UMAP + MAPPER

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UMAPPER

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UMAP and MAPPER are both data visualization methods

Can we combine them?

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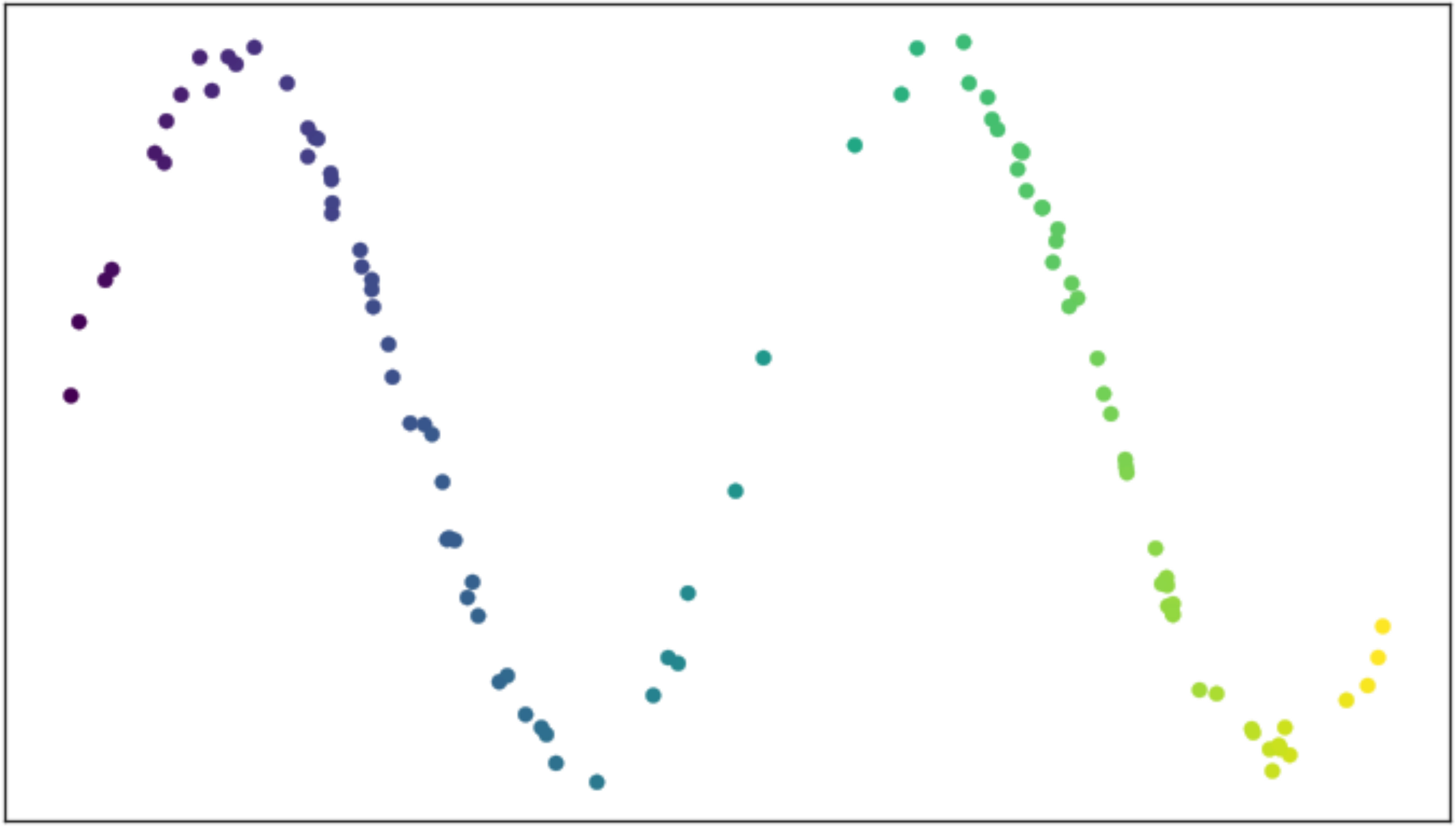
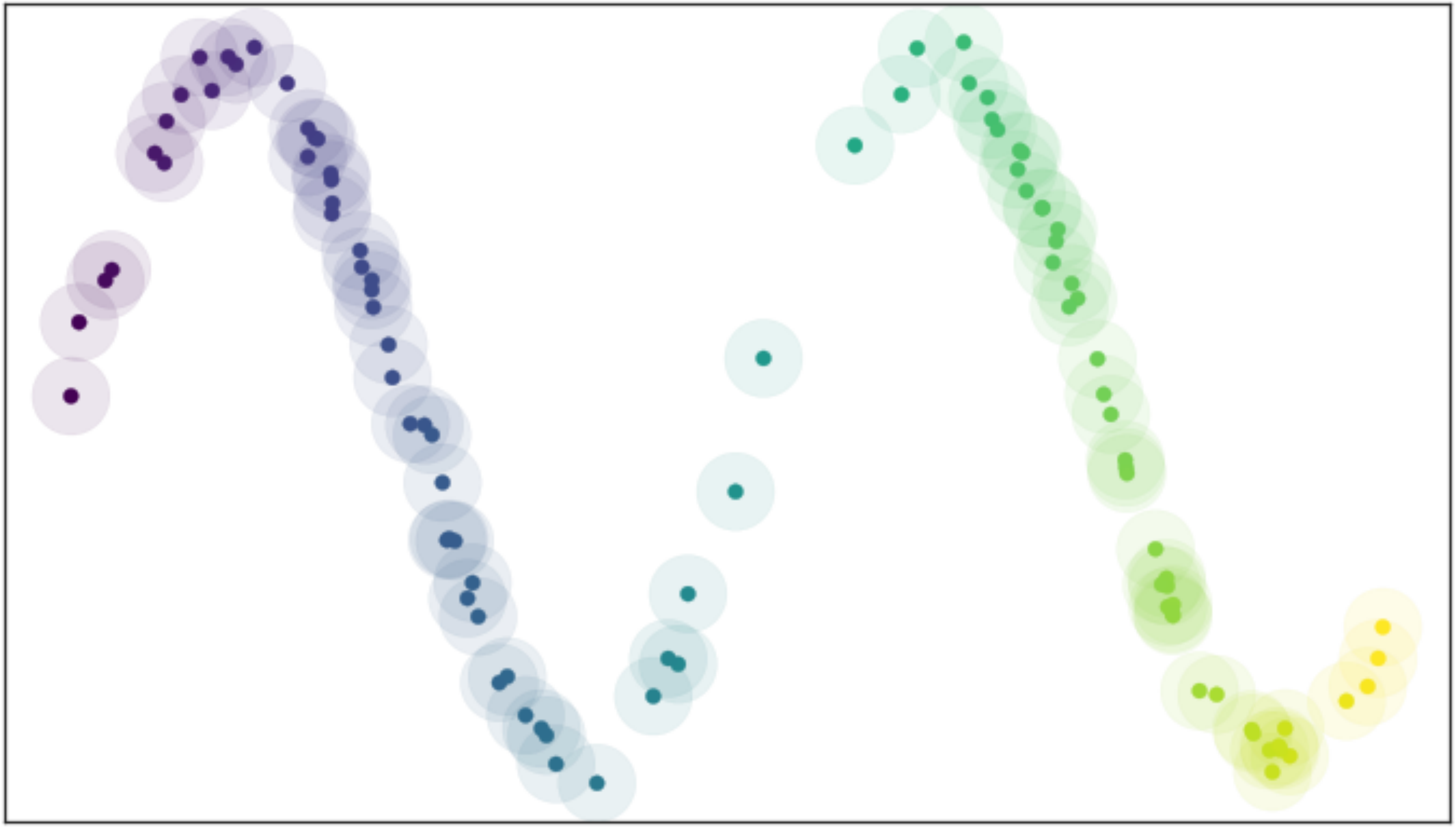
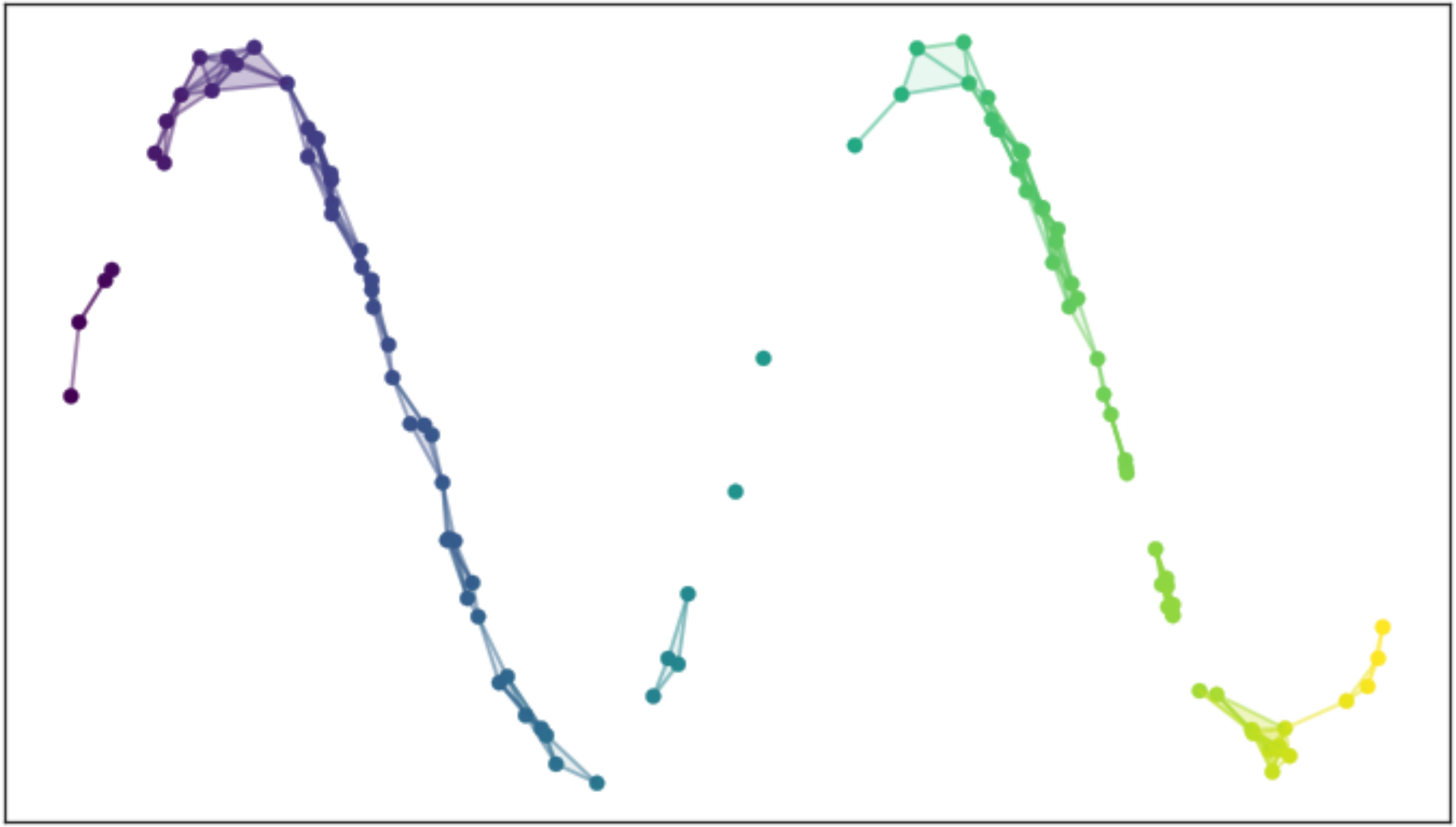
UMAP

McInnes, Healy and Melville 2018

UMAP is a dimension reduction technique using basic topology







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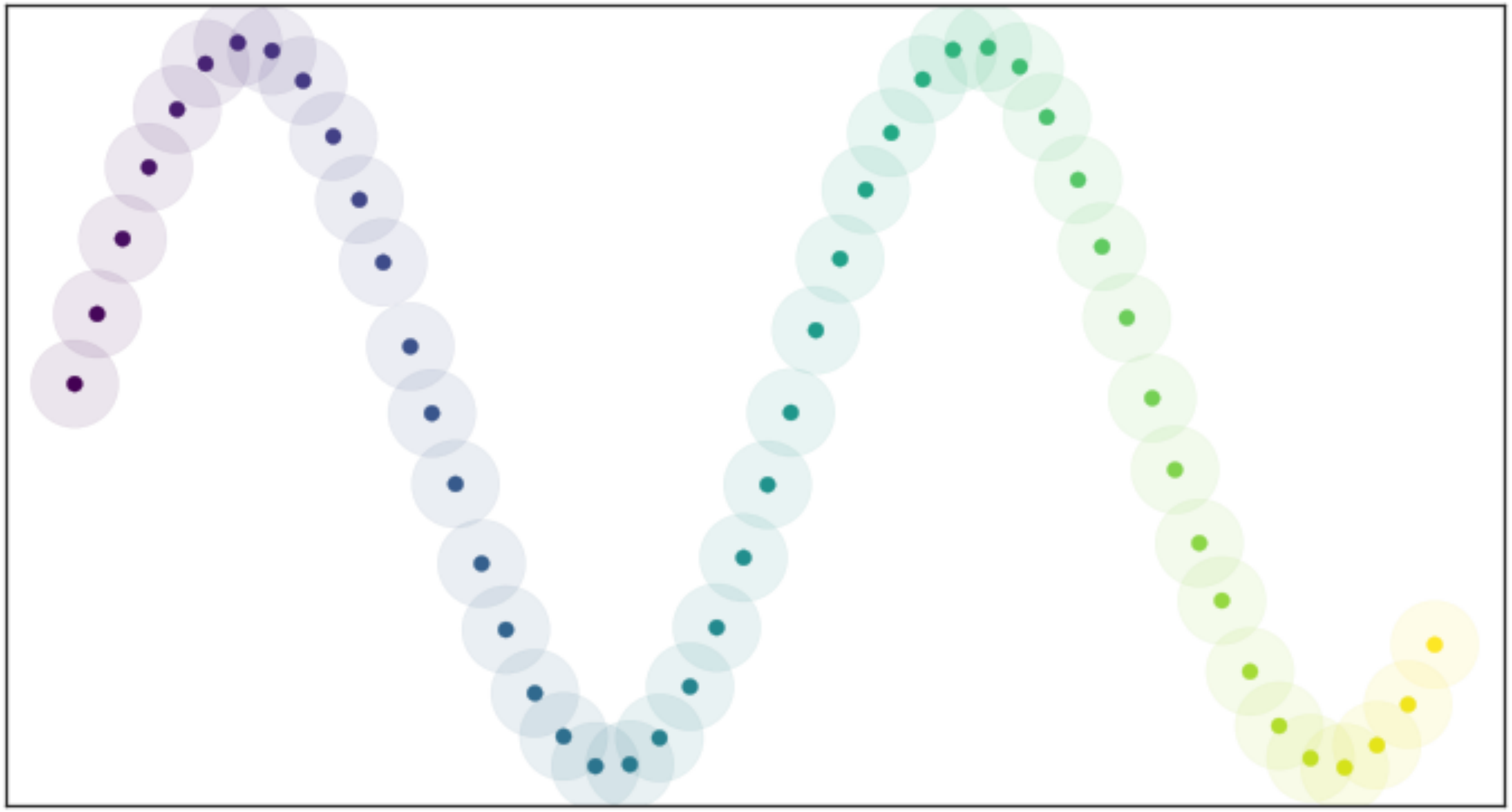
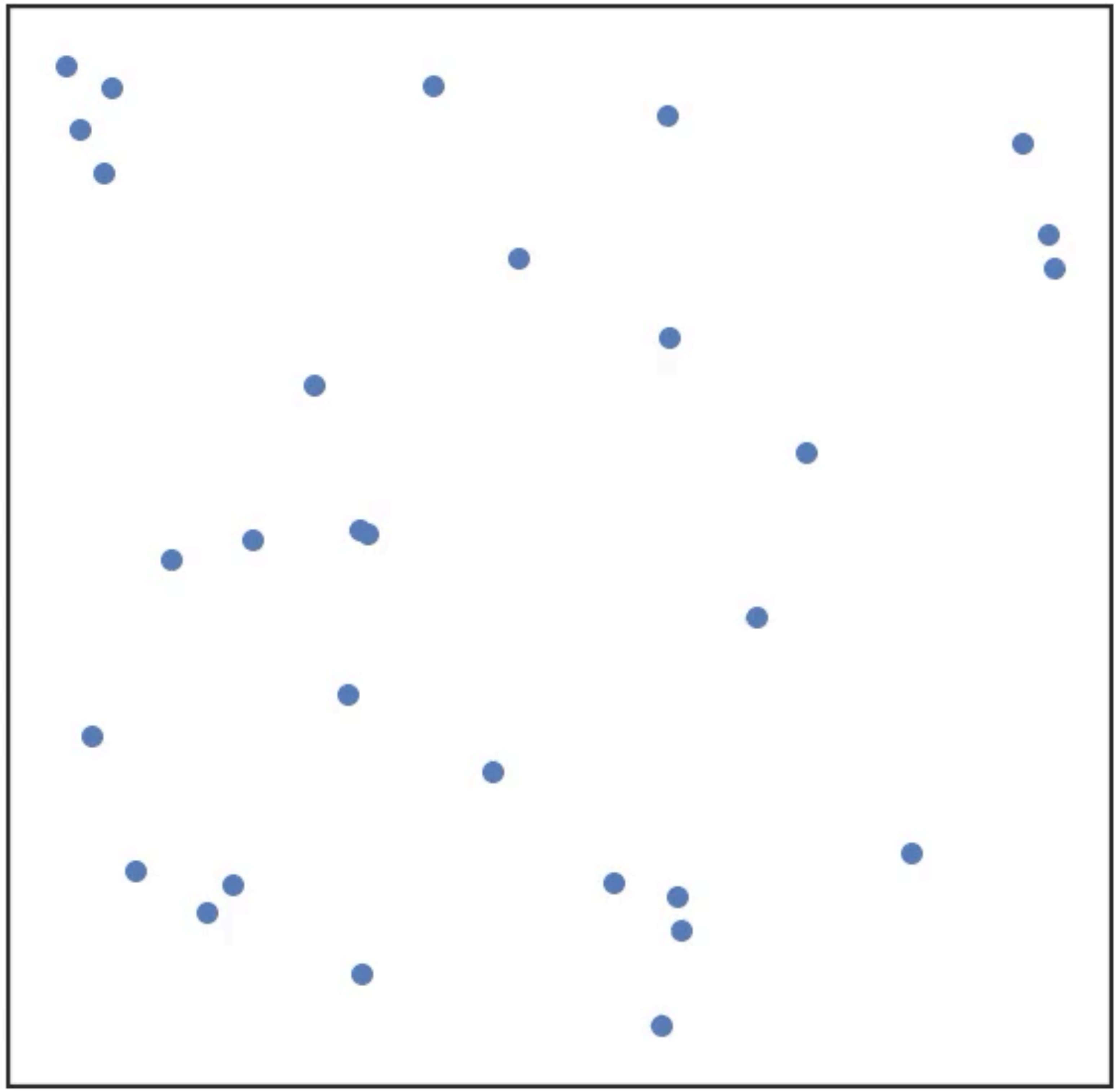
If the data is uniformly distributed on the manifold then the cover will be "good"



Vary the notion of distance according to the density



We can derive probabilistic weights to simplices based on when they form

Suppose we were given a low dimensional representation

We can apply the same process to get a probabilistic graph!

Now measure the distance between the graphs using cross-entropy and optimize

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$$\sum_{a \in A} \mu(a) \log\left(\frac{\mu(a)}{\nu(a)}\right) + (1 - \mu(a)) \log\left(\frac{1 - \mu(a)}{1 - \nu(a)}\right)$$

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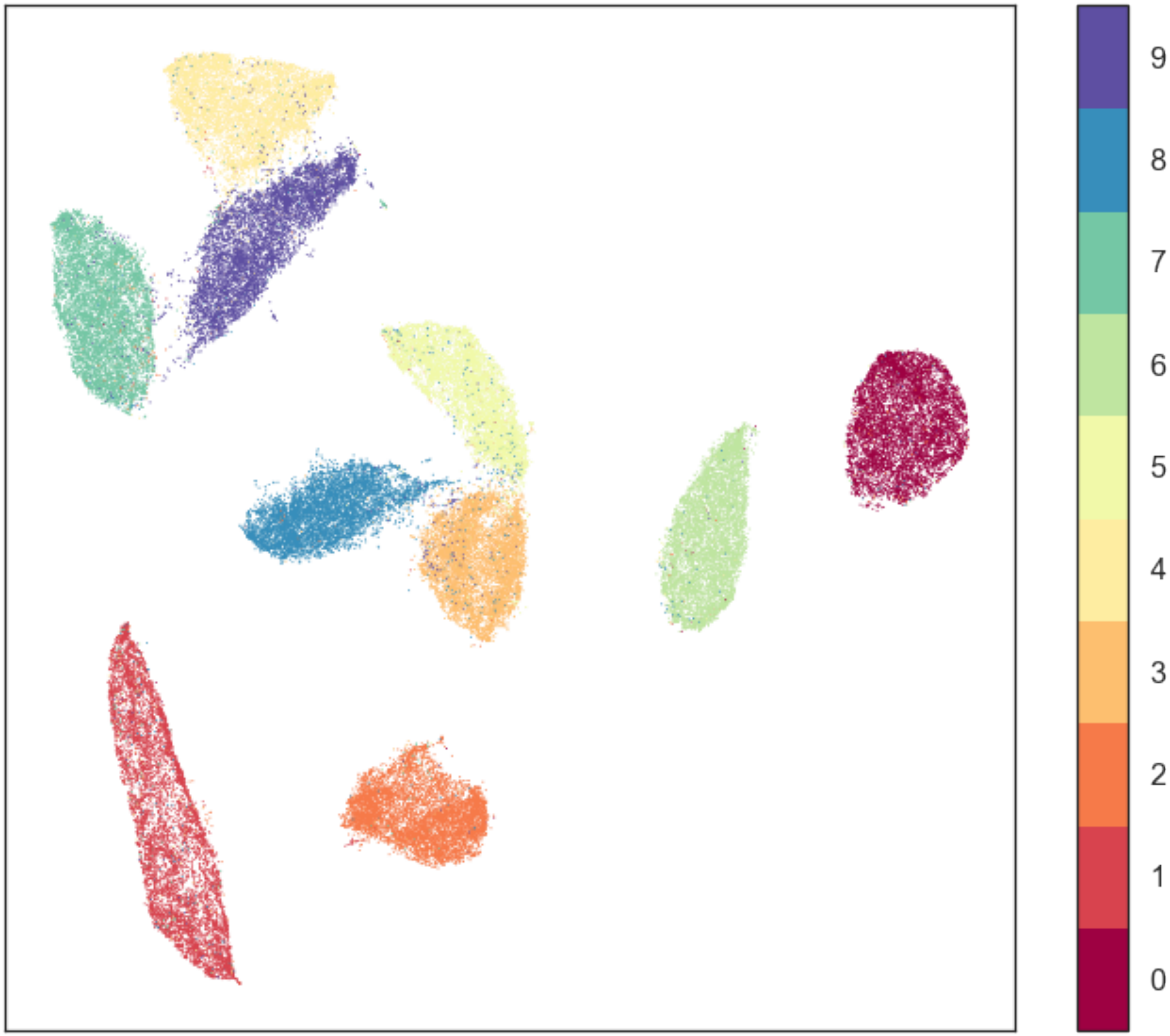
We are just embedding the graph

$$\overbrace{\sum_{a \in A} \mu(a) \log\left(\frac{\mu(a)}{\nu(a)}\right)}^{\text{Get the clumps right}} + \underbrace{(1-\mu(a)) \log\left(\frac{1-\mu(a)}{1-\nu(a)}\right)}_{\text{Get the gaps right}}$$

UMAP on MNIST digits



MAPPER

Singh, Memoli and Carlsson, 2007

Reeb Graphs

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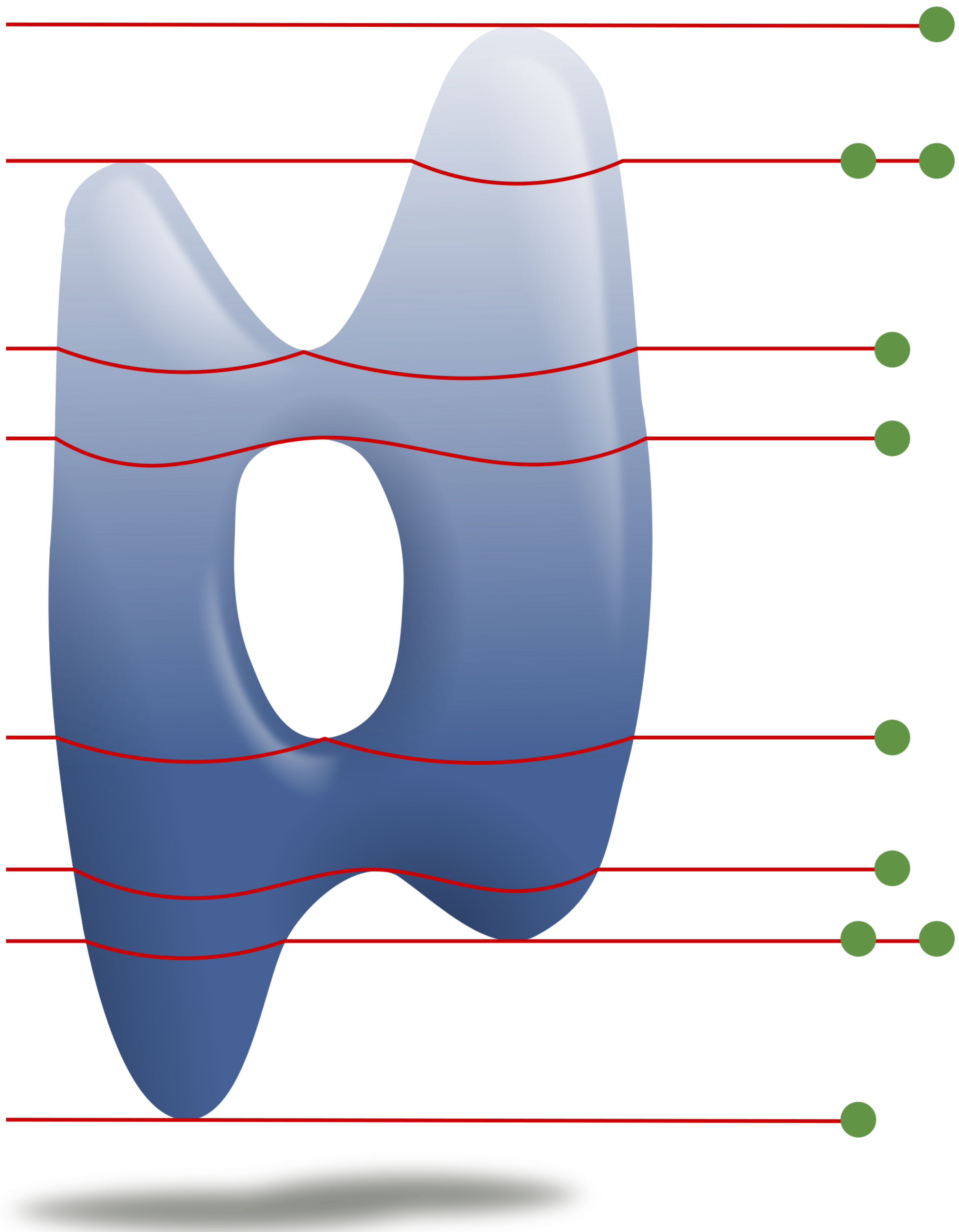

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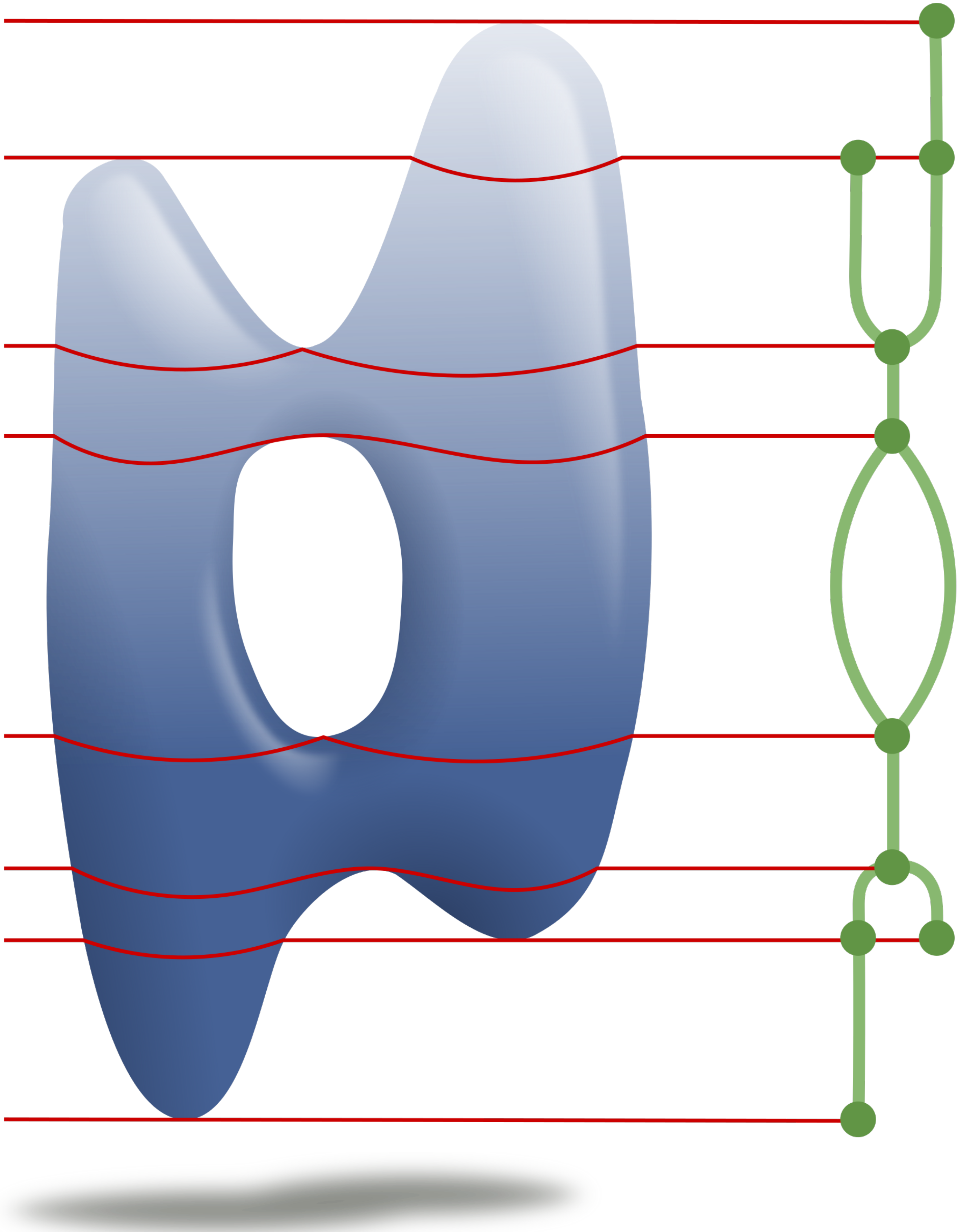
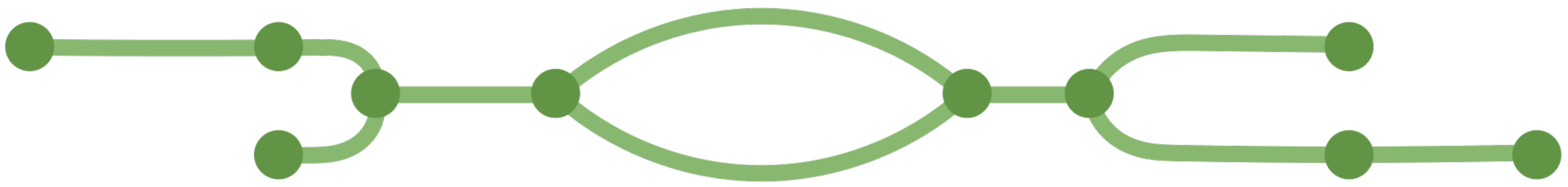
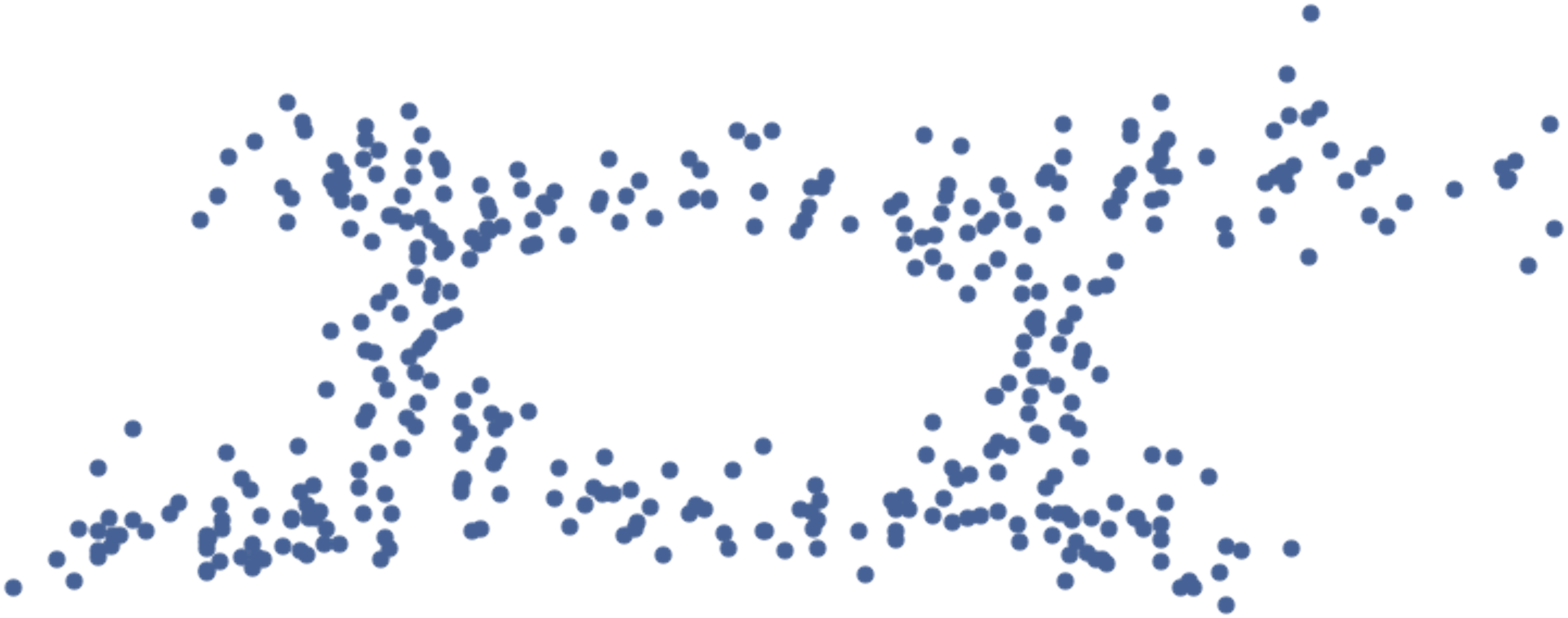
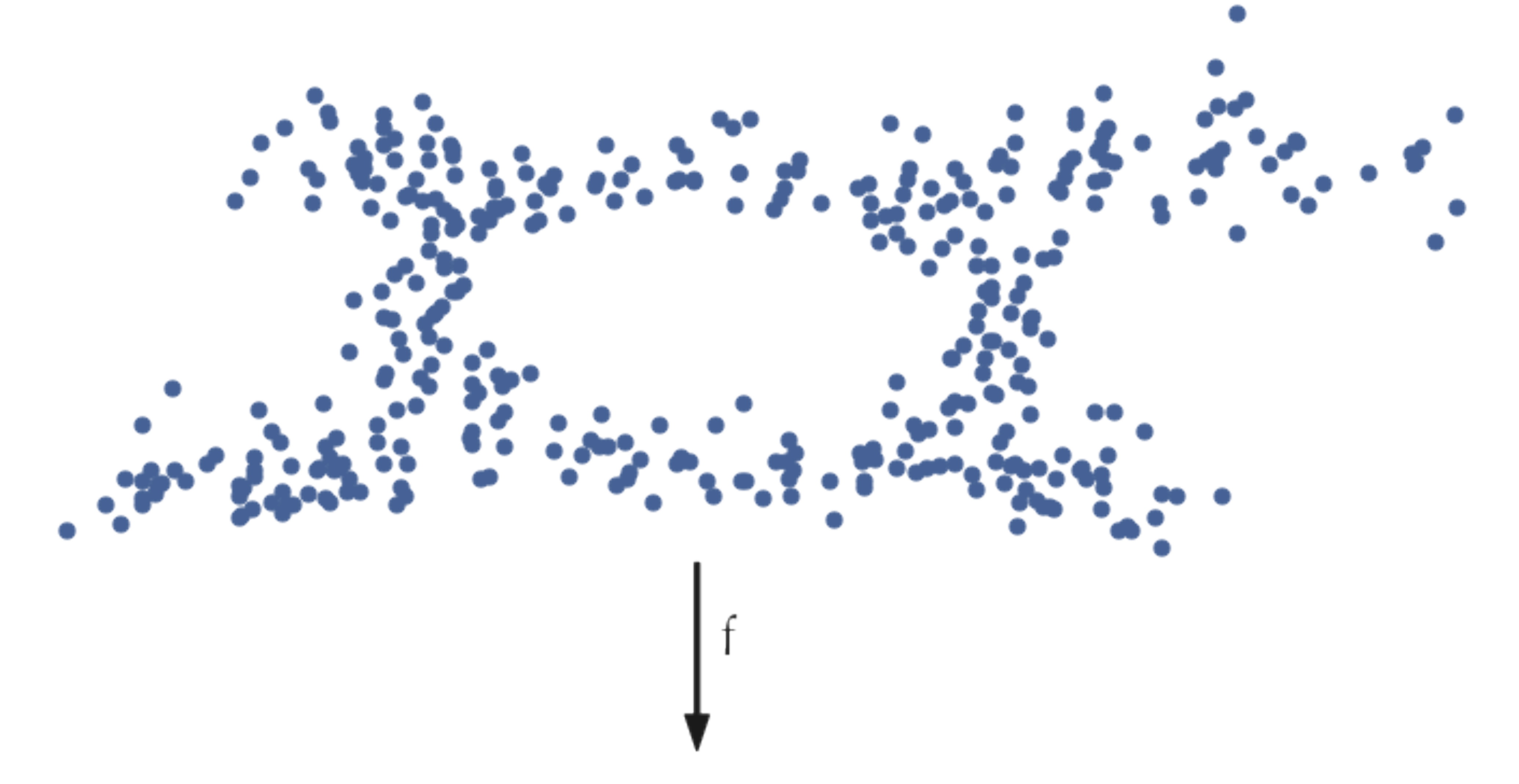




Approximating Reeb Graphs

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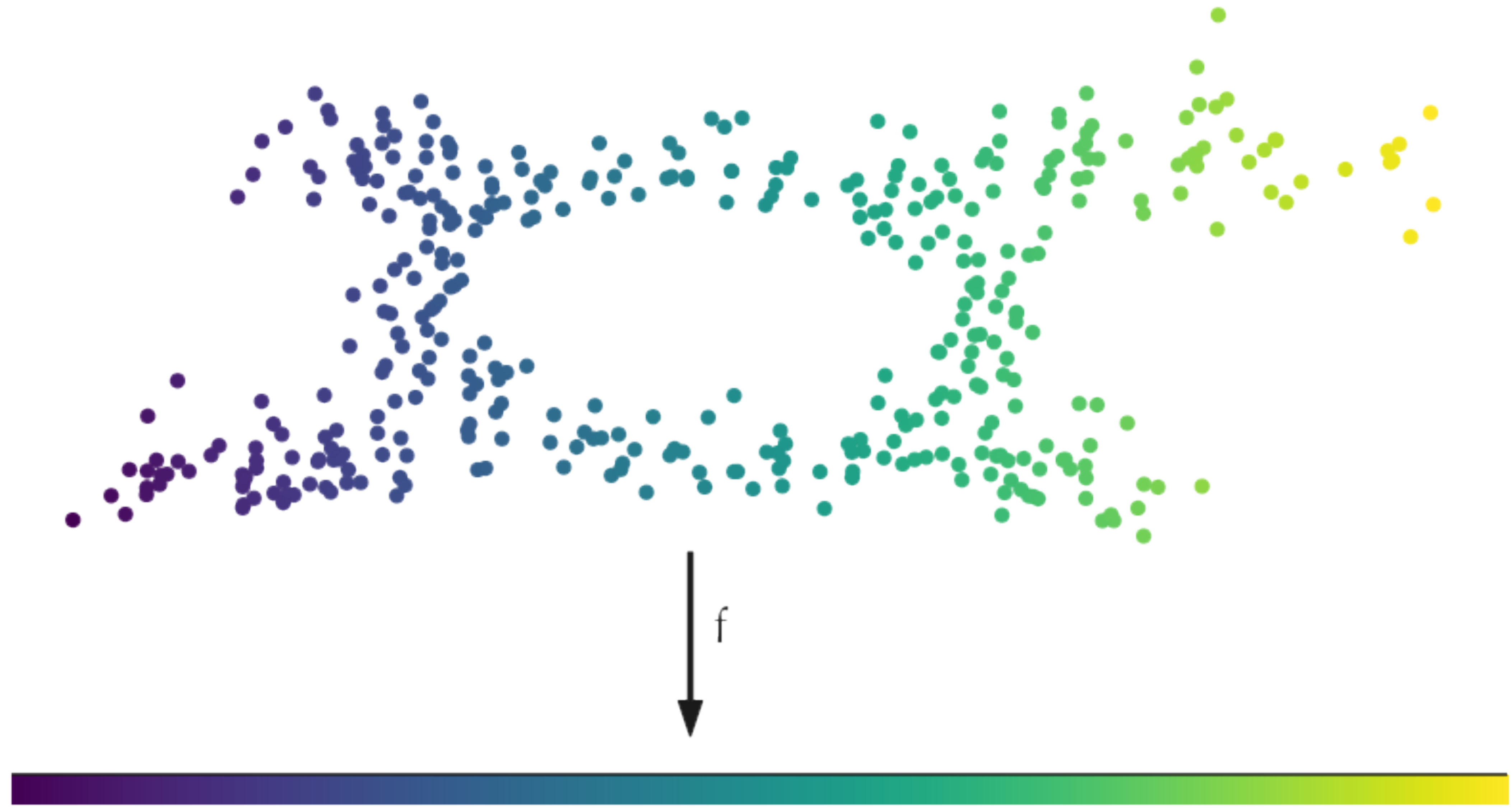

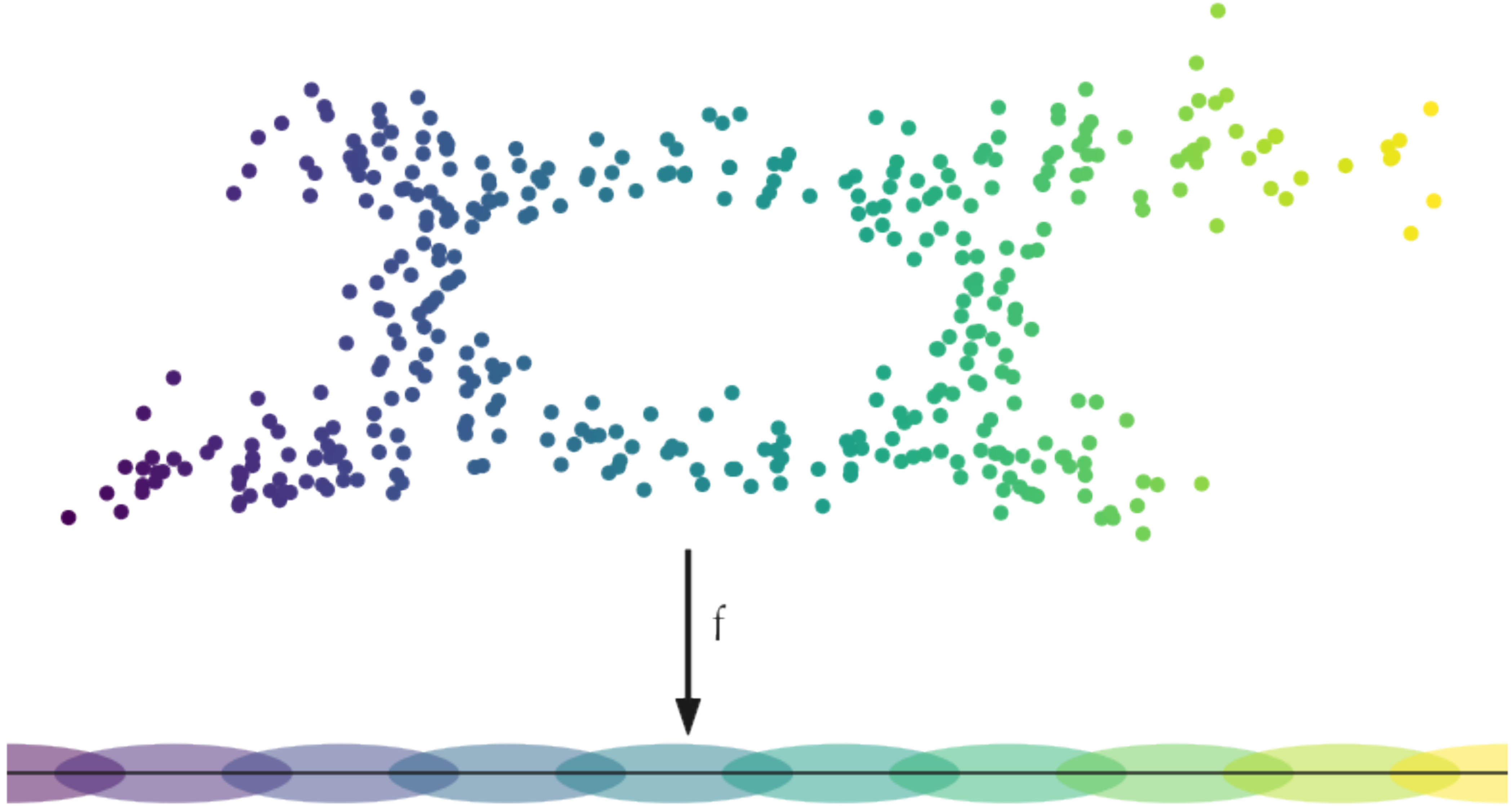
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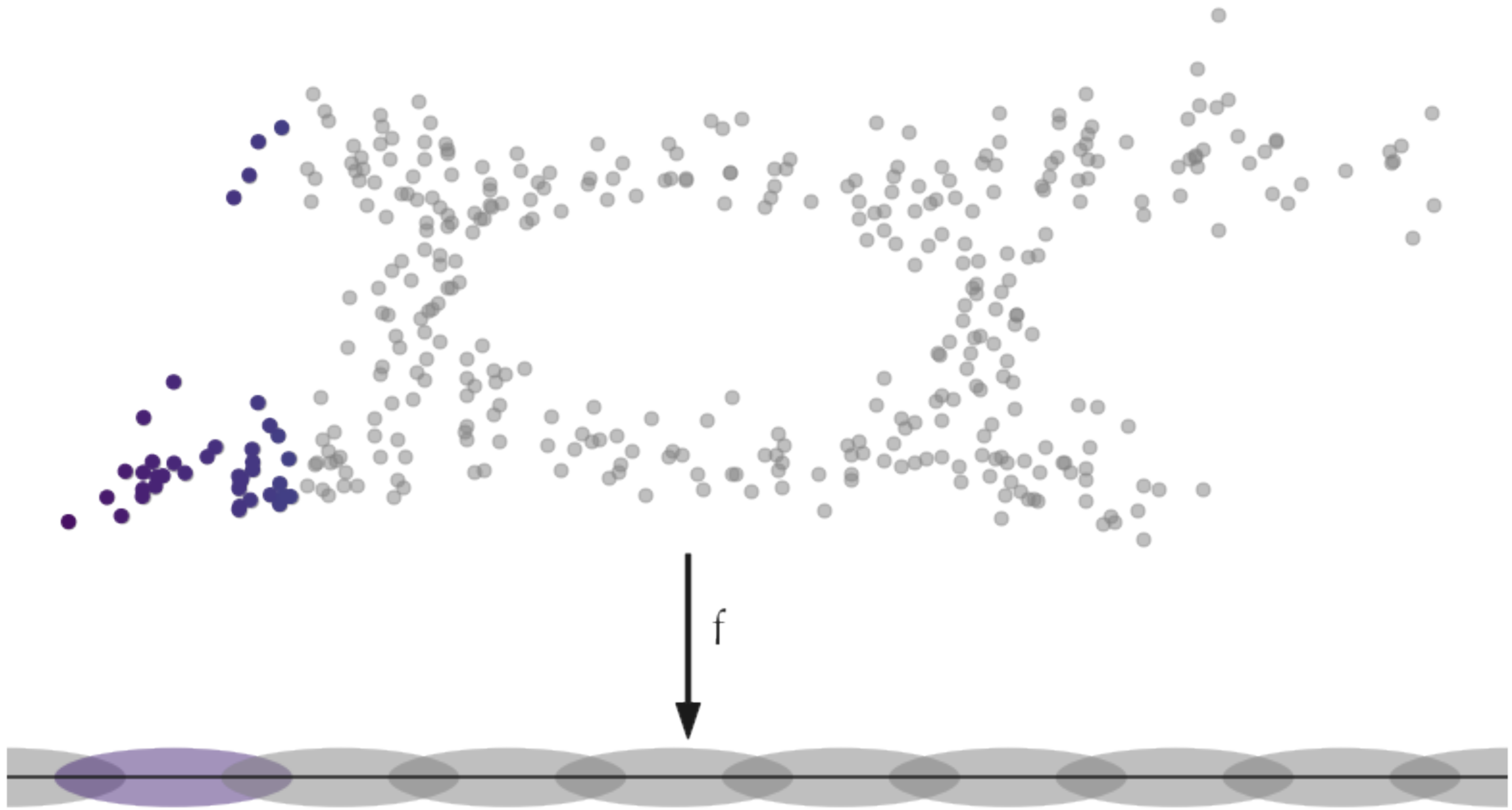
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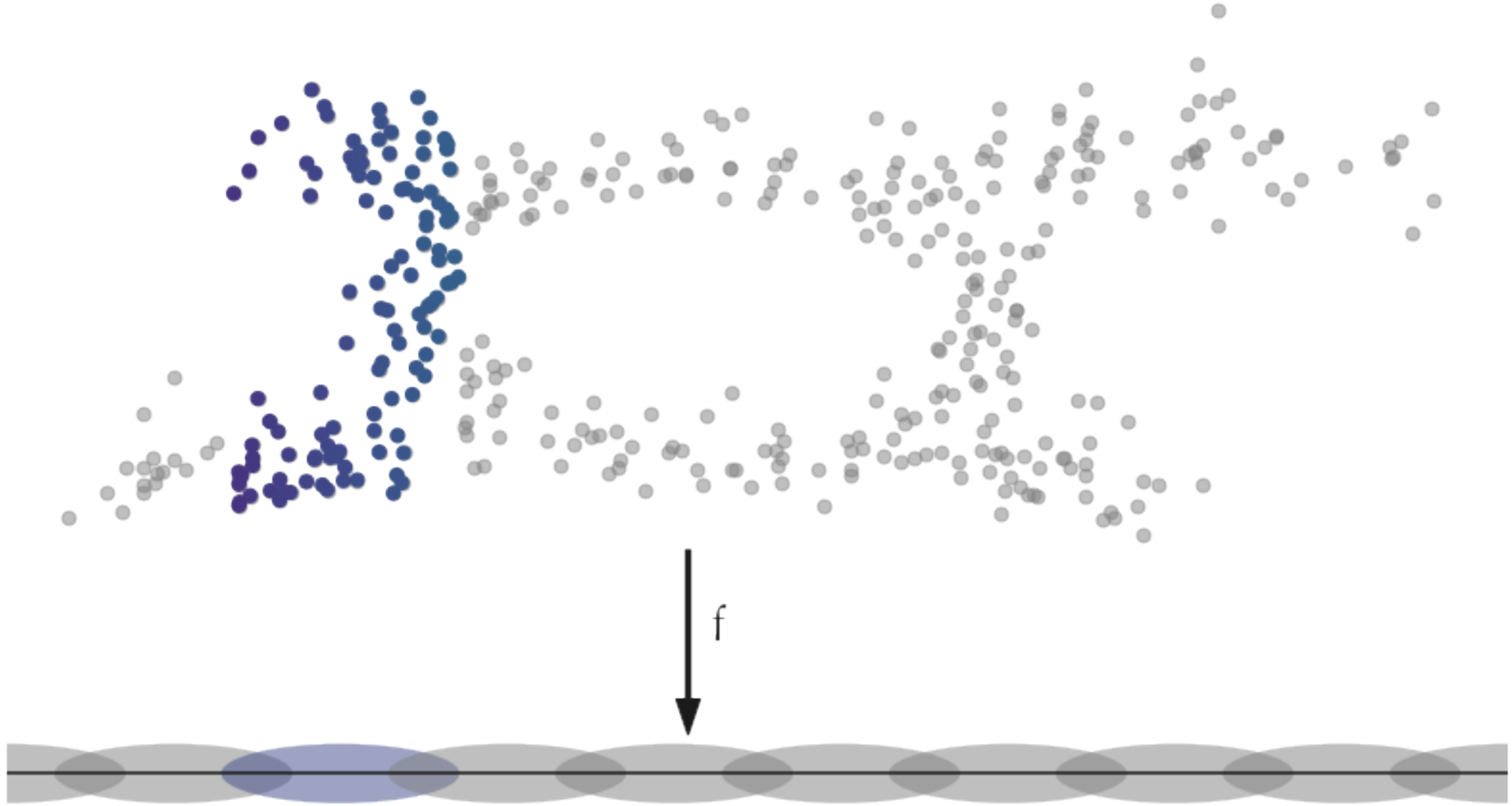

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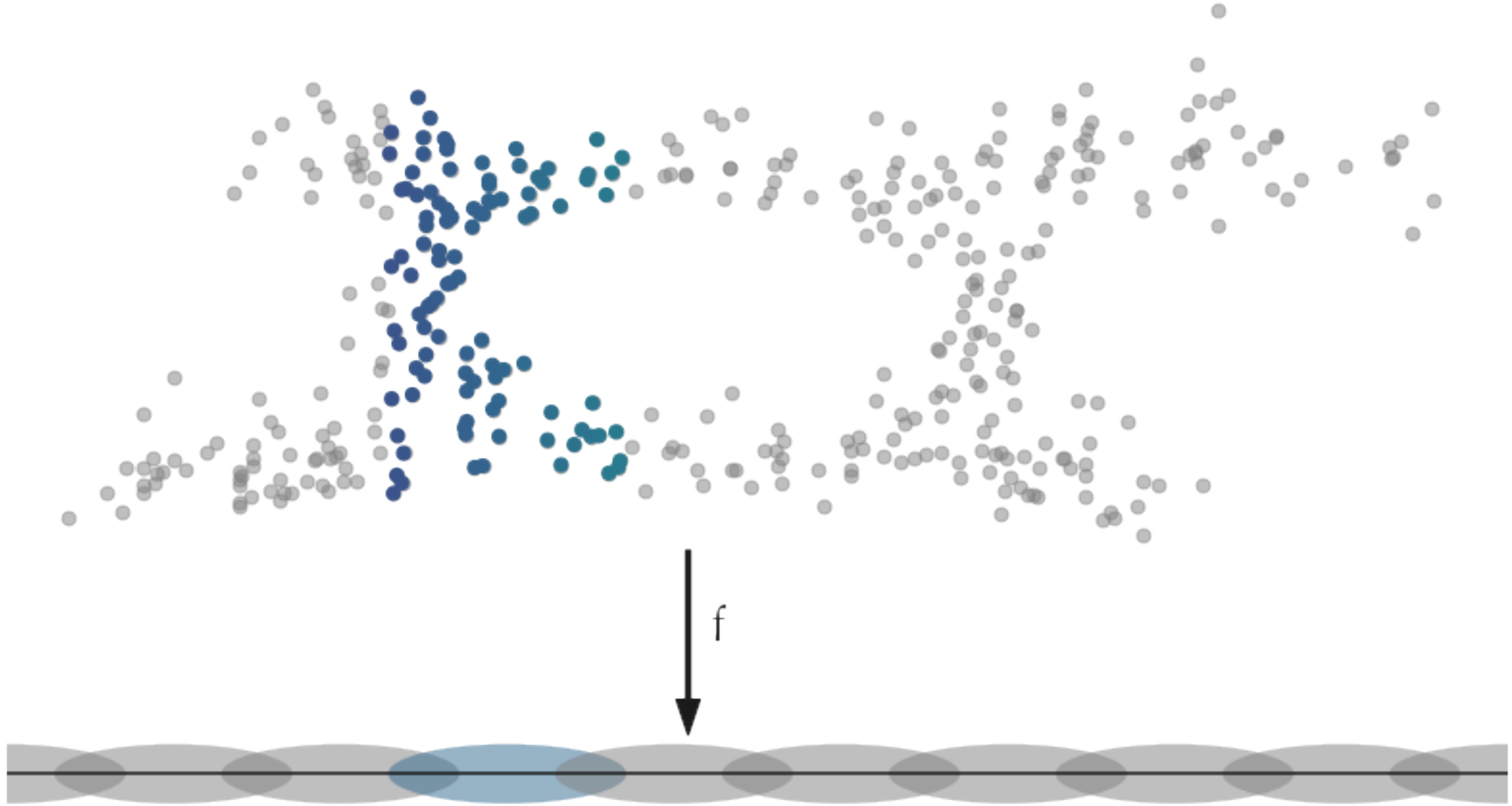

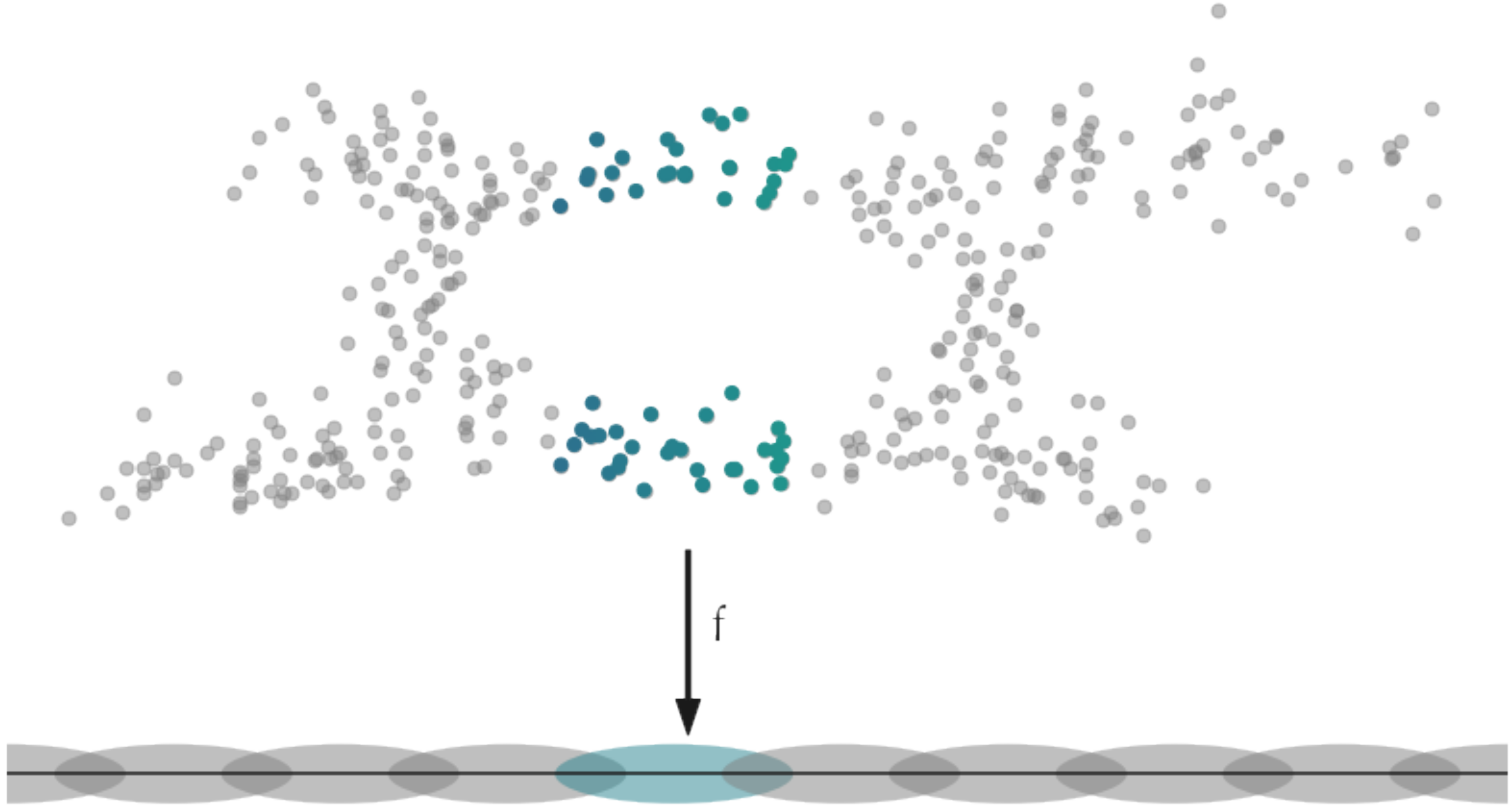
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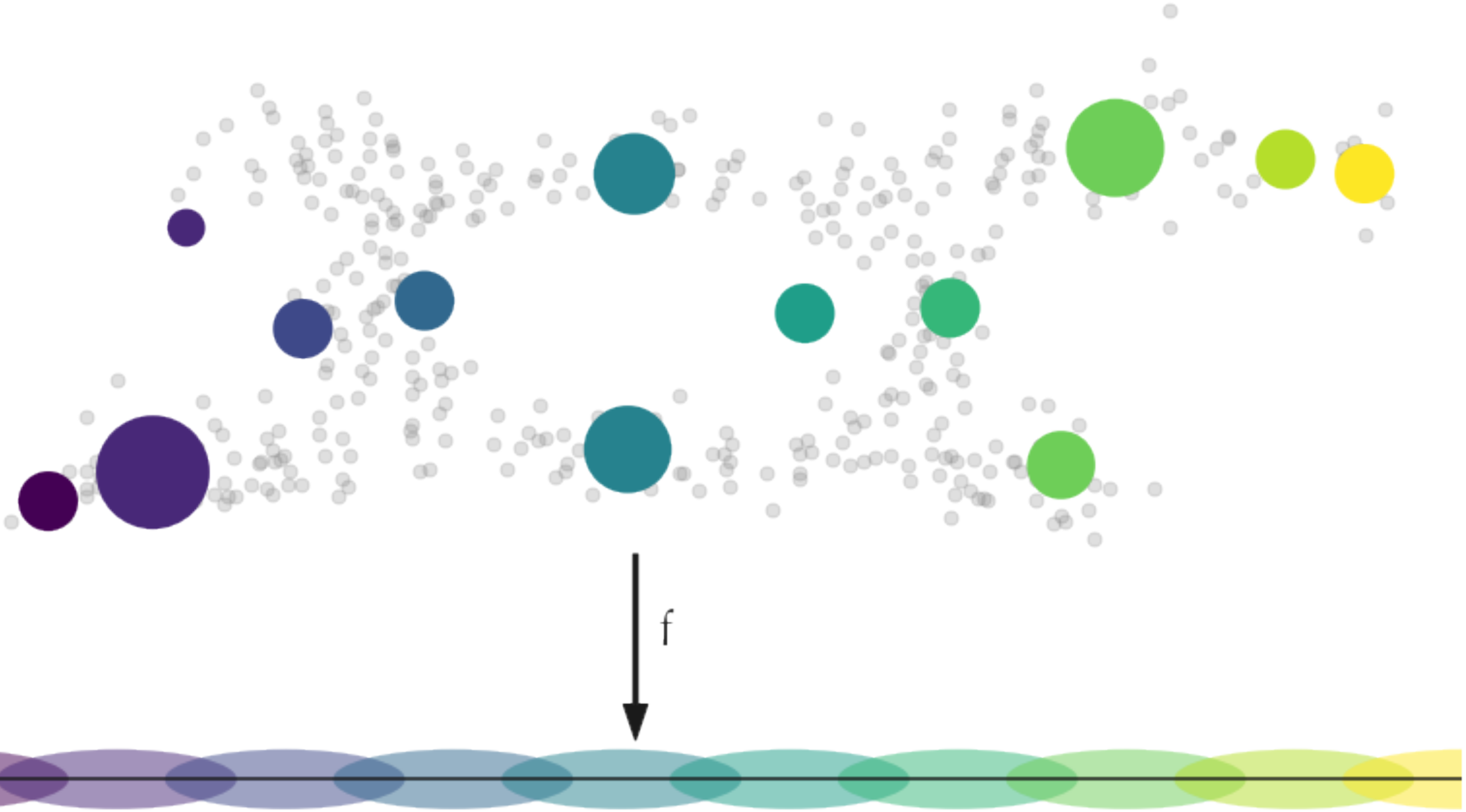

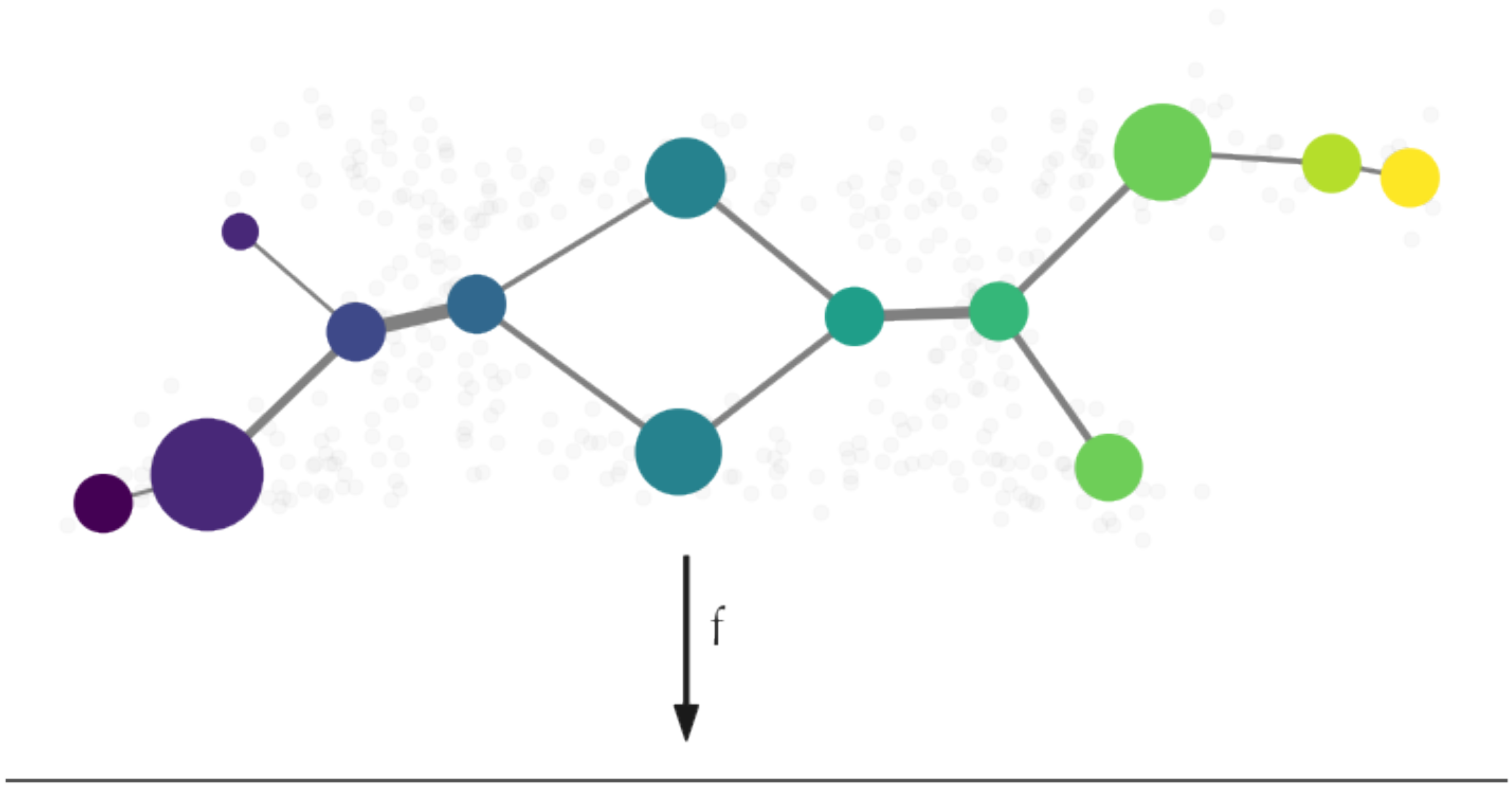
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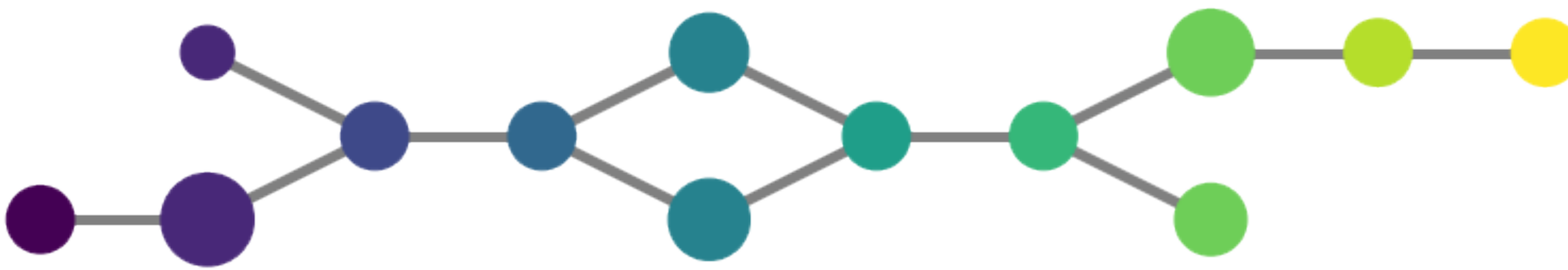

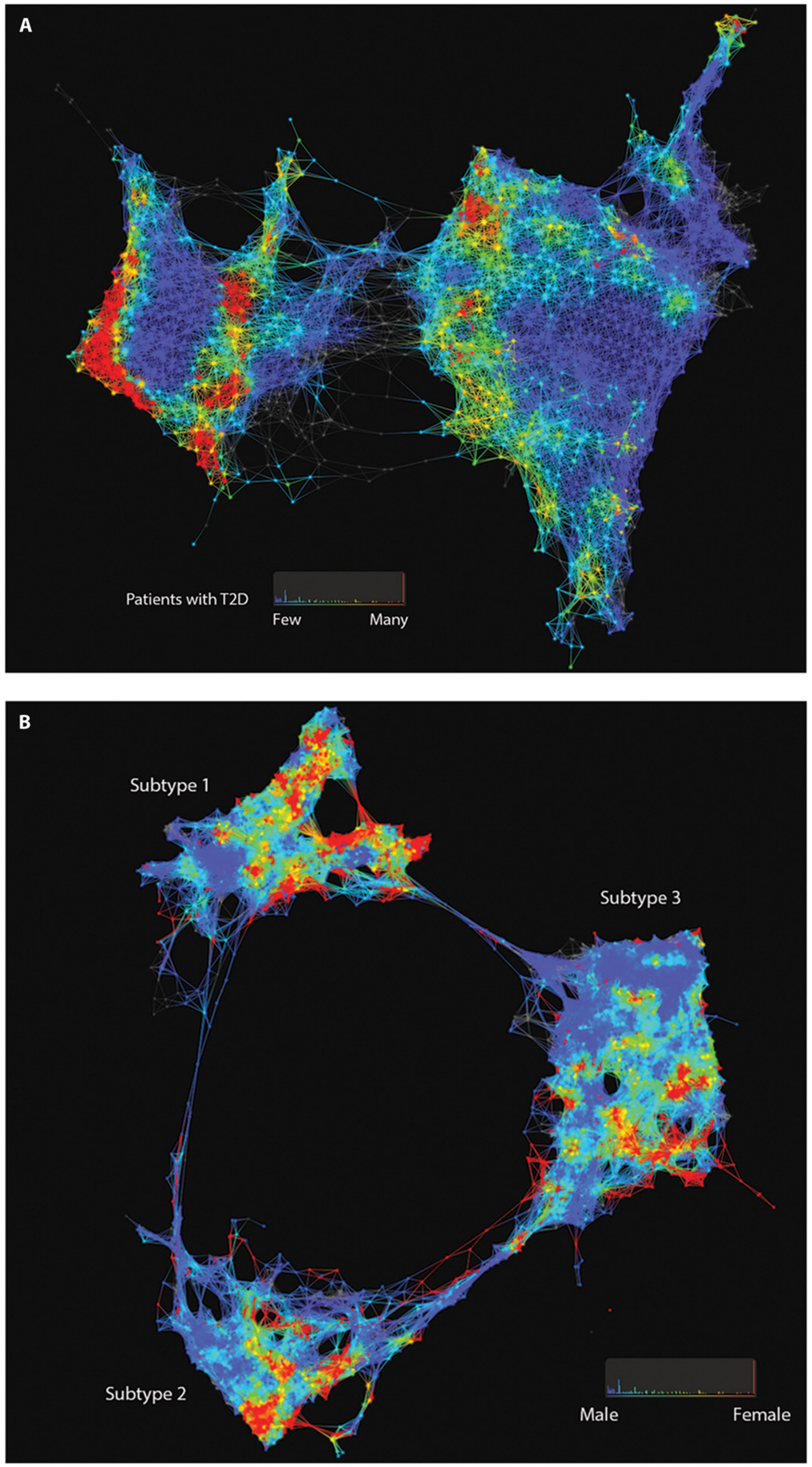

Identification of type 2 diabetes subgroups through topological analysis of patient similarity, Li et al, 2015

UMAPPER

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UMAP provides exact positioning and relationships among all points

UMAP doesn't require a filter function to operate

MAPPER is very expressive for suitable filter functions

UMAP can't make use of a filter function

Can we get the benefits of both?

What if we apply UMAP instead of clustering?

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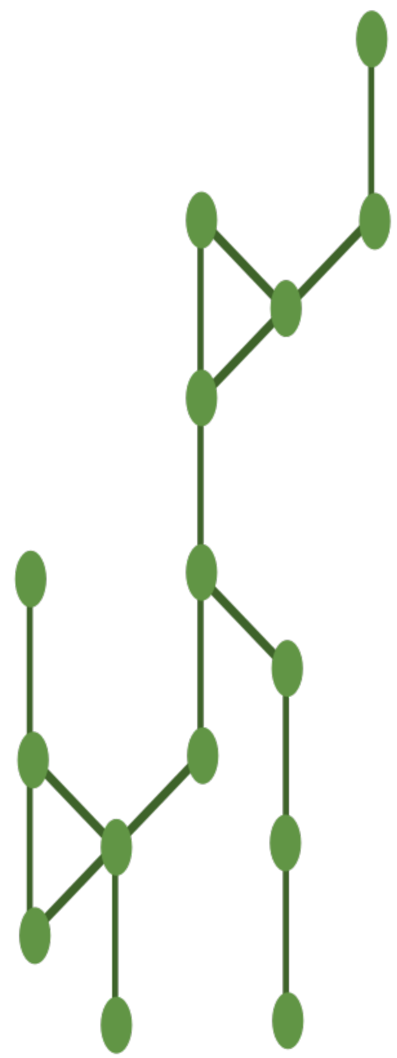

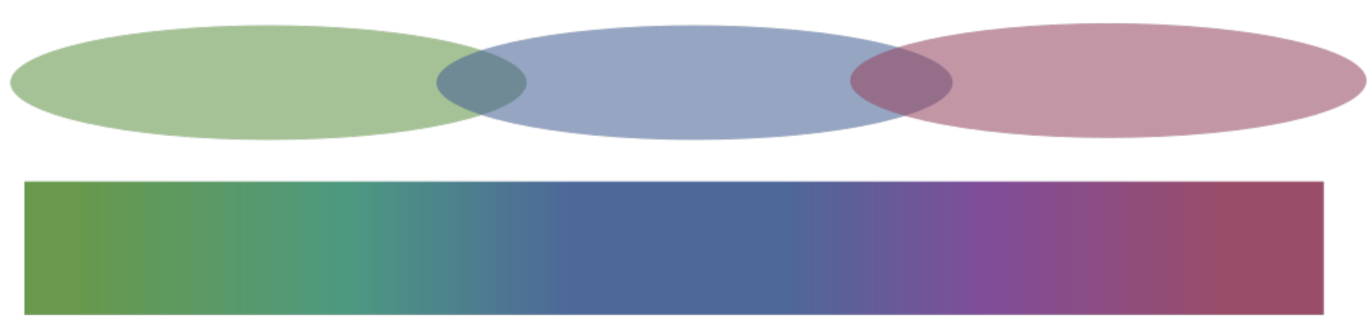

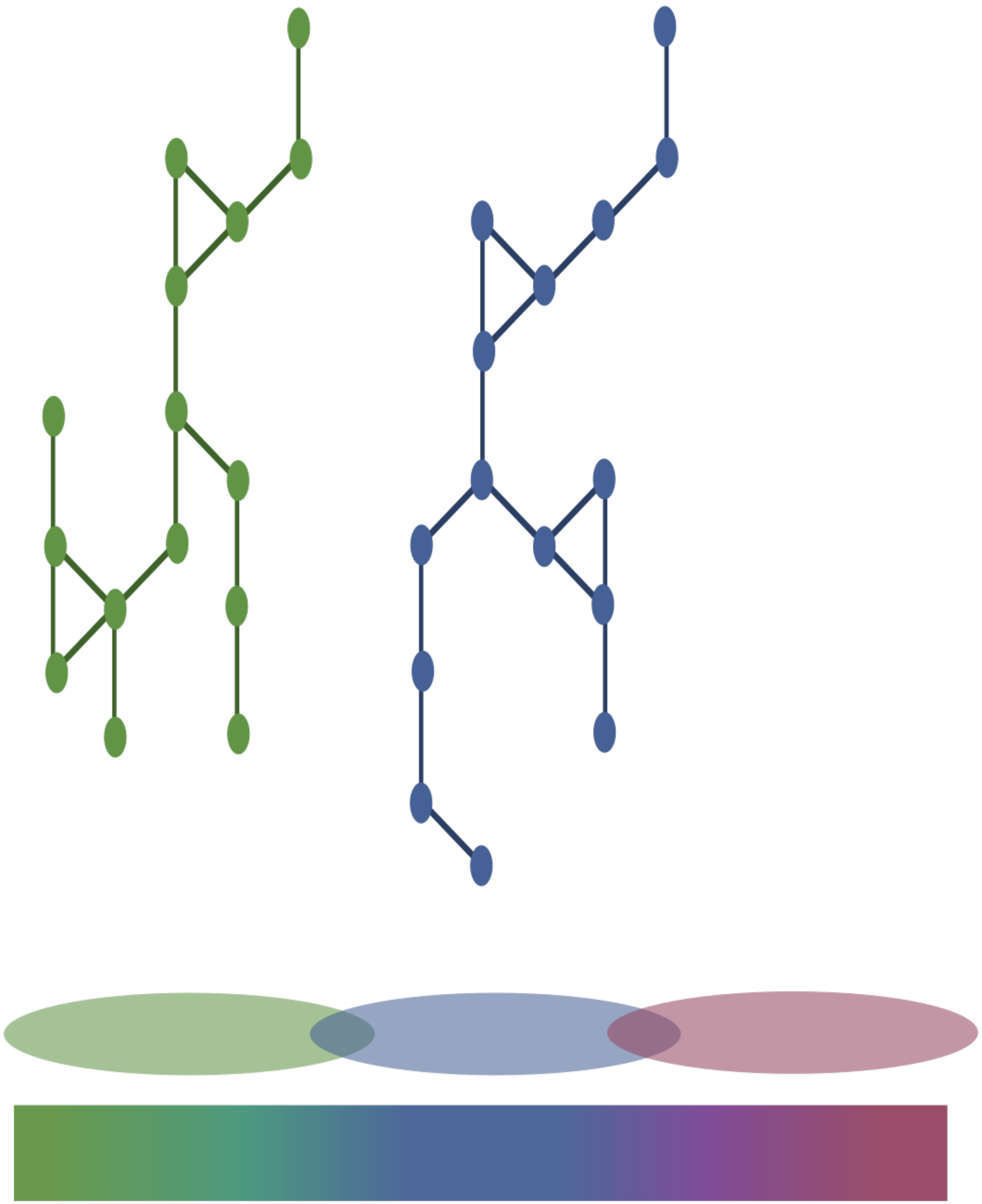

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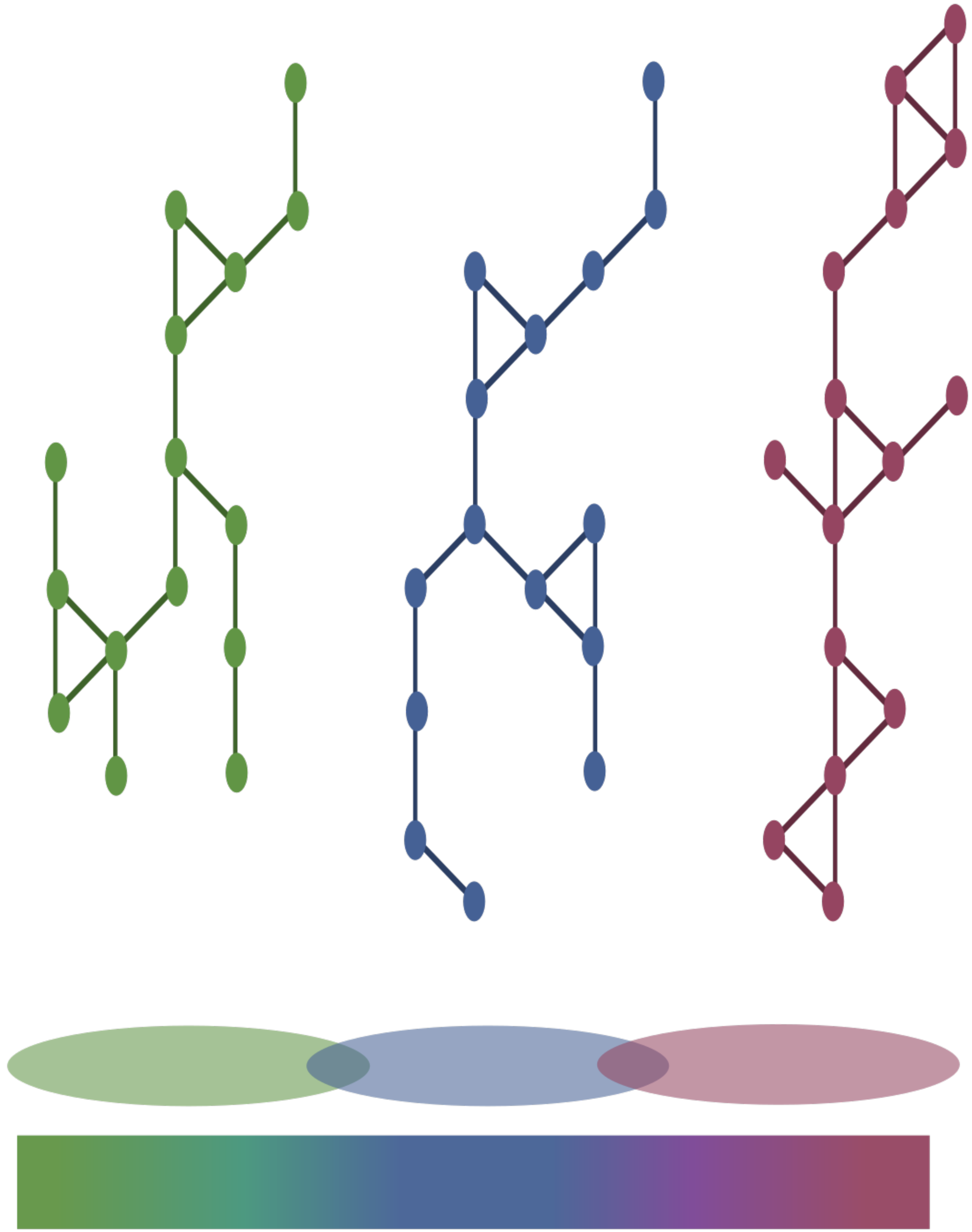
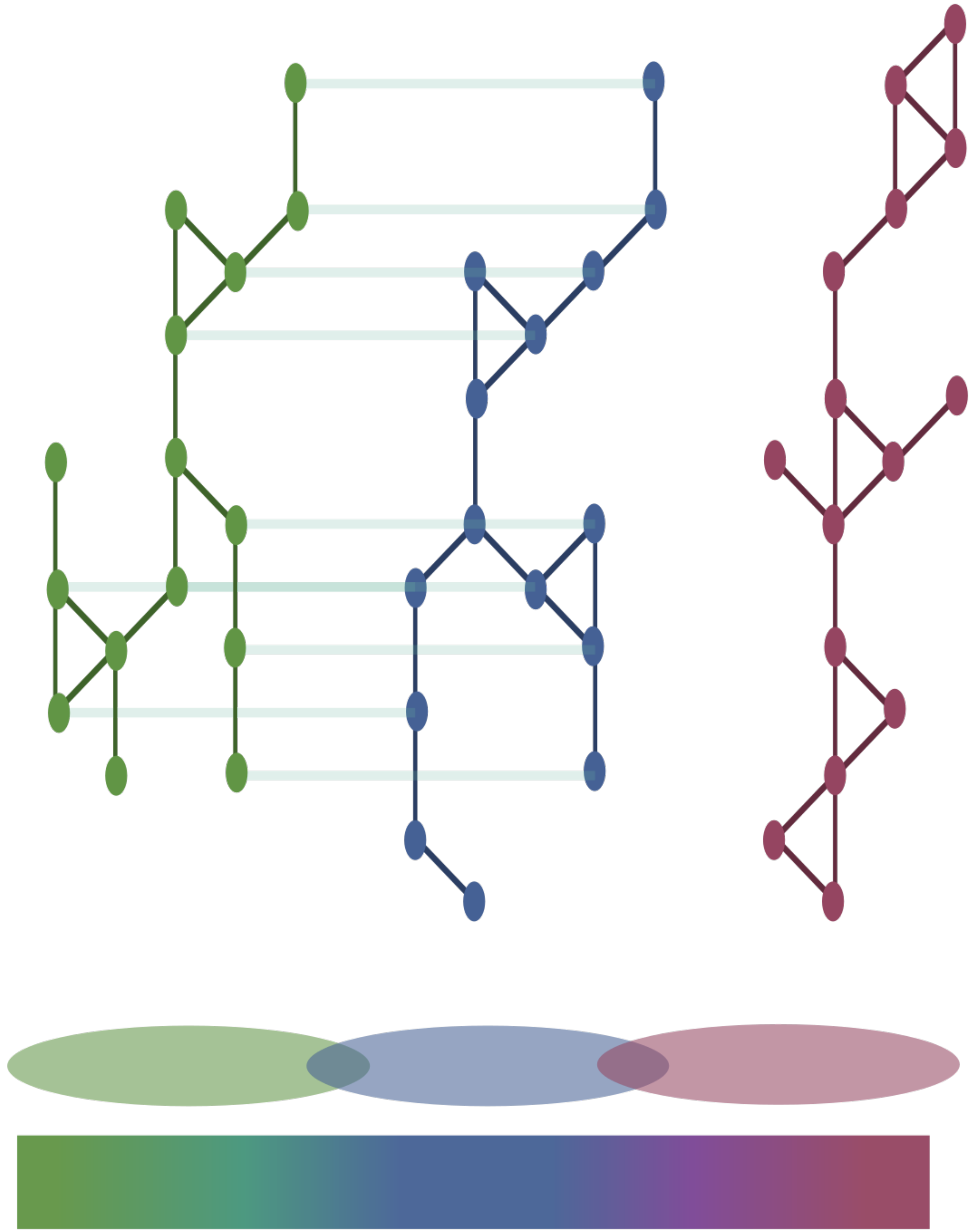
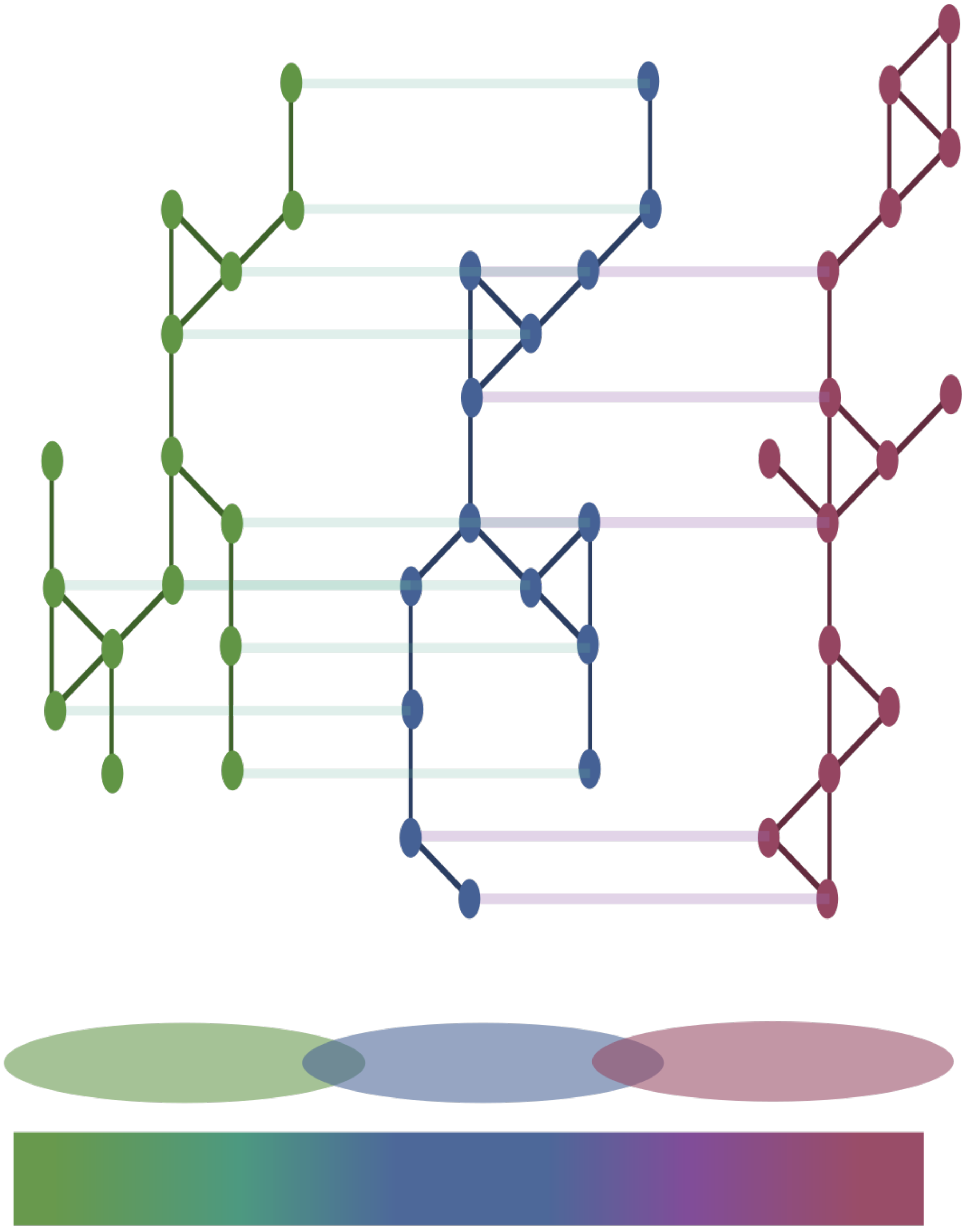


Can we build a MAPPER simplicial structure?





A bi-simplicial structure?

Optimize the UMAP representations simultaneously, using MAPPER simplices for alignment

U_i be the 1-skeleton in the i^{th} UMAP complex

M be the 1-simplices in the MAPPER complex

Let

$$C_i = \sum_{u \in U_i} \mu(u) \log\left(\frac{\mu(u)}{\nu(u)}\right) + (1 - \mu(u)) \log\left(\frac{1 - \mu(u)}{1 - \nu(u)}\right)$$

and

$\ell oc(\partial_i(m))$ be the current location of the zero simplex $\partial_i(m)$

Optimize

$$\sum_i C_i + \lambda \sum_{m \in M} \| \ell oc(\partial_0(m)) - \ell oc(\partial_1(m)) \|_2^2$$

Can we have a notion of membership strength on MAPPER edges?

In standard MAPPER we might use Jaccard Index between clusters

Apply Jaccard Index to "neighborhoods"

For $x \in U_i$ let $N_{\rightarrow}(x)$ denote the neighbours of x in U_i that are faces of simplices in M spanning U_i and U_{i+1}

For $x \in U_i$ let $N_{\leftarrow}(x)$ denote the neighbours of x in U_i that are faces of simplices in M spanning U_i and U_{i-1}

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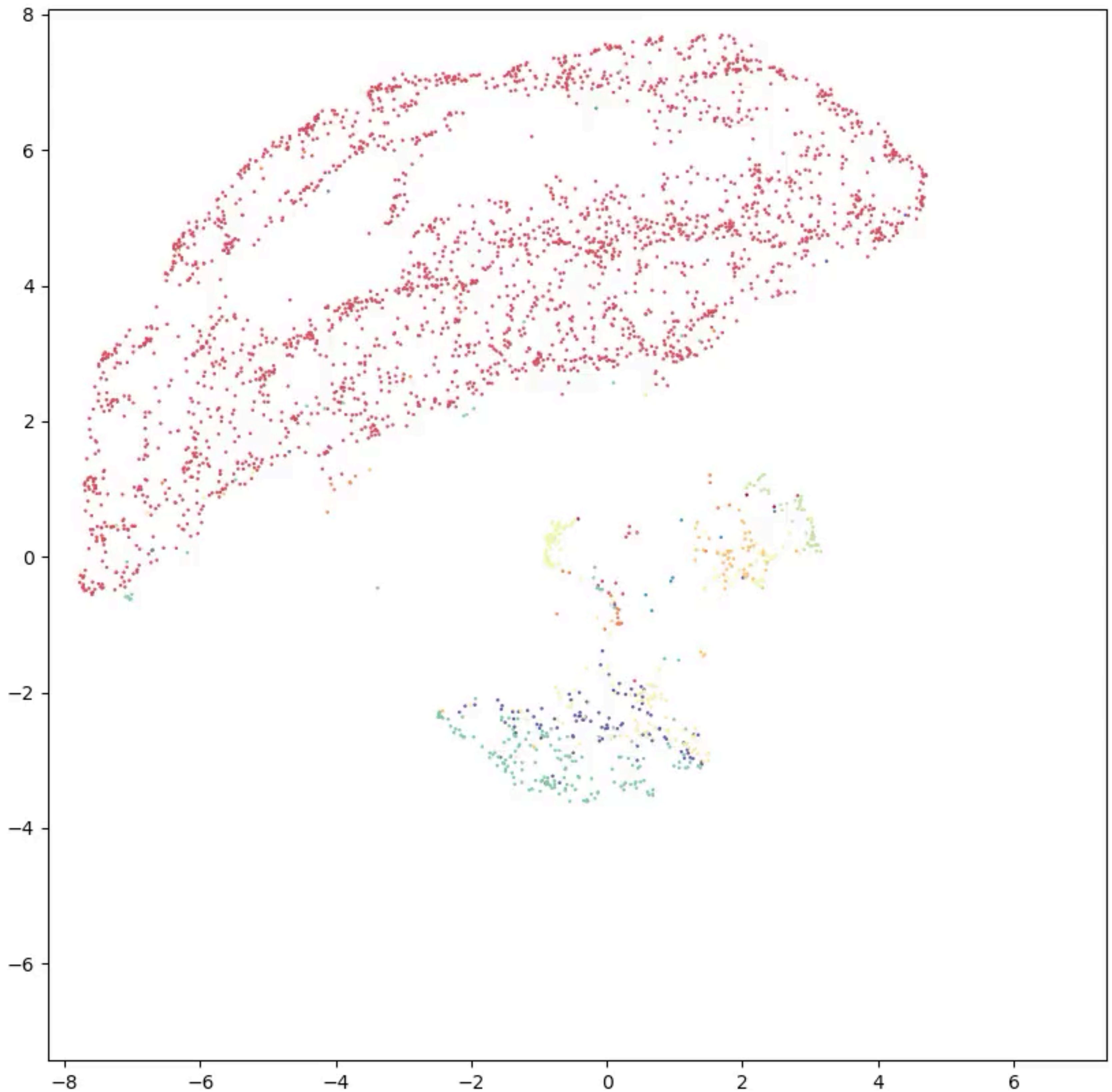
$$\mathrm{Jacc}(m) := \frac{\left| N_{\rightarrow}(\partial_0(m)) \cap N_{\leftarrow}(\partial_1(m)) \right|}{\left| N_{\rightarrow}(\partial_0(m)) \cup N_{\leftarrow}(\partial_1(m)) \right|}$$

Optimize

$$\sum_i C_i + \lambda \sum_{m \in M} \mathrm{Jacc}(m) \| \ell oc(\partial_0(m)) - \ell oc(\partial_1(m)) \|_2^2$$

We can still do this with stochastic gradient descent!



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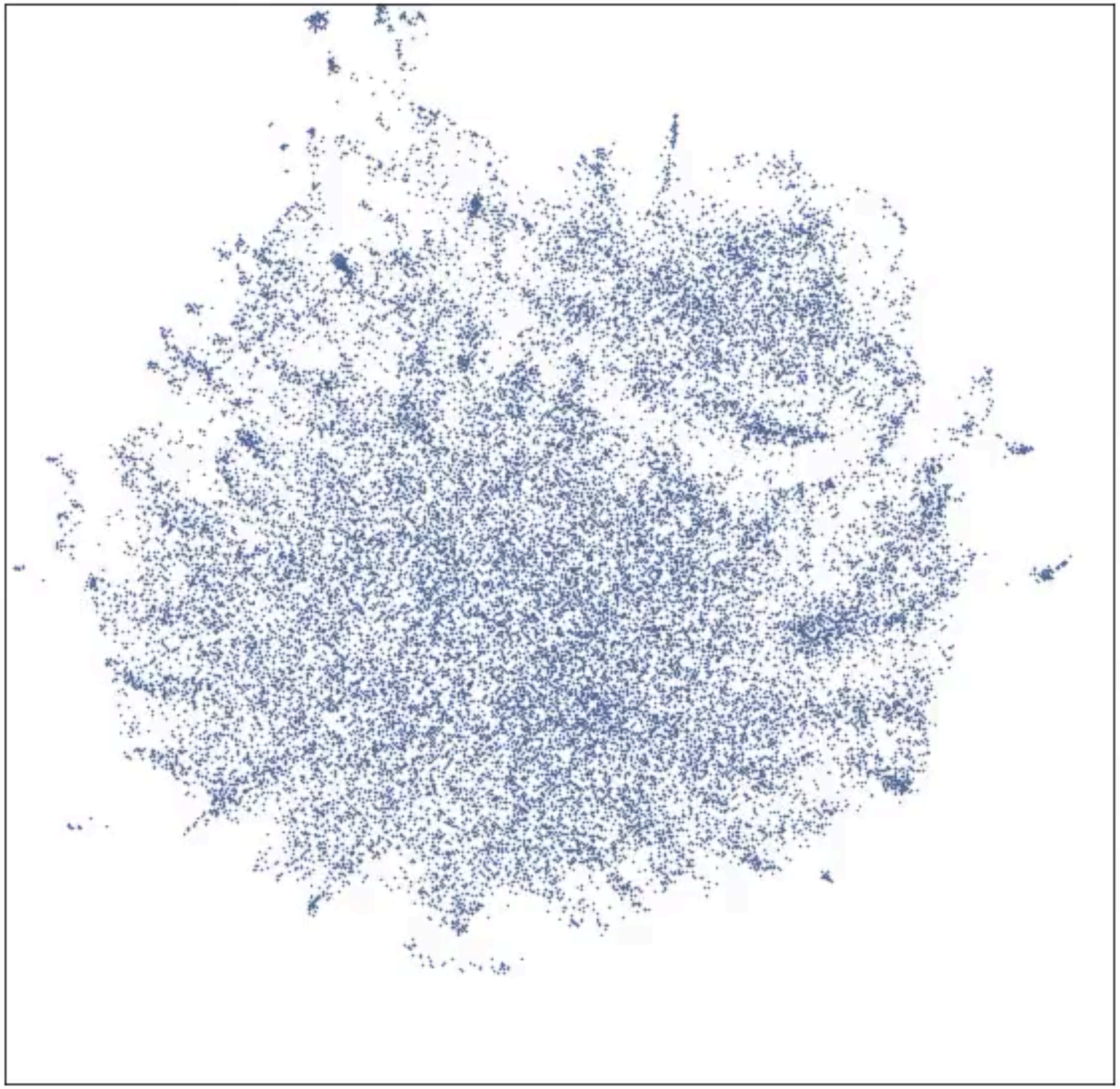

Conclusions

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It is possible to combine the strengths of UMAP and MAPPER and provide rich data visualizations

Richer topological structures and more advanced approaches are possible

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https://github.com/lmcinnes/umap/tree/0.5dev

demo: https://bit.ly/2zxcWsZ