DLI Accelerated Data Science Teaching Kit

Lecture 15.5 - t-SNE

t-SNE

t-distributed Stochastic Neighbor Embedding

- Non-linear dimensionality reduction method developed for visualizing high-dimensional data in low-dimensional space (e.g., 2D, 3D) [1]
- Widely used in numerous fields and applications
- Main ideas
    - Models similarities between data points as joint probabilities
        - Similar (dissimilar) points assigned a higher (lower) probability
    - Represents each high-dimensional point by a low-dimensional version (e.g., 2D)
    - Minimizes KL divergence between the joint probabilities between originally high-dimensional data and low-dimensional representation

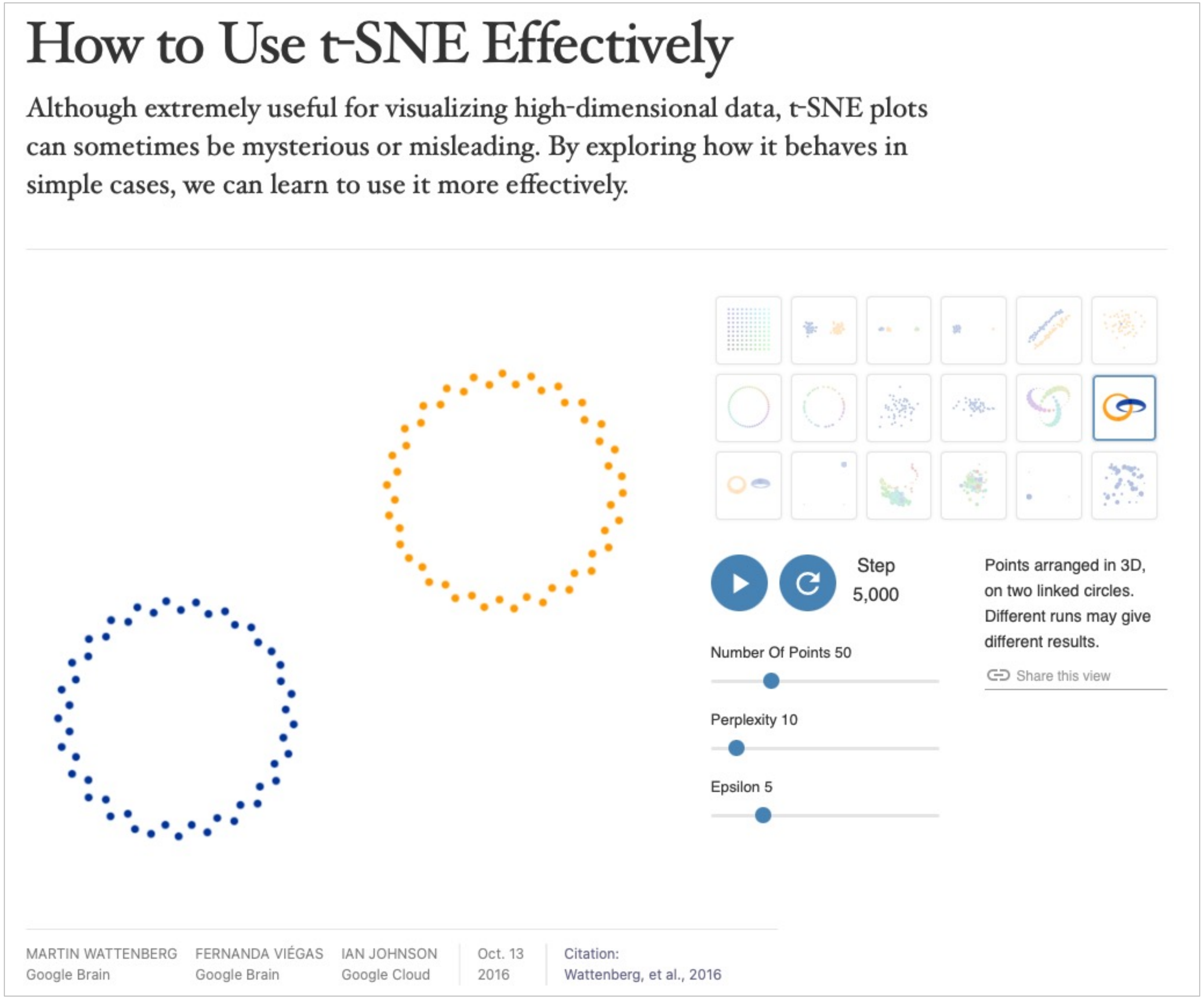
[1] L. v. d. Maaten and G. Hinton. Visualizing data using t-sne. Journal of machine learning research, 9(Nov):2579–2605, 2008.

t-SNE

t-distributed Stochastic Neighbor Embedding

- For super-high dimensional data, typically first apply another dimensionality reduction method (e.g., SVD)
- Can help discover patterns other techniques cannot (e.g., when linear assumptions violated for PCA)
- Extension over SNE
    - t-SNE uses heavy-tailed t-distribution (vs Gaussian)
    - Suitable for reducing to a very low dimensions (e.g., 2D)
- Used to be considered a “slow” method (solving n-body problem)
- Now has fast approximate algorithms, and GPU acceleration (available in RAPIDS)

[1] L. v. d. Maaten and G. Hinton. Visualizing data using t-sne. Journal of machine learning research, 9(Nov):2579–2605, 2008.



How to Use t-SNE Effectively

Although extremely useful for visualizing high-dimensional data, t-SNE plots can sometimes be mysterious or misleading. By exploring how it behaves in simple cases, we can learn to use it more effectively.

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Citation: Wattenberg, et al., 2016

Important Considerations when Using t-SNE

Try at https://distill.pub/2016/misread-tsne/

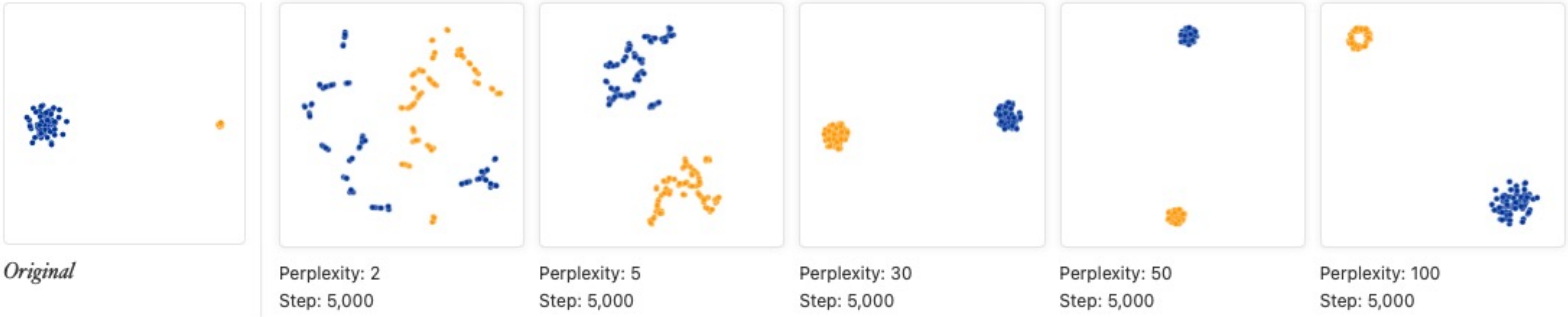
1. Hyperparameters really matter

Perplexity recommended to be 5-50. Should be smaller than number of data points.

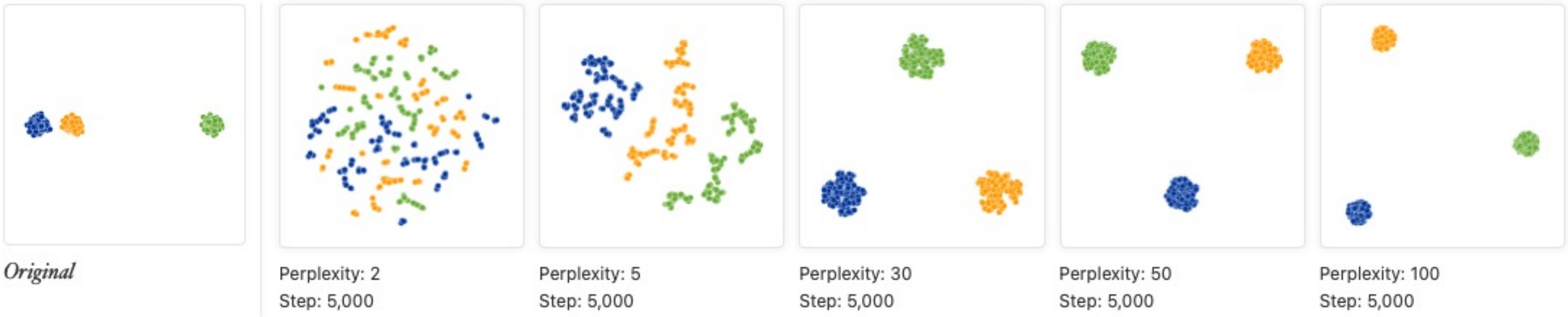
1. Hyperparameters really matter

“Pinched” may indicate stopping too early. Should wait until convergence.

2. Cluster sizes in a t-SNE plot mean nothing



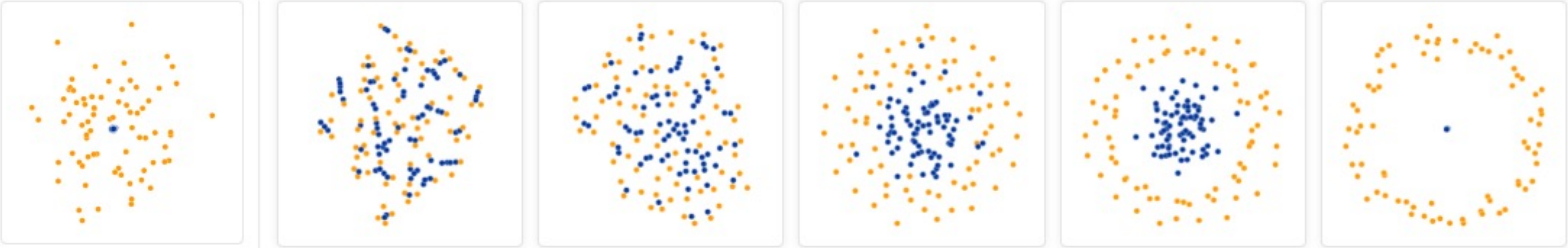
3. Distances between clusters might not mean anything



5. You can see some shapes, sometimes

See shapes as “right” perplexity. t-SNE tends to magnify dense regions.

6. For topology, you may need more than one plot



Original

Perplexity: 2
Step: 5,000

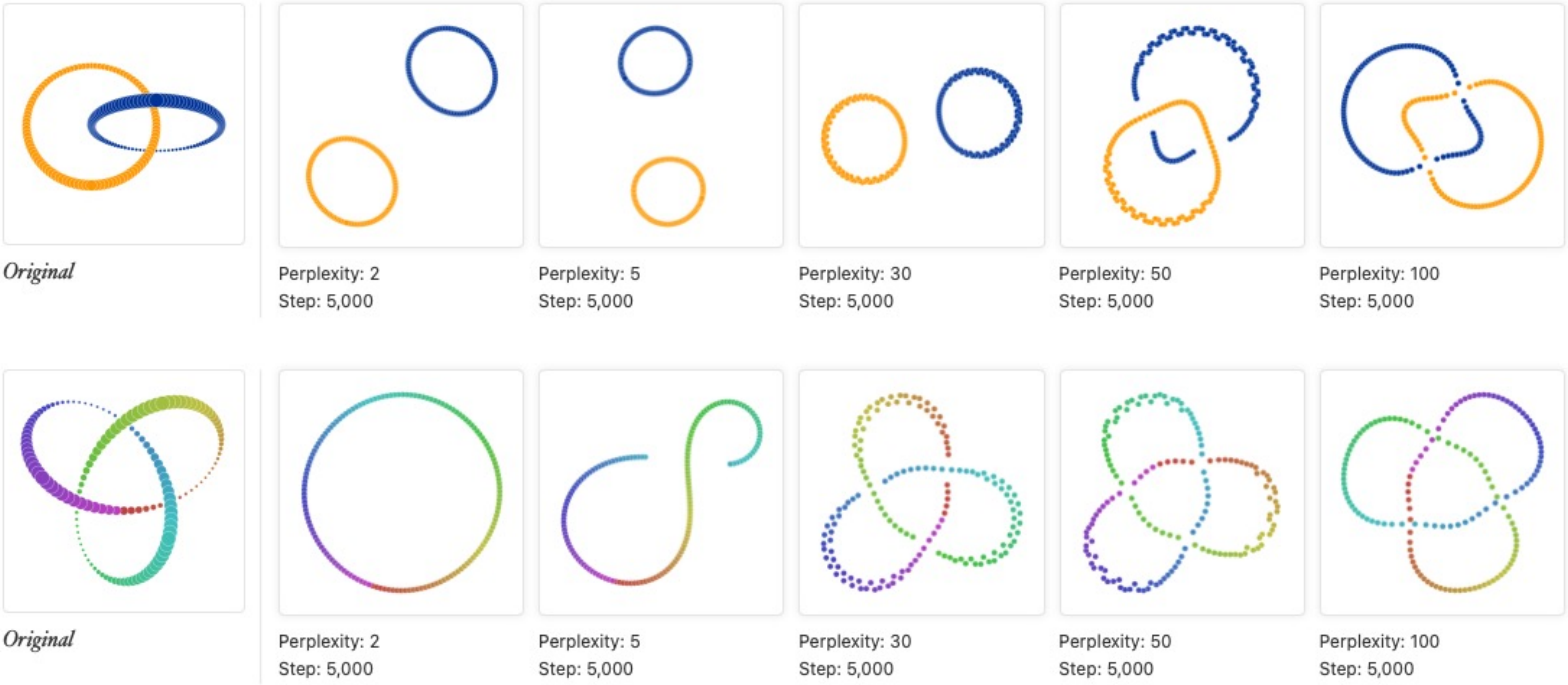
Perplexity: 5
Step: 5,000

Perplexity: 30
Step: 5,000

Perplexity: 50
Step: 5,000

Perplexity: 100
Step: 5,000

6. For topology, you may need more than one plot



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Thank You