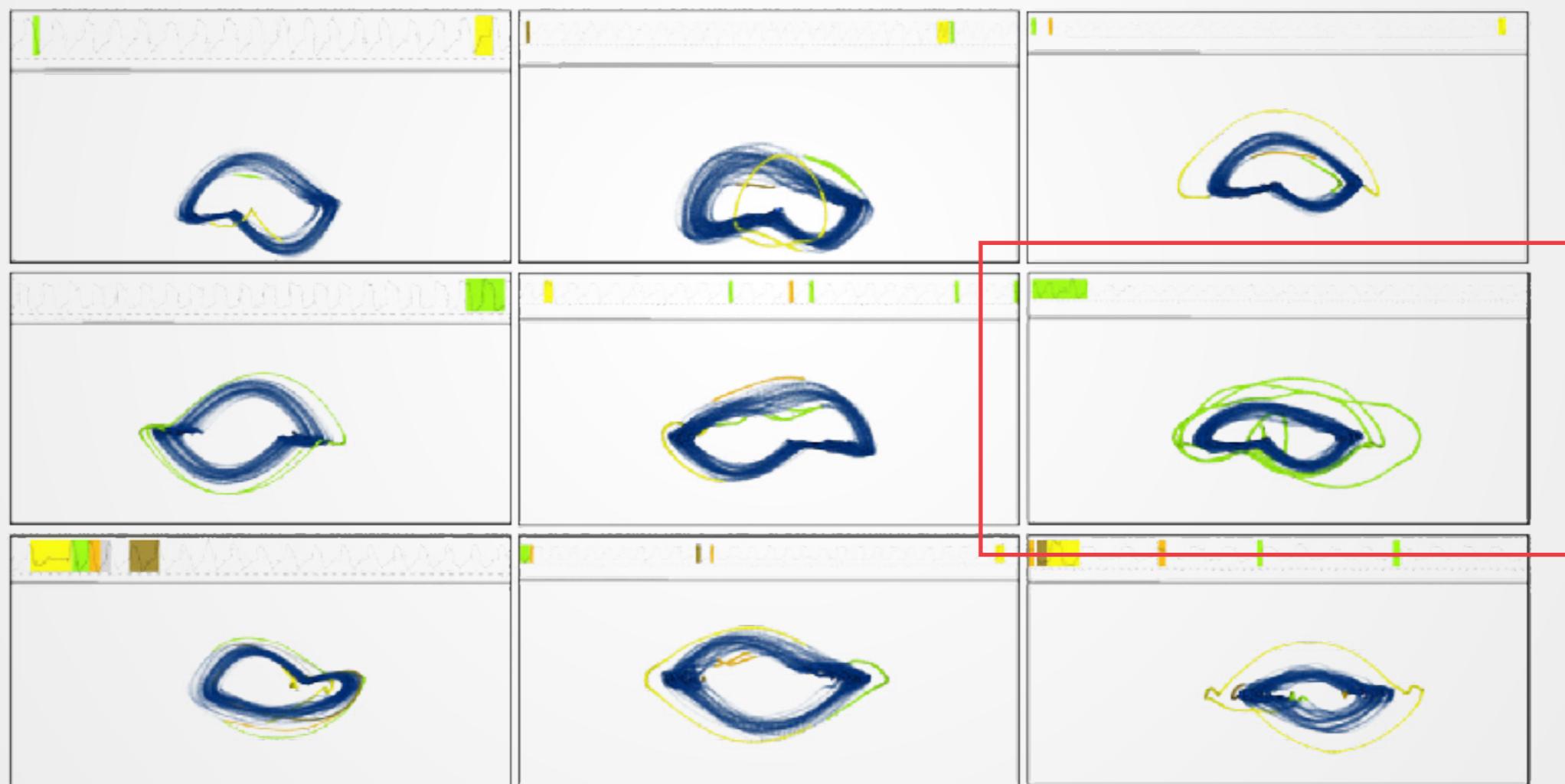


Source: Ali, M., Jones, M.W., Xie, X. et al. TimeCluster: dimension reduction applied to temporal data for visual analytics. *Vis Comput* 35, 1013–1026 (2019). <https://doi.org/10.1007/s00371-019-01673-y>



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## UMAP bottomline

- Useful dimension reduction technique
- Can serve as intermediate step to increase classification accuracy of high dimensional data
- Computationally fast
- Recovers local and global structure



## Cost function

*t*-SNE: KL-divergence

Impossible to preserve global  
distances

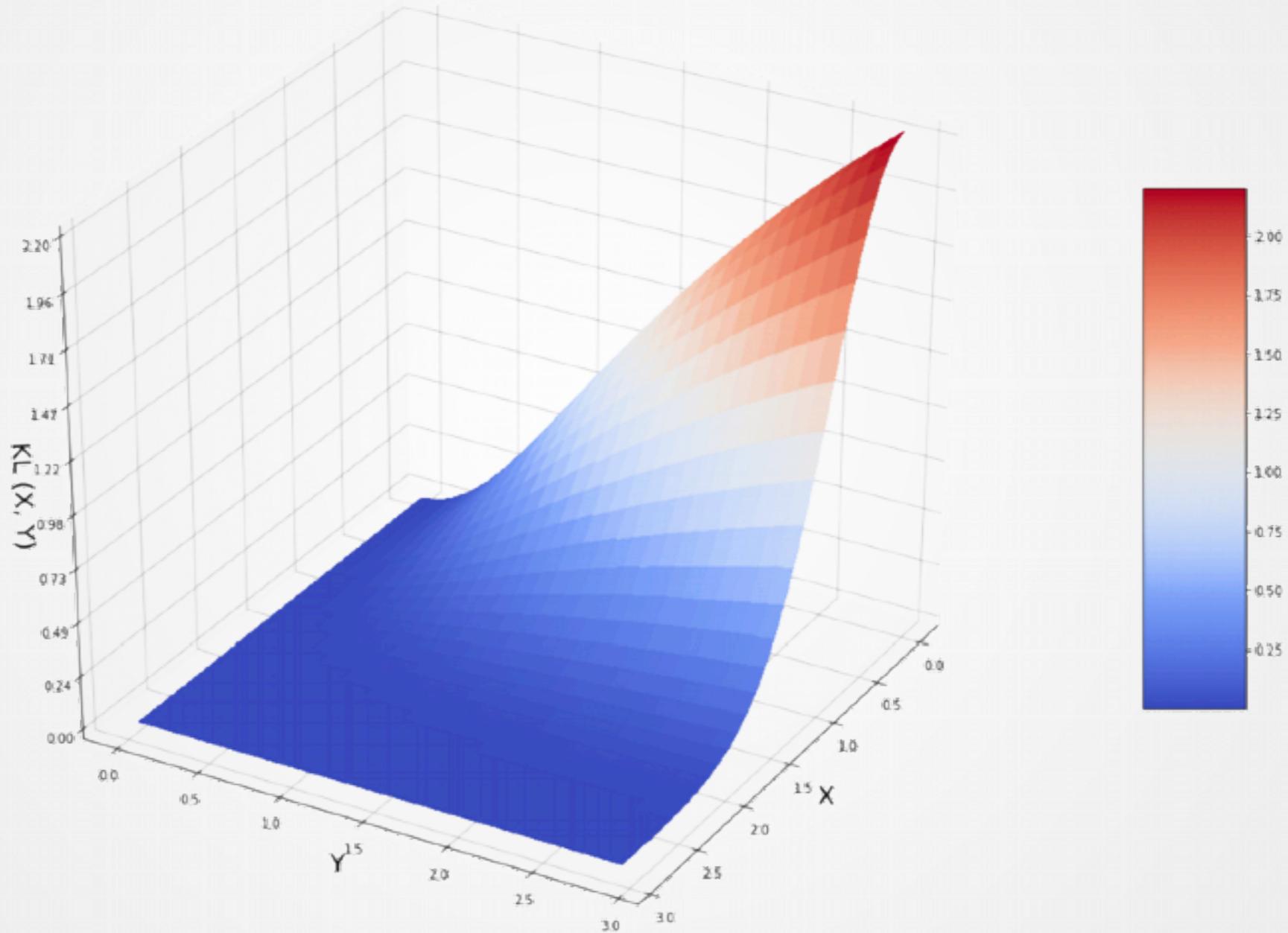
UMAP: Cross Entropy (CE)

Smarter cost function to preserve  
global distances



## KL-divergence

- Large X does not guarantee a large Y



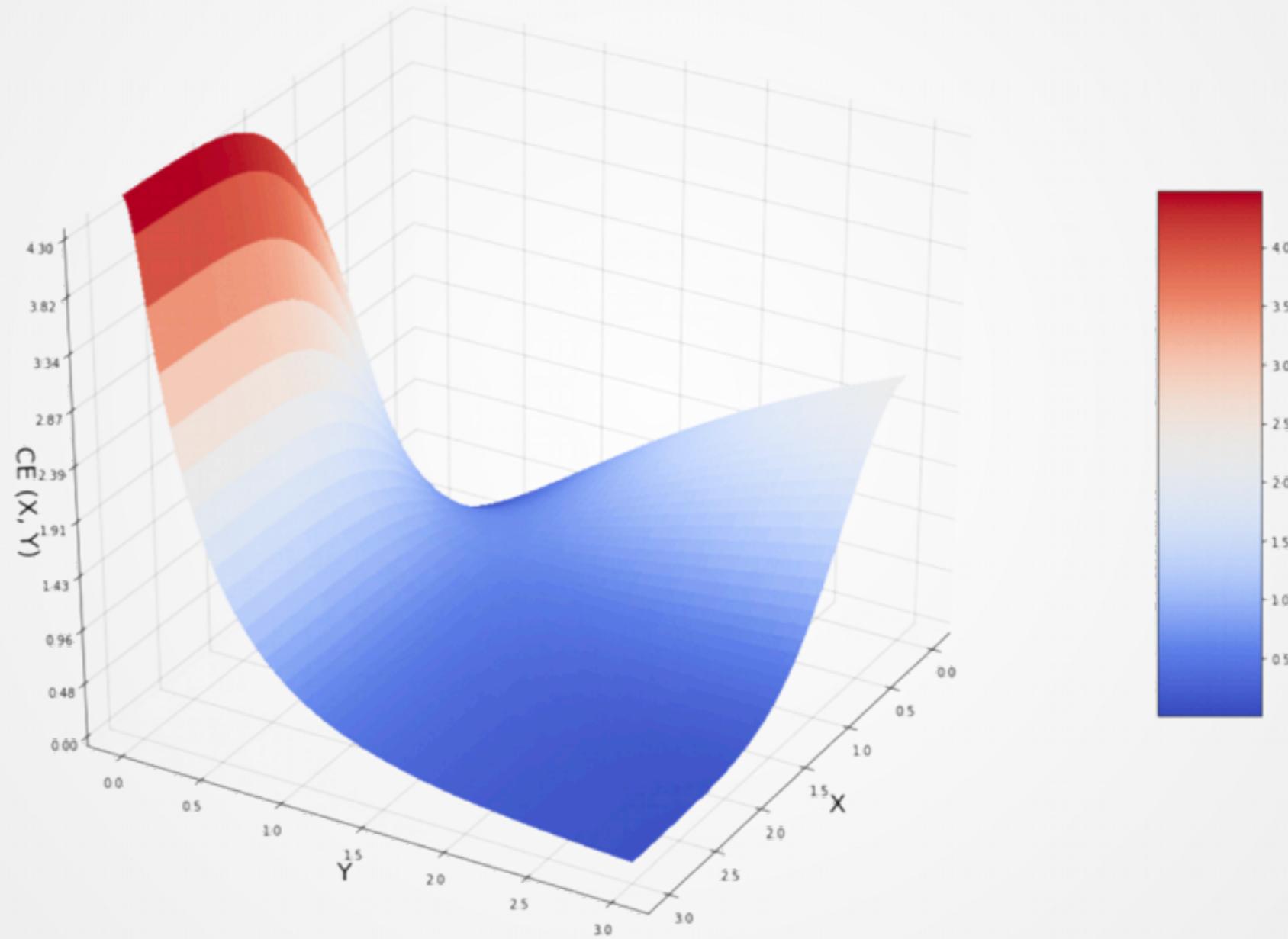
X: distance between points in high dimensions

Y: distance between points in low dimensions



## Cross Entropy (CE)

- Large X, get a huge CE penalty when Y is small

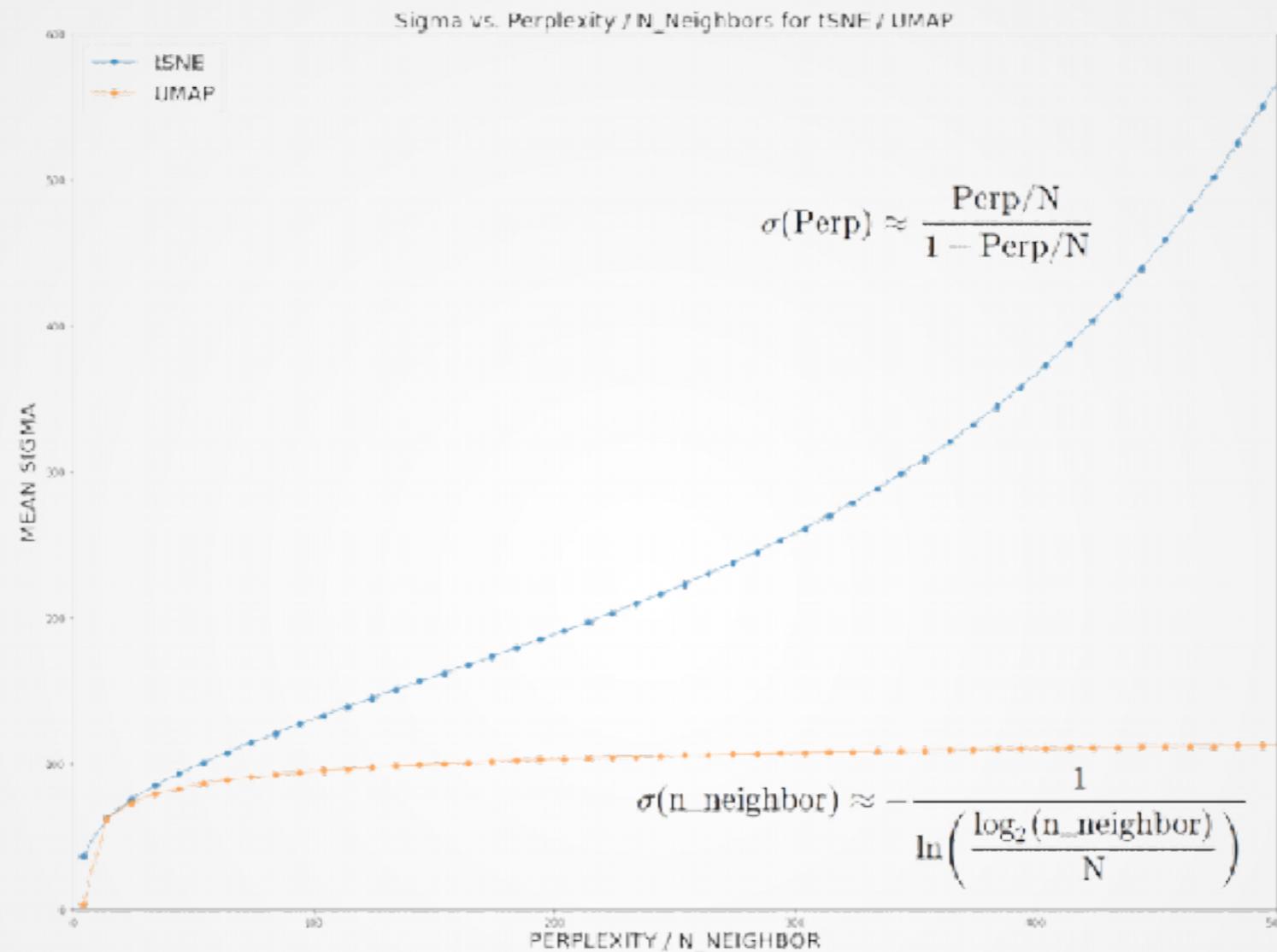


X: distance between points in high dimensions

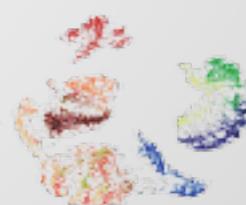
Y: distance between points in low dimensions



## Sensitivity towards hyperparameters

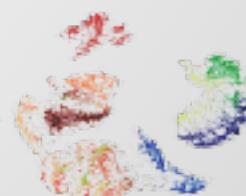


*t*-SNE is much more sensitive towards perplexity than UMAP towards *n\_neighbor*



## References

- <http://www.sci.utah.edu/~beiwang/teaching/cs6965-fall-2019/>
- <https://towardsdatascience.com/dimensionality-reduction-for-data-visualization-pca-vs-tsne-vs-umap-be4aa7b1cb29>
- <http://www.sci.utah.edu/~beiwang/teaching/cs6965-fall-2019/Lecture02-DR.pdf>
- [https://nbisweden.github.io/excelerate-scRNAseq/saession-dim-reduction/lecture\\_dimensionality\\_reduction.pdf](https://nbisweden.github.io/excelerate-scRNAseq/saession-dim-reduction/lecture_dimensionality_reduction.pdf)
- [https://github.com/deniederhut/Slides-SciPyConf-2018/blob/master/umap/SciPy2018\\_UMAP.pdf](https://github.com/deniederhut/Slides-SciPyConf-2018/blob/master/umap/SciPy2018_UMAP.pdf)
- <https://speakerdeck.com/lmcinnes/umap-uniform-manifold-approximation-and-projection-for-dimension-reduction?slide=59>



## References

- <http://www.sci.utah.edu/~beiwang/teaching/cs6965-fall-2019/>
- <https://towardsdatascience.com/dimensionality-reduction-for-data-visualization-pca-vs-tsne-vs-umap-be4aa7b1cb29>
- <http://www.sci.utah.edu/~beiwang/teaching/cs6965-fall-2019/Lecture02-DR.pdf>
- [https://nbisweden.github.io/excelerate-scRNAseq/saession-dim-reduction/lecture\\_dimensionality\\_reduction.pdf](https://nbisweden.github.io/excelerate-scRNAseq/saession-dim-reduction/lecture_dimensionality_reduction.pdf)
- [https://github.com/deniederhut/Slides-SciPyConf-2018/blob/master/umap/SciPy2018\\_UMAP.pdf](https://github.com/deniederhut/Slides-SciPyConf-2018/blob/master/umap/SciPy2018_UMAP.pdf)
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