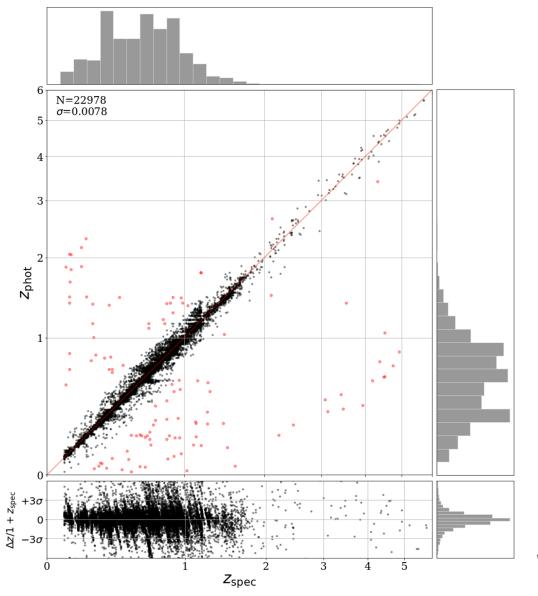
Photometric Redshifts Usually Work...

Hovis-Afflerbach, Steinhardt et al. 2020





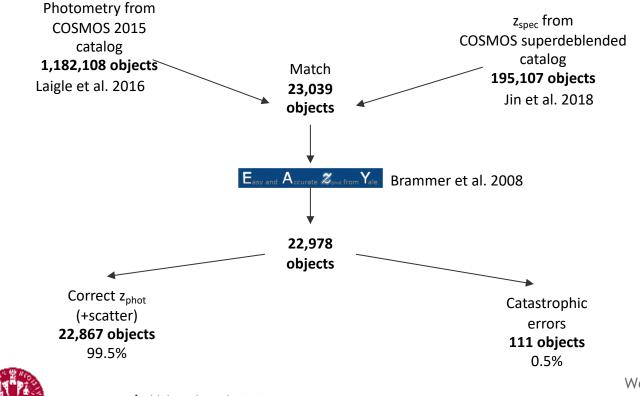


...But Not Always!

About 5% of objects fail template fitting¹

Can we identify these objects without comparing with spectroscopy?

Can we fix these objects and determine the correct properties?



Wednesday May 4, 2022

¹Hildebrandt et al. 2010:

COSMIC DAWN CENTER

DAWN

12 photo-z methods tested on objects with 18 bands, between 4.9% and 29% of objects had dz/(1+z) > 0.15

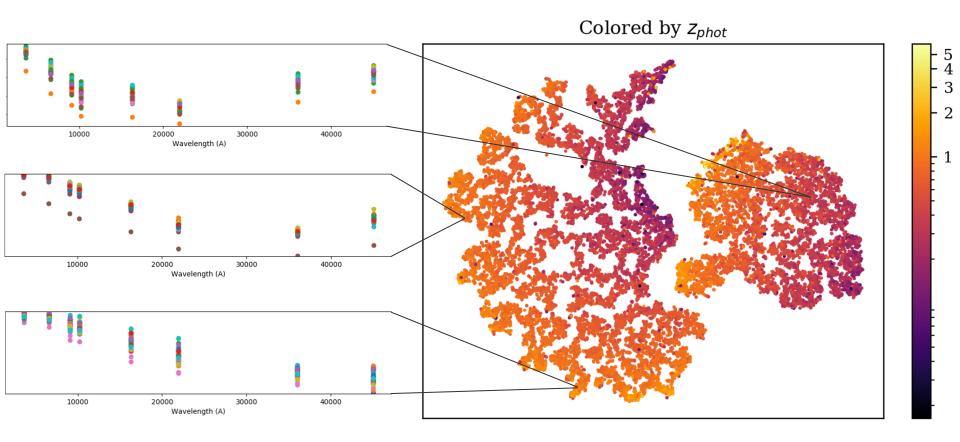
Two Three Fundamental Assumptions for Photometry

- 1. If an object is sufficiently well-measured, there is a surjective (one-to-one or many-to-one, but not one-to-many) mapping from photometric fluxes to astrophysical properties.
- 2. Objects with sufficiently similar photometry should be mapped to similar astrophysical properties.
- 3. We can map objects from the full, n-dimensional space with all bands to a smaller one with many neighbors, and the other two assumptions will continue to hold.



t-SNE Map for COSMOS/Spec-z Dataset

Hovis-Afflerbach, Steinhardt et al. 2020

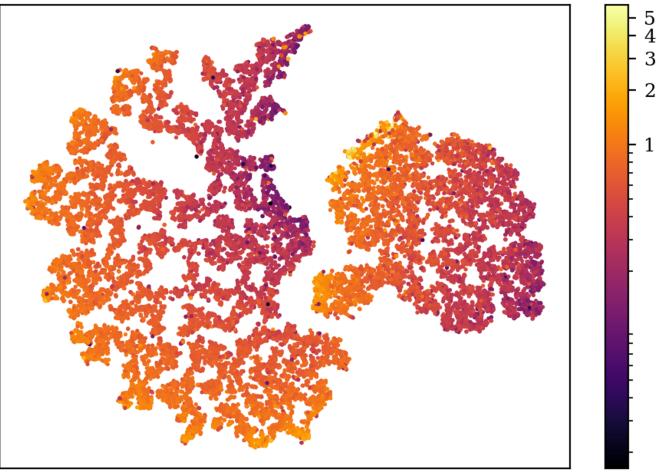




t-SNE Map for COSMOS/Spec-z Dataset

Hovis-Afflerbach, Steinhardt et al. 2020

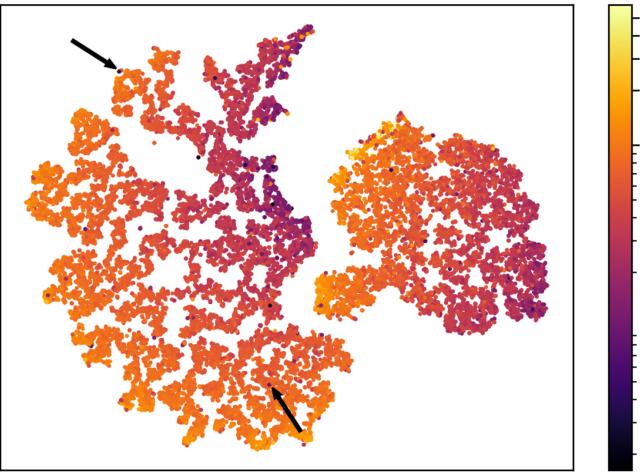
Colored by *z*_{phot}





Hovis-Afflerbach, Steinhardt et al. 2020

Colored by *z*_{phot}





5 4

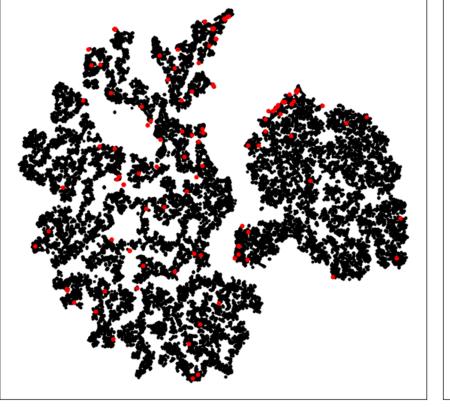
3

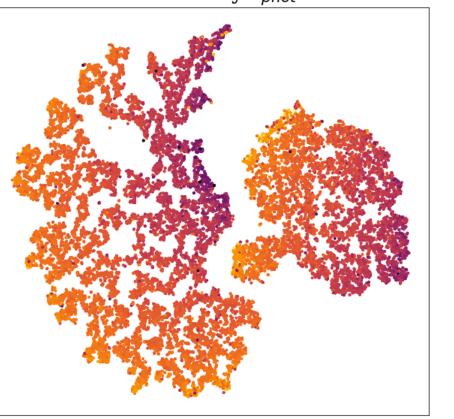
2

Hovis-Afflerbach, Steinhardt et al. 2020

Catastrophic errors in red

Colored by *z*_{phot}







Wednesday May 4, 2022

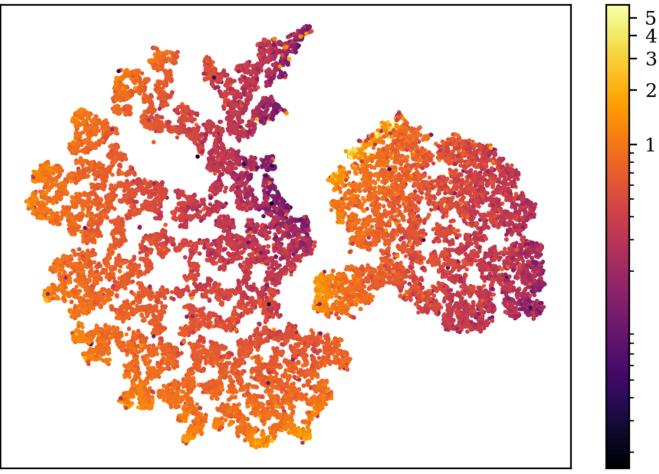
5 4 3

2

1

Hovis-Afflerbach, Steinhardt et al. 2020

Colored by z_{phot}

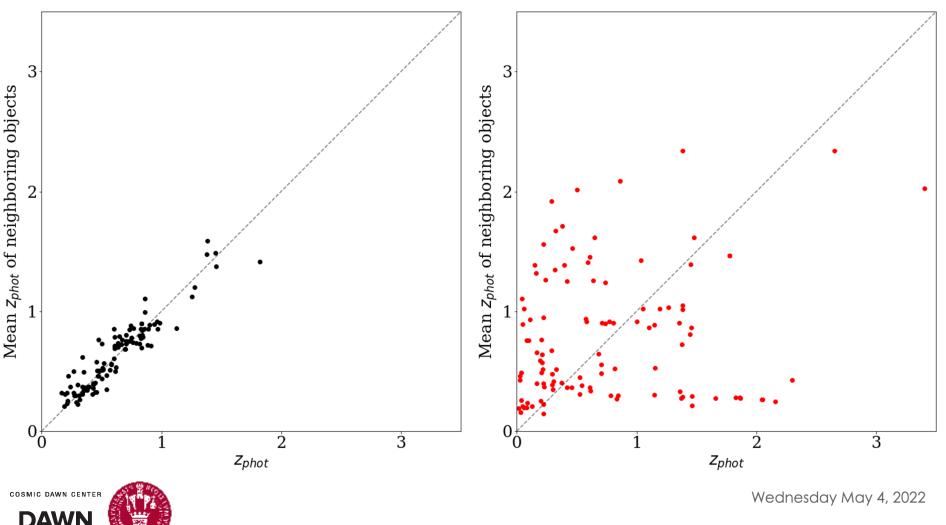




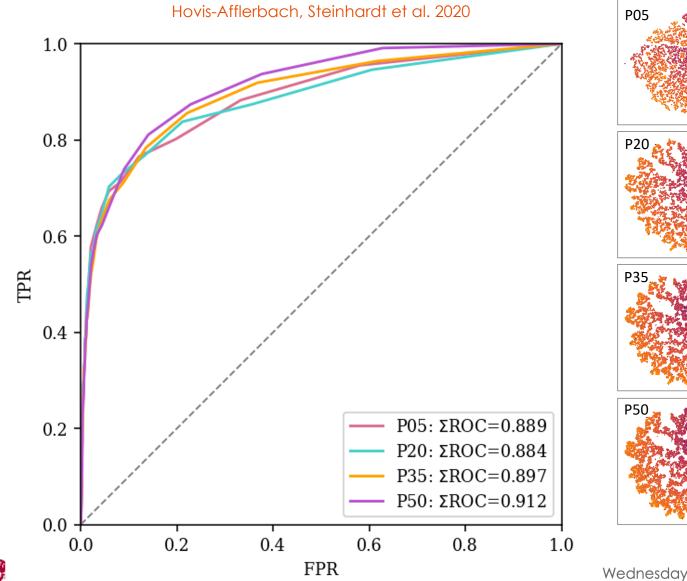
Hovis-Afflerbach, Steinhardt et al. 2020

Sample with correct phot-z

Sample with wrong phot-z



ROC Curve for Catastrophic Errors

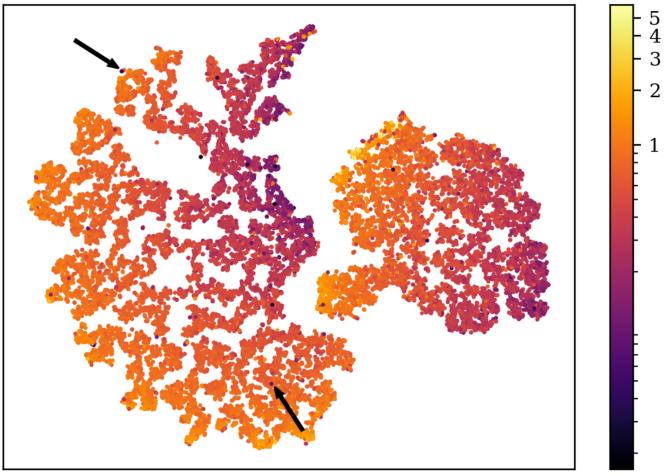




Can we fix it?

Hovis-Afflerbach, Steinhardt et al. 2020

Colored by z_{phot}

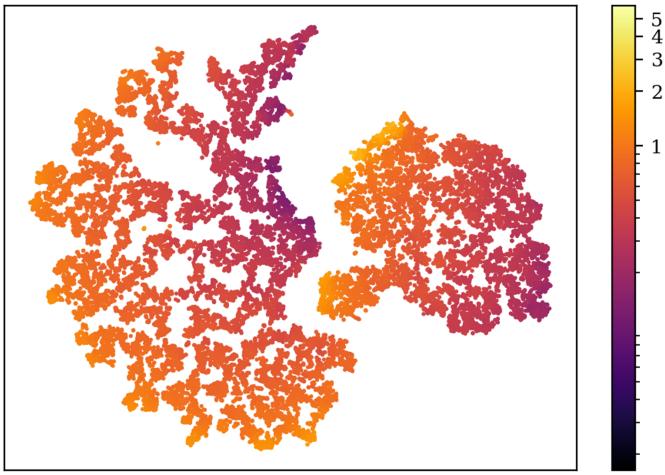




Can we fix it?

Hovis-Afflerbach, Steinhardt et al. 2020

Colored by *z_{mean}*





Two Three Fundamental Assumptions for Photometry

- 1. If an object is sufficiently well-measured, there is a surjective (one-to-one or many-to-one, but not one-to-many) mapping from photometric fluxes to astrophysical properties.
- 2. Objects with sufficiently similar photometry should be mapped to similar astrophysical properties.
- 3. We can map objects from the full, n-dimensional space with all bands to a smaller one with many neighbors, and the other two assumptions will continue to hold.



OK, but can you tell me how t-SNE actually works?



t-Stochastic Neighbor Embedding (t-SNE)

N. Oskolkov, towardsdatascience.com

$$p_{j|i} = \frac{\exp\left(-||x_i - x_j||^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-||x_i - x_k||^2 / 2\sigma_i^2\right)}, \quad p_{ij} = \frac{p_{i|j} + p_{j|i}}{2N} \quad (1)$$

$$-\sum_{j} p_{j|i} \log_2 p_{j|i}$$
Perplexity = 2 (2)
$$q_{ij} = \frac{\left(1 + ||y_i - y_j||^2\right)^{-1}}{\sum_{k \neq l} \left(1 + ||y_k - y_l||^2\right)^{-1}} \quad (3)$$

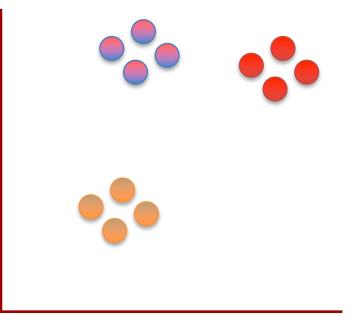
$$KL(P_i||Q_i) = \sum_{i} \sum_{j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}, \quad \frac{\partial KL}{\partial y_i} = 4 \sum_{j} (p_{ij} - q_{ij})(y_i - y_j) \left(1 + ||y_i - y_j||^2\right)^{-1} \quad (4)$$



Wait...I'm a visual learner. Maybe in a cartoon?



Here's a basic 2-D scatter plot.

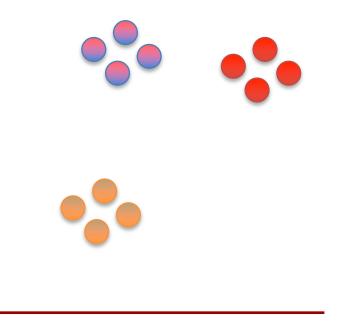




Copyright 2017 Joshua Starmer, https://statauest.org

Here's a basic 2-D scatter plot.

Let's do a walk through of how t-SNE would transform this graph...





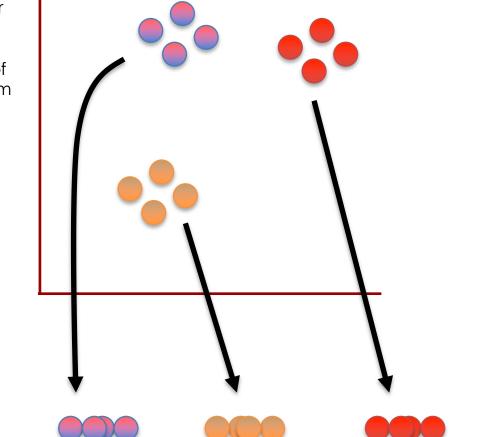
Copyright 2017 Joshua Starmer, https://statauest.org

Here's a basic 2-D scatter plot.

Let's do a walk through of how t-SNE would transform this graph...

...into a flat, 1-D plot on

a number line.



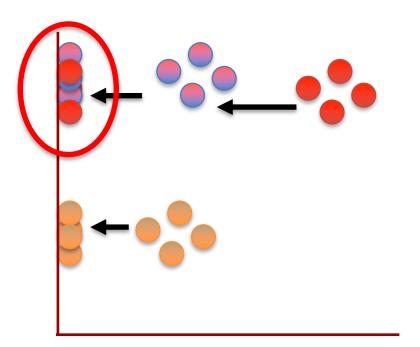


Copyright 2017 Joshua Starmer, https://statauest.org

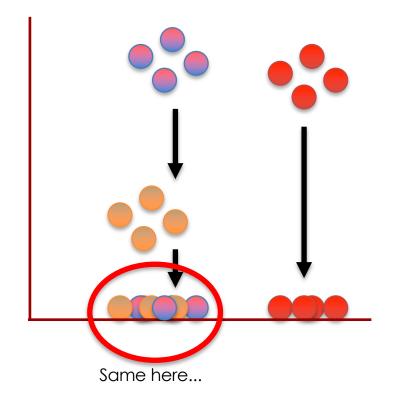
NOTE: If we just projected the data onto one of the axes, we'd just get a big mess that doesn't preserve the original clustering.



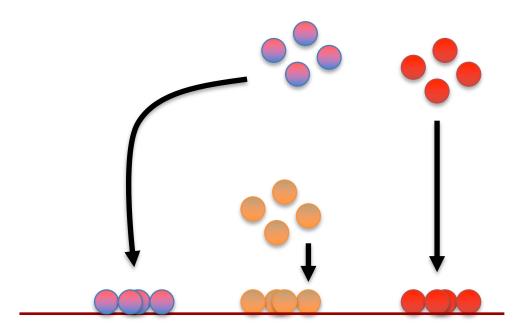
Instead of two distinct clusters, we just see a mishmash.





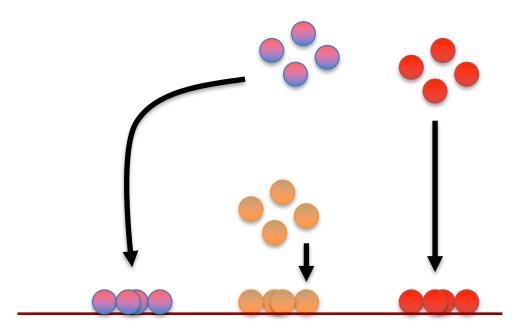






What t-SNE does is find a way to project data into a low dimensional space (in this case, the 1-D number line) so that the clustering in the high dimensional space (in this case, the 2-D scatter plot) is preserved.

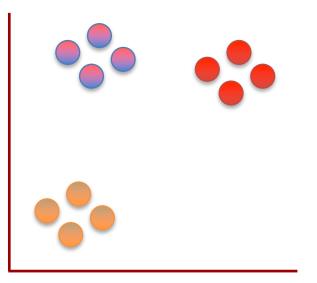




So let's step through the basic ideas of how t-SNE does this.



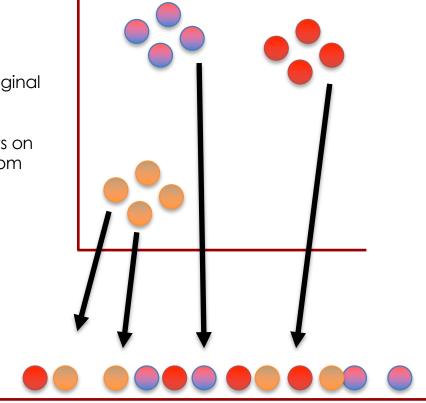
We'll start start with the original scatter plot...



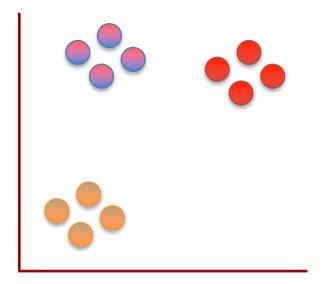


We'll start start with the original scatter plot...

... then we'll put the points on the number line in a random order.



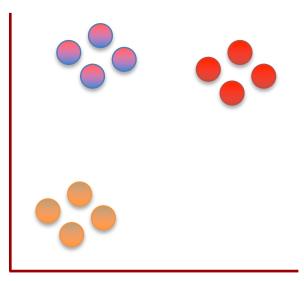




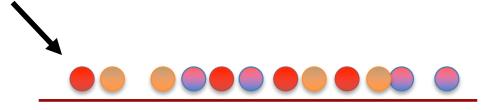


From here on out, t-SNE moves these points, a little bit at a time, until it has clustered them.

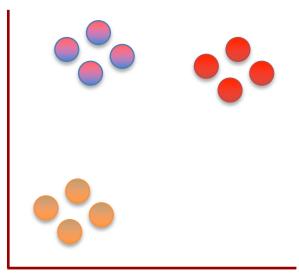




Let's figure out where to move this first point...





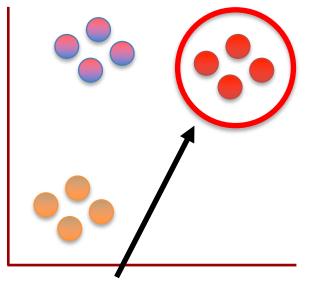


Let's figure out where to move this first point...

Should it move a little to the left or to the right?



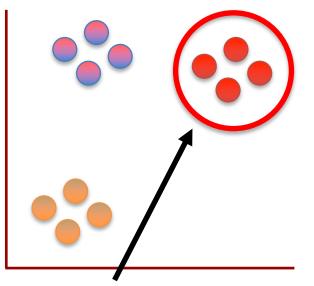




Because it is part of this cluster...

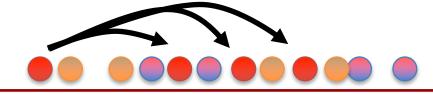




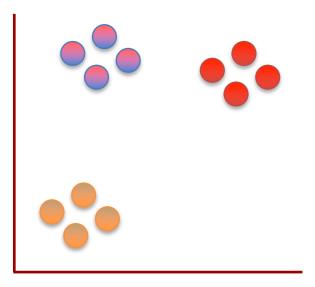


Because it is part of this cluster...





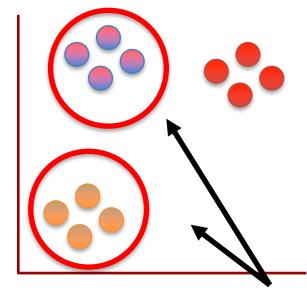




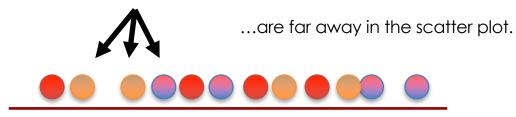
But at the same time, these points...



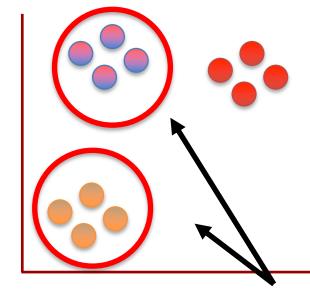




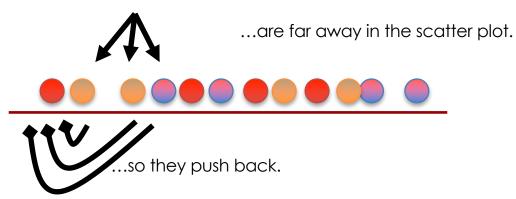
But at the same time, these points...



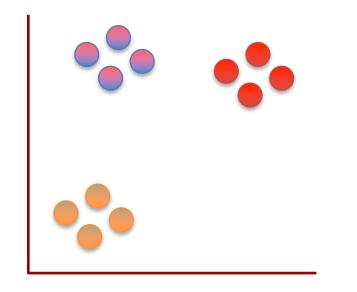


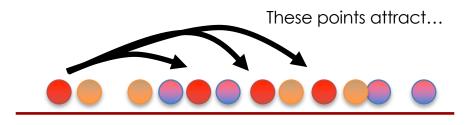


But at the same time, these points...

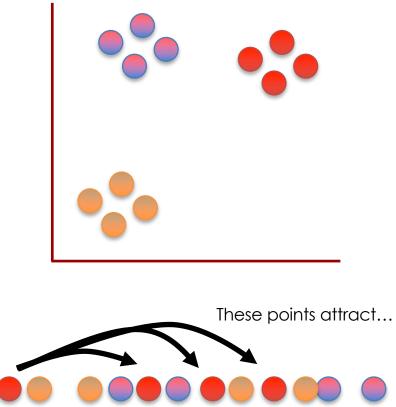






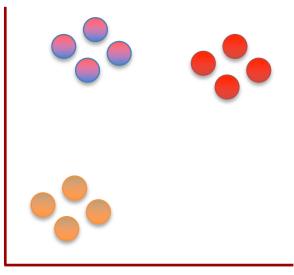






...while these points repel.

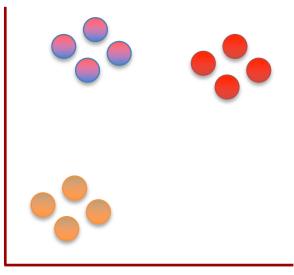




In this case, the attraction is strongest, so the point moves a little to the right.



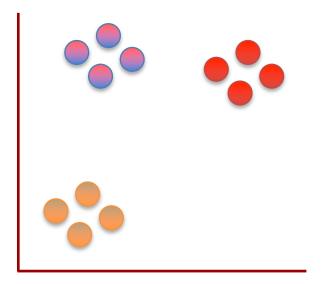




In this case, the attraction is strongest, so the point moves a little to the right.



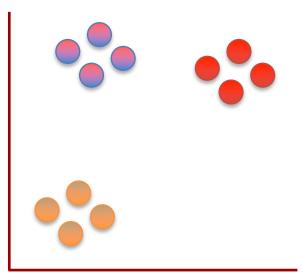




BAM!



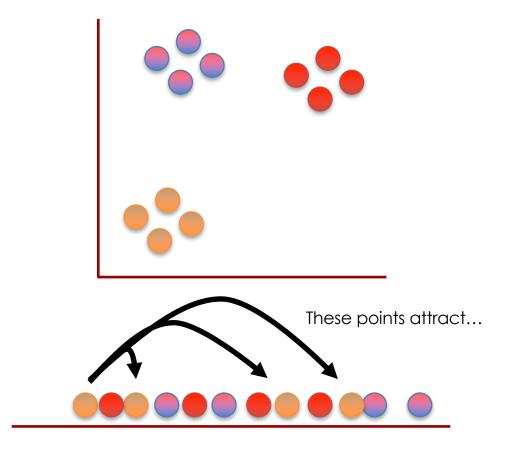




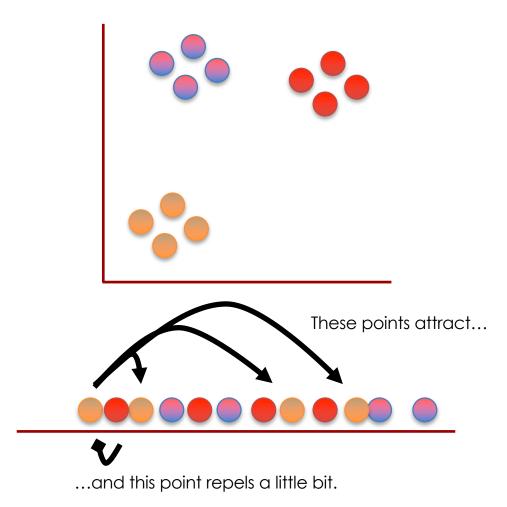
Now let's move this point a little bit...



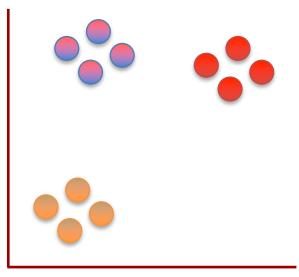








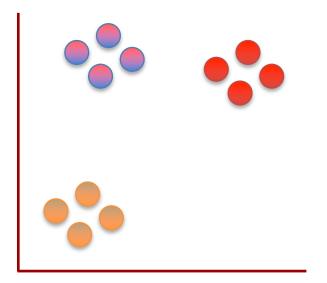




So it moves a little to closer to the other orange points.



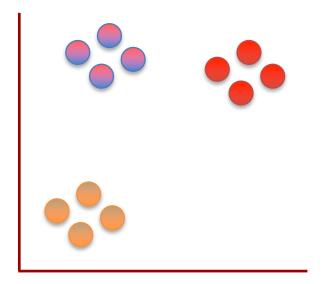




Double BAM!



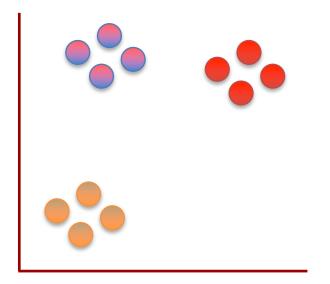






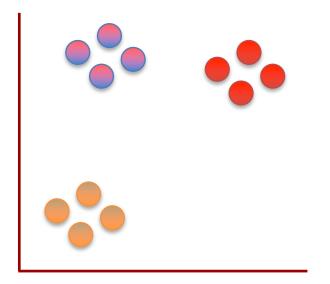
At each step, a point on the line is attracted to points it is near in the scatter plot, and repelled by points it is far from...





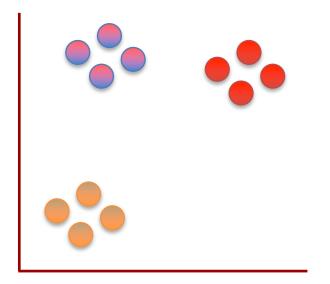






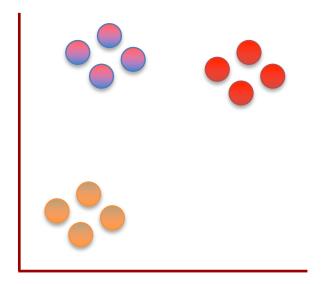






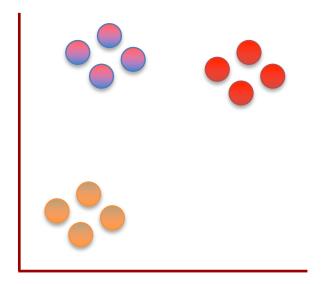






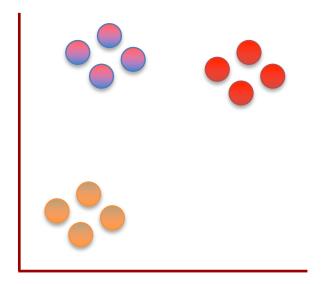






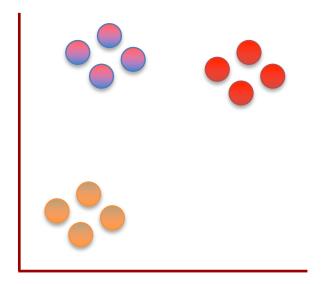






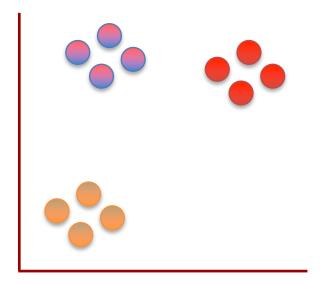






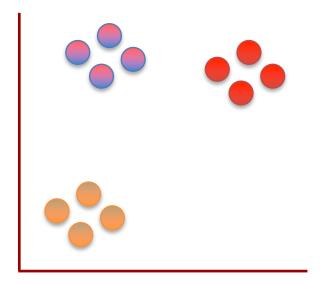






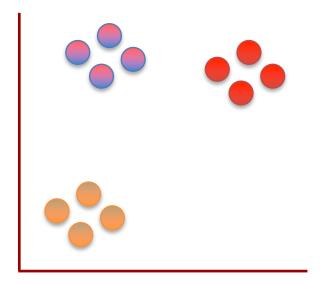






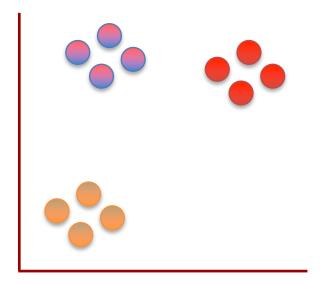






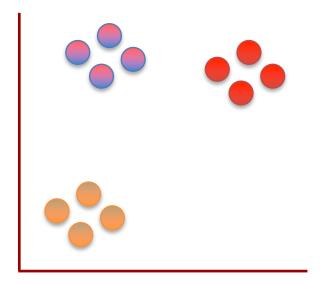






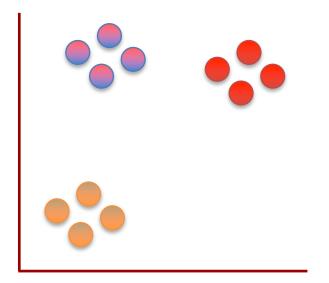






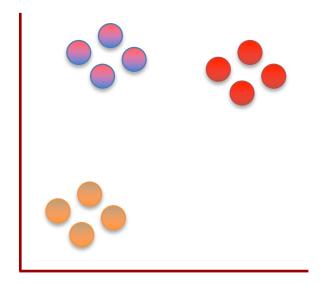






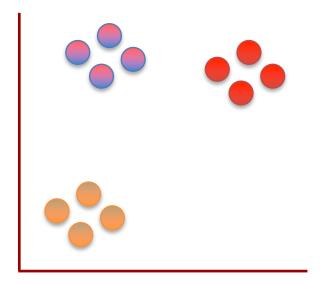






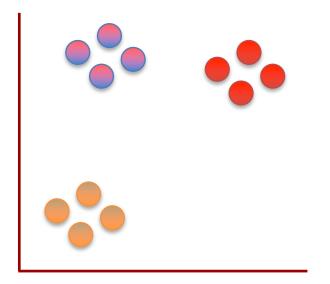






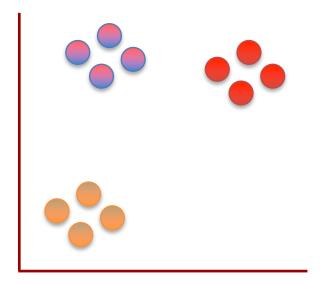






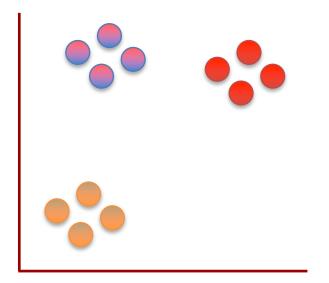






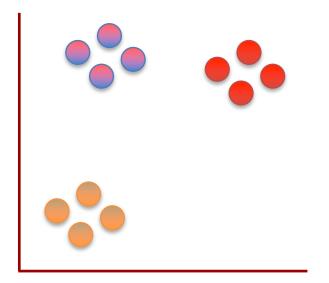






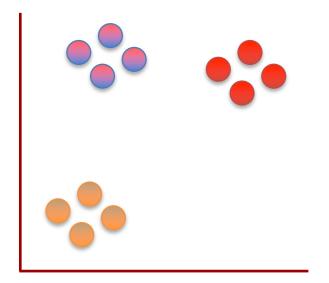






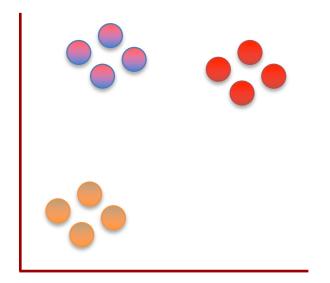






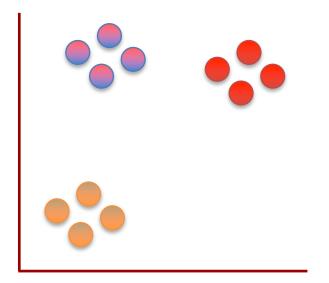






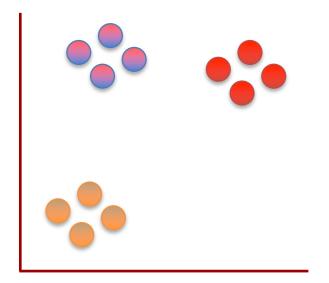






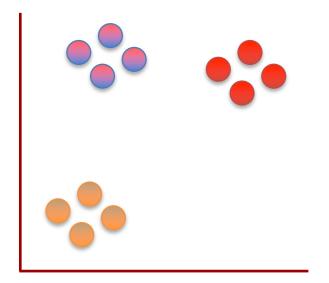






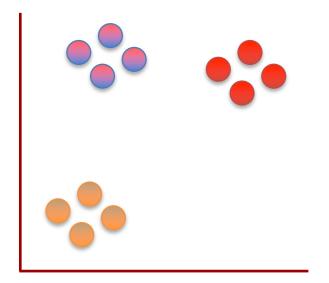






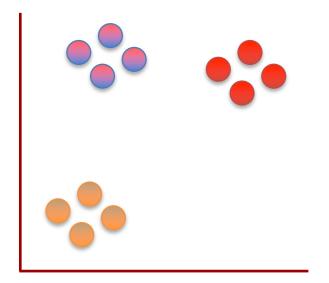






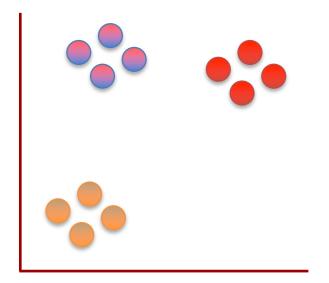






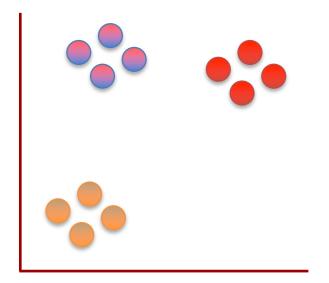






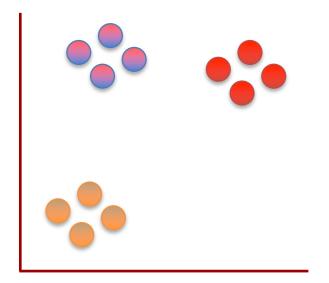






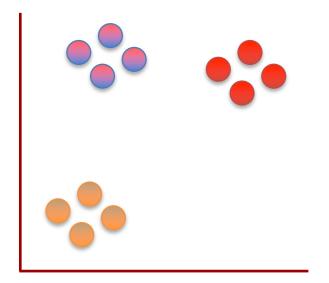






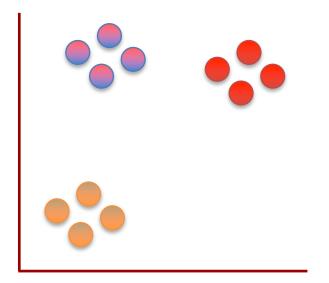






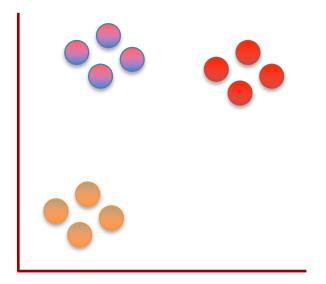












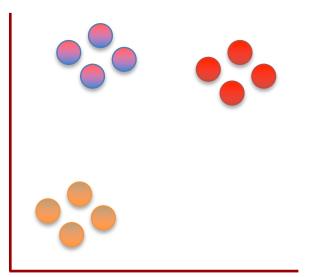
Triple BAM!!!!!





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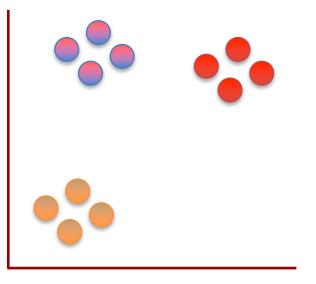
Now that we've seen the what t-SNE tries to do, let's dive into the nitty-gritty details of how it does what it does.





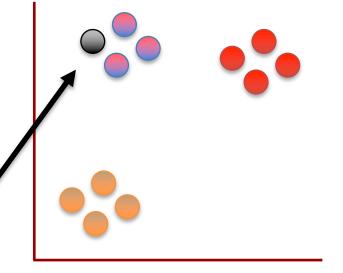


Step 1: Determine the "similarity" of all the points in the scatter plot.



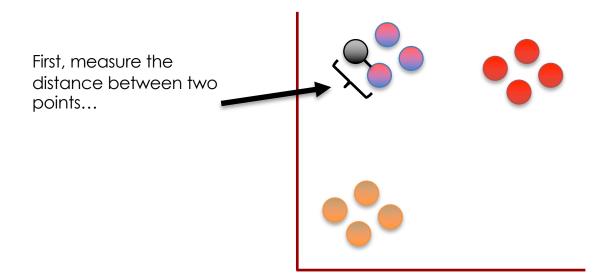


Step 1: Determine the "similarity" of all the points in the scatter plot.

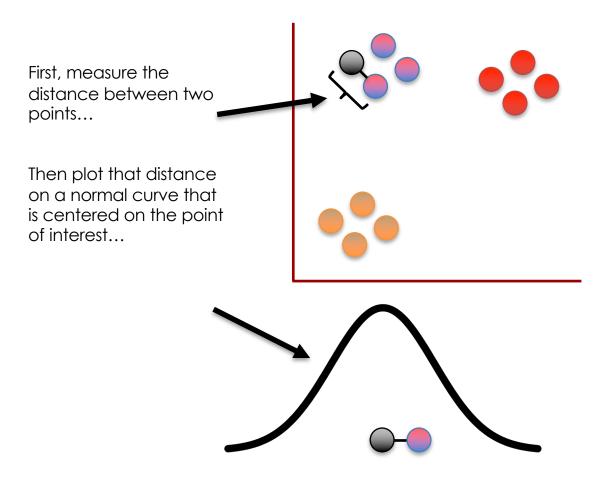


For this example, let's focus on determining the similarities between this point and all of the other points.

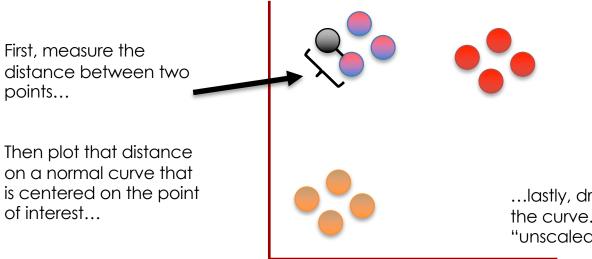




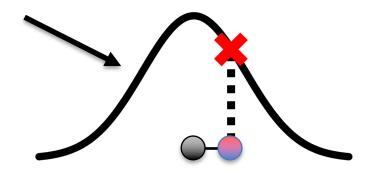






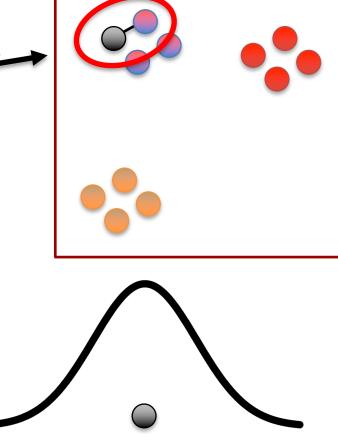


...lastly, draw a line from the point to the curve. The length of that line is the "unscaled similarity".

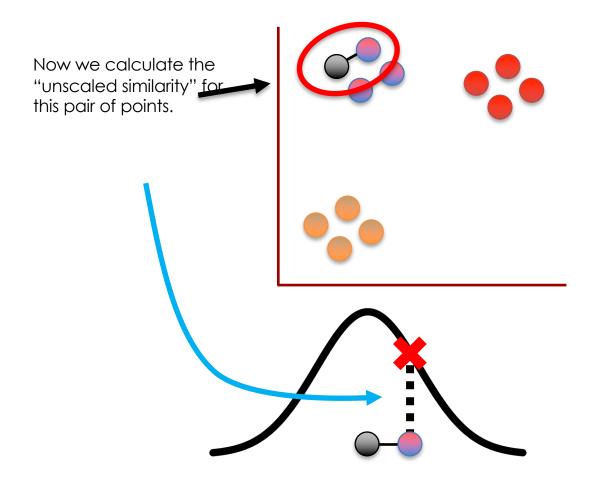




Now we calculate the "unscaled similarity" for this pair of points.

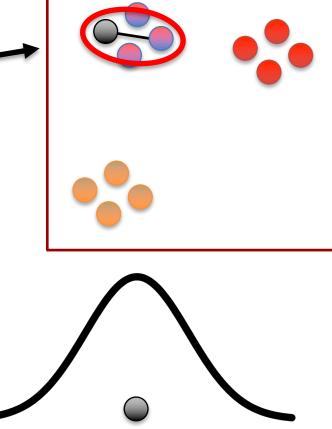






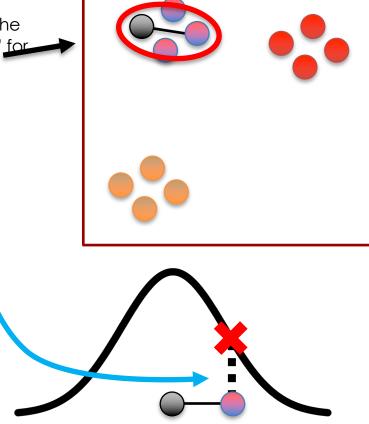


Now we calculate the "unscaled similarity" for this pair of points.

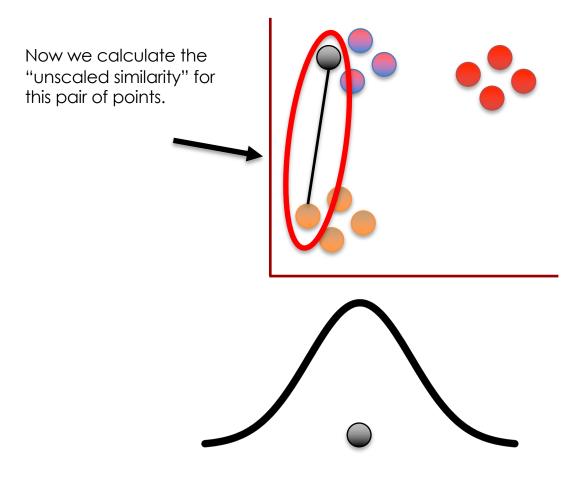




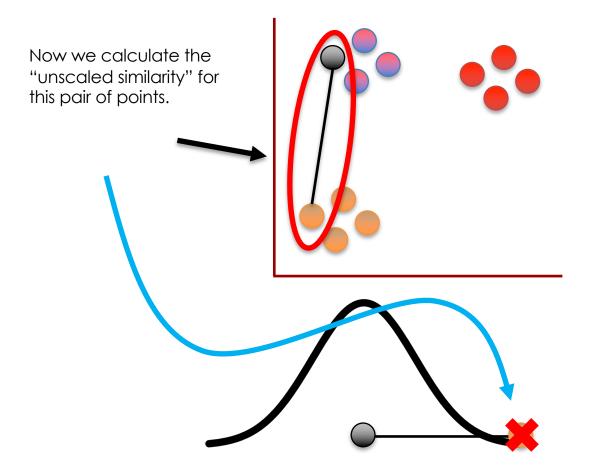
Now we calculate the "unscaled similarity" <u>for</u> this pair of points.



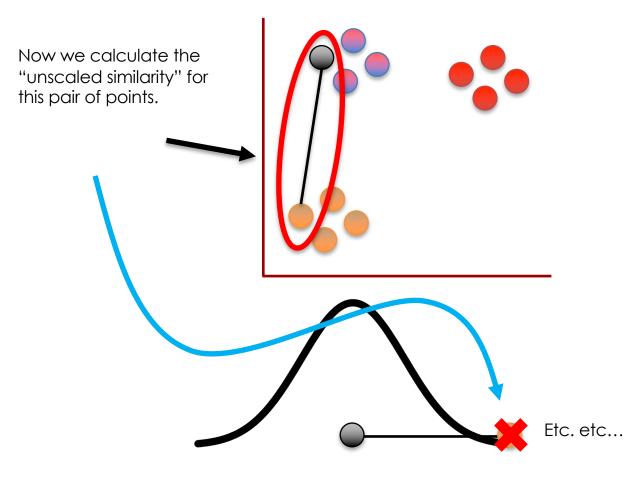




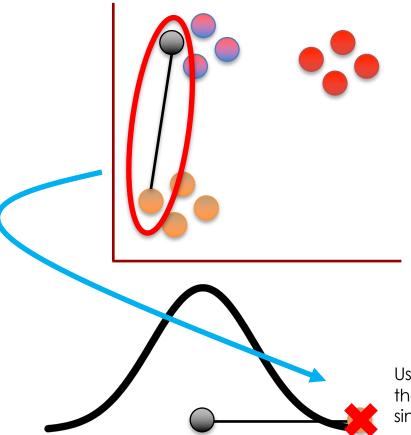






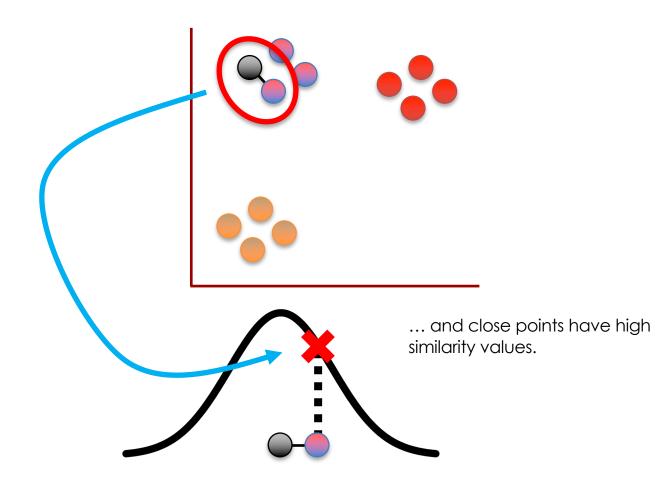






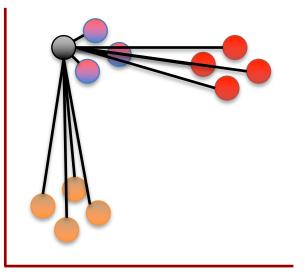
Using a normal distribution means that distant points have very low similarity values....



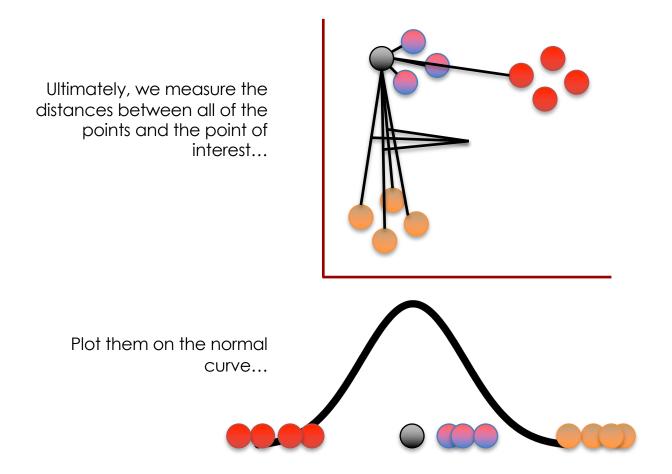




Ultimately, we measure the distances between all of the points and the point of interest...









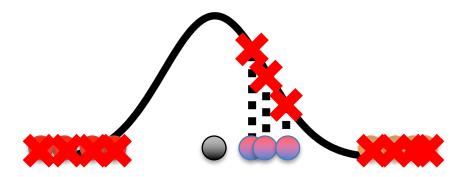
Ultimately, we measure the distances between all of the points and the point of interest... Plot them on the normal curve...

...and then measure the distances from the points to the curve to get the unscaled similarity scores with respect to the point of interest.



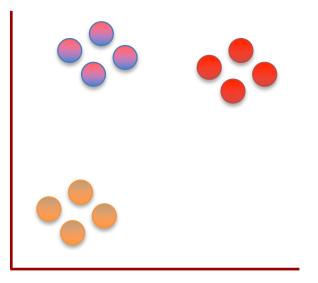
The next step is to scale the unscaled similarities so that they add up to 1.

Umm... Why do the similarity scores need to add up to 1?



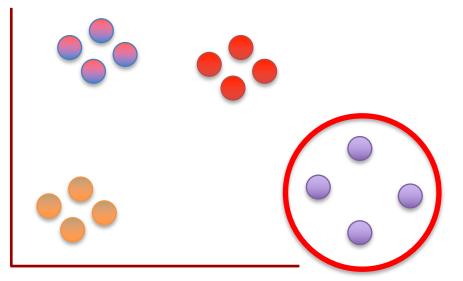


It has to do with something I didn't tell you earlier...



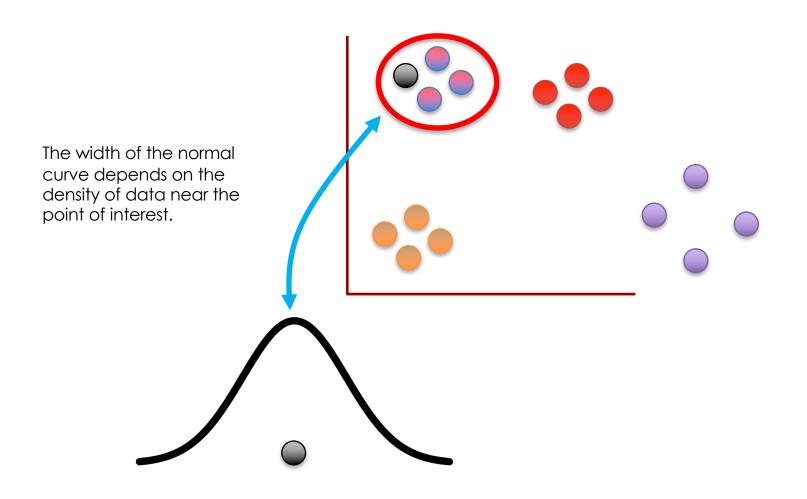


It has to do with something I didn't tell you earlier...

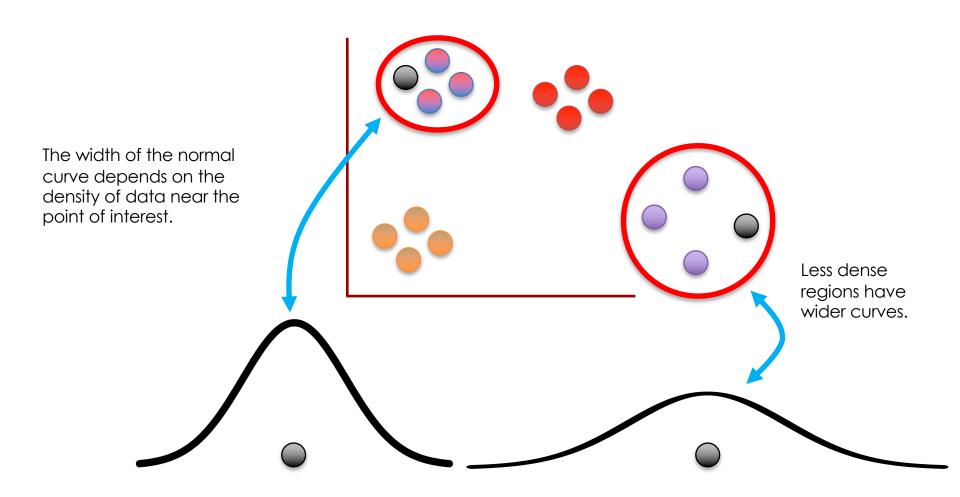


...and to illustrate the concept, I need to add a cluster that is half as dense as the others.

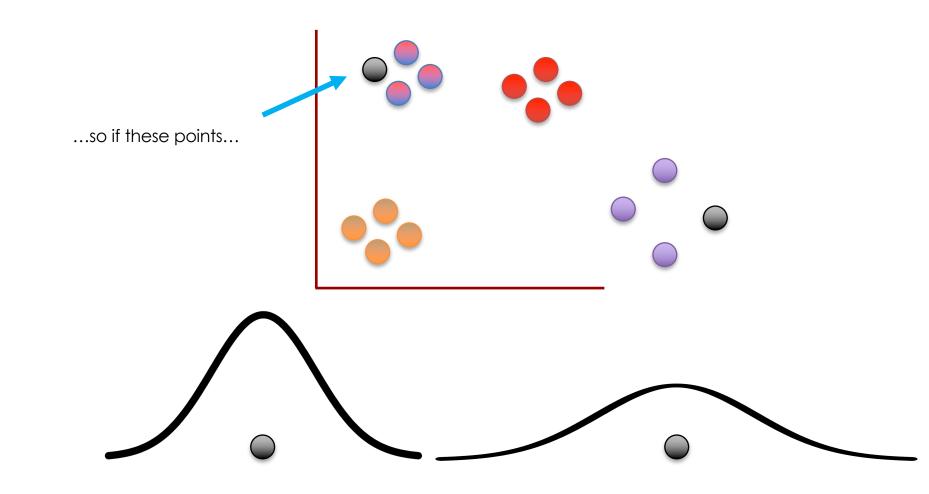




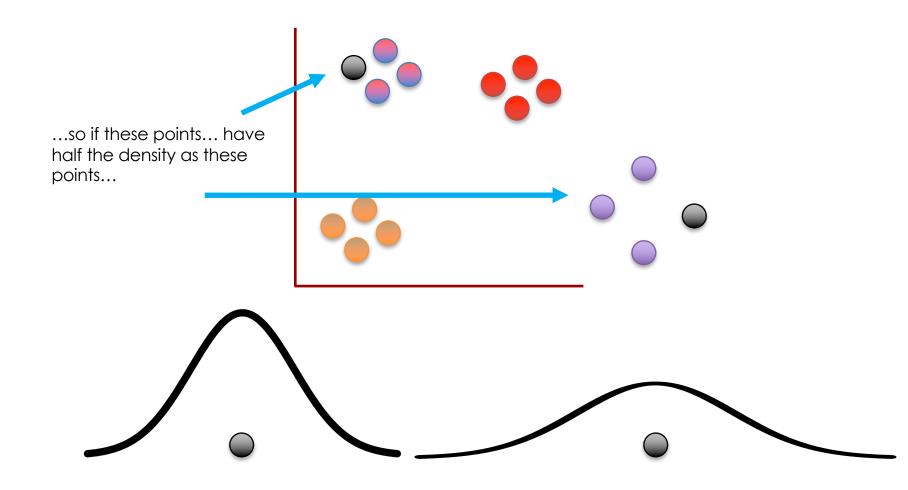




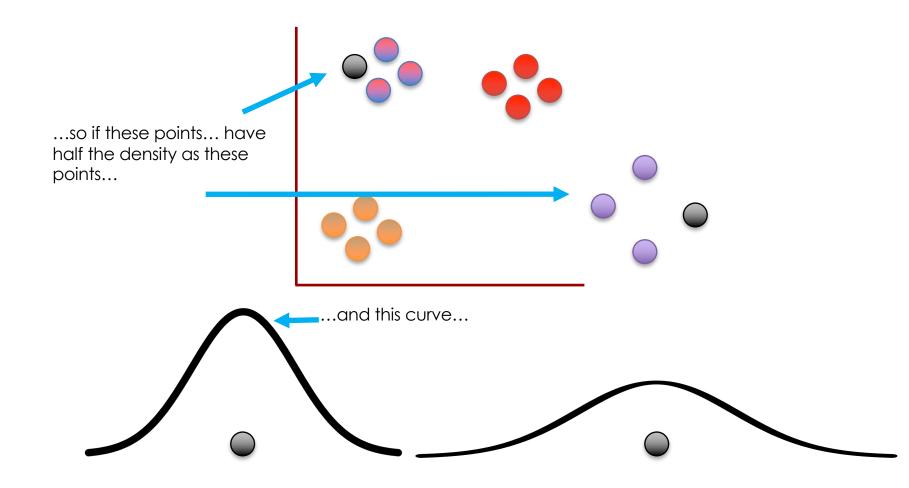




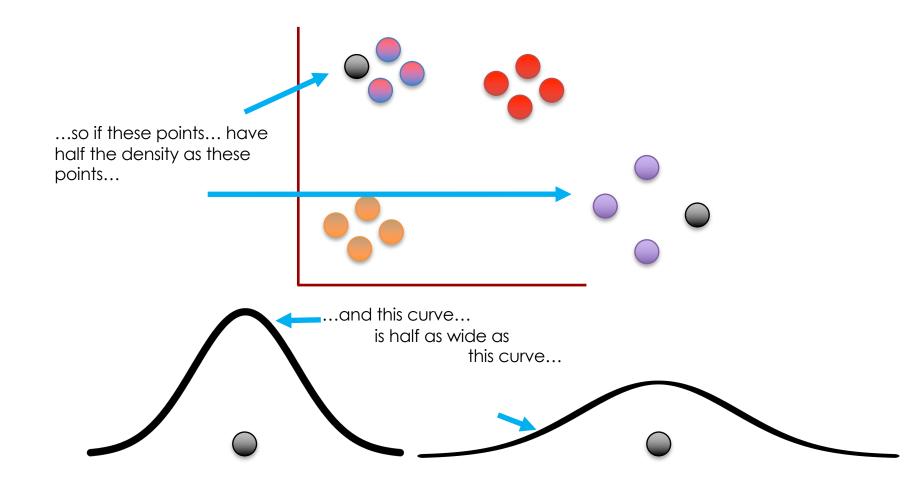




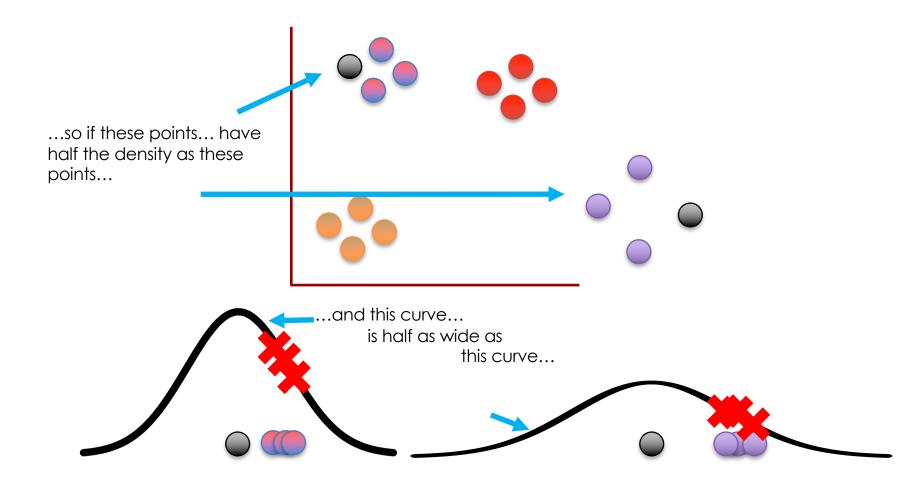












...then scaling the similarity scores will make them the same for both clusters.

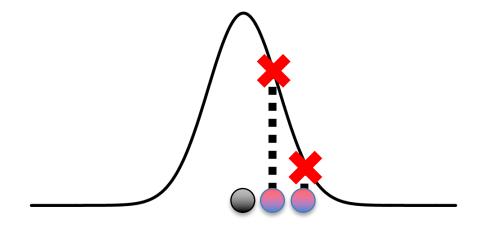


Here's an example...

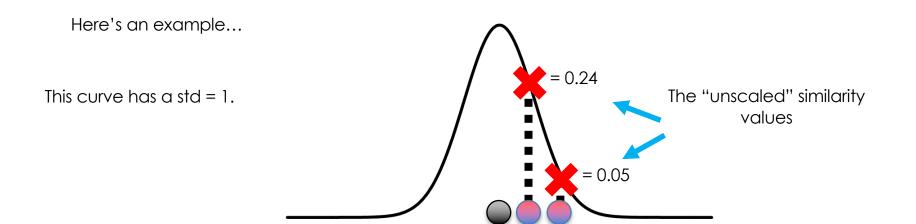


Here's an example...

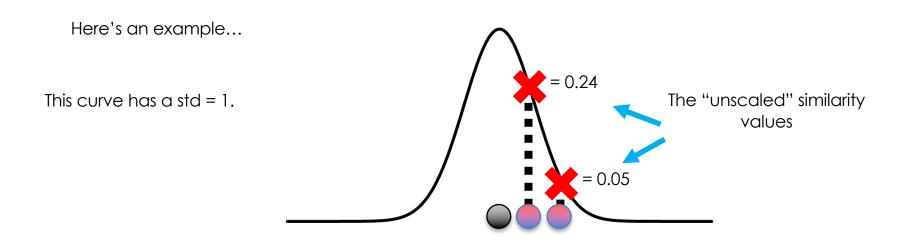
This curve has a std = 1.



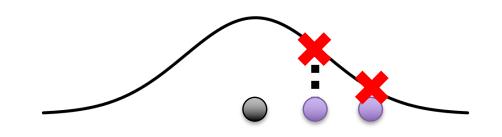




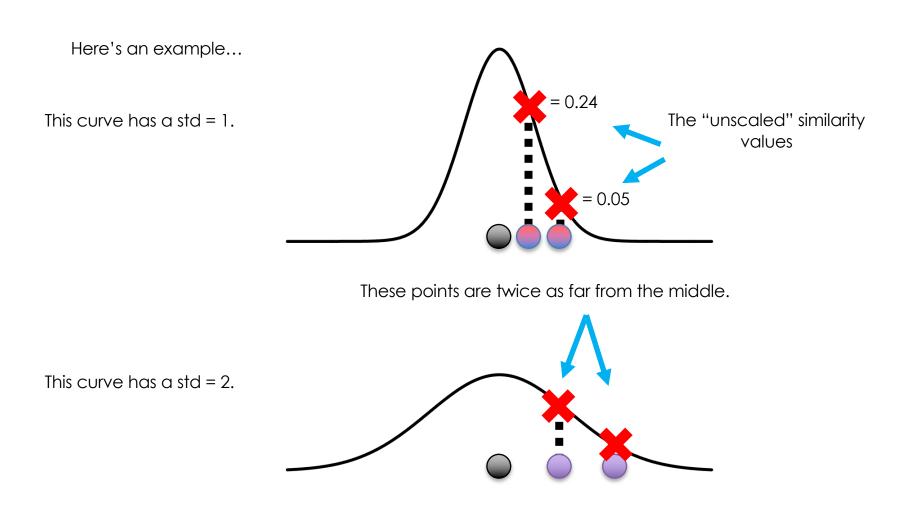




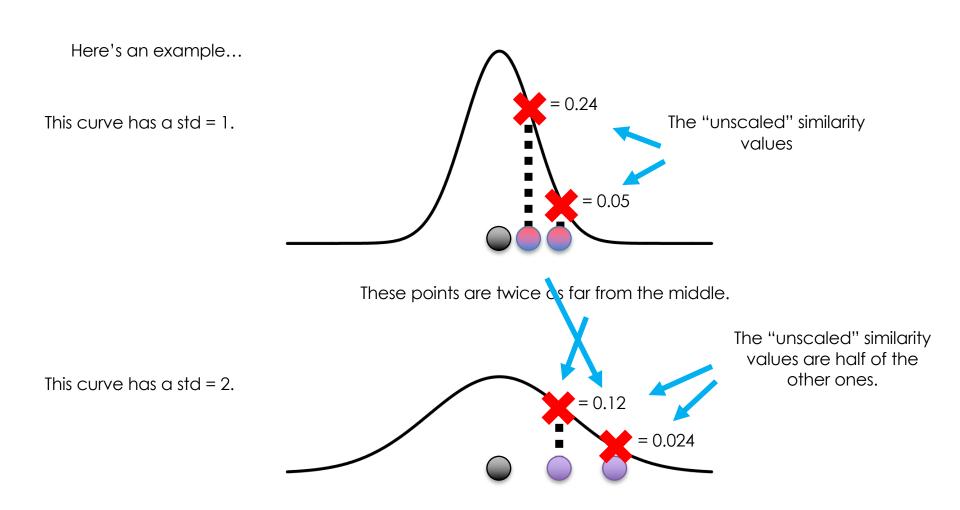
This curve has a std = 2.



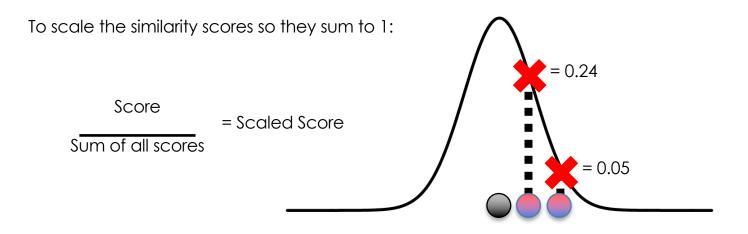


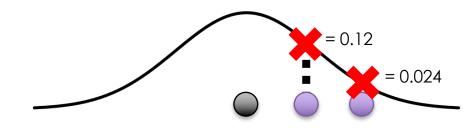




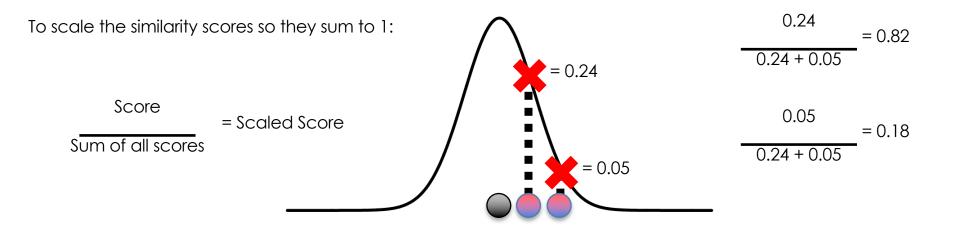


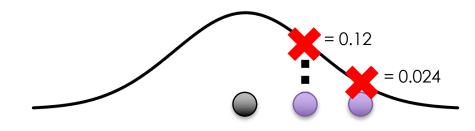




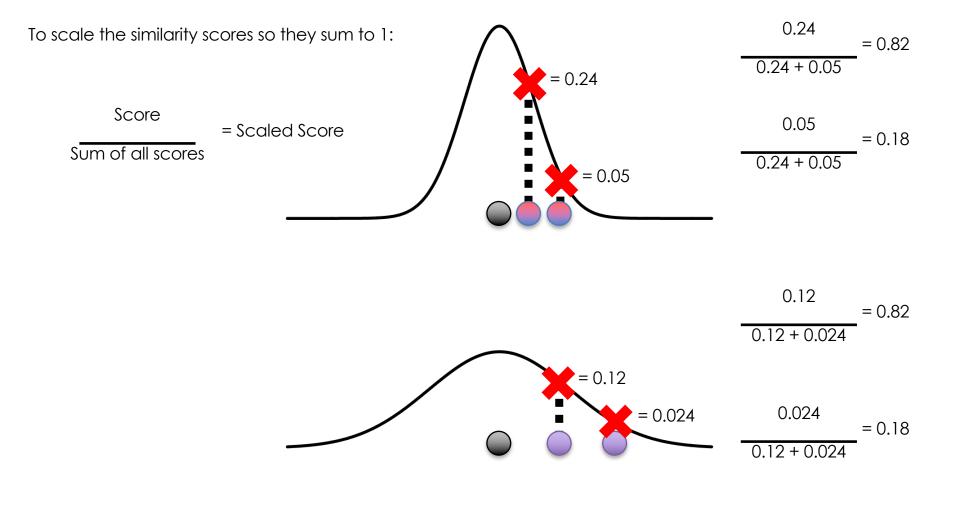




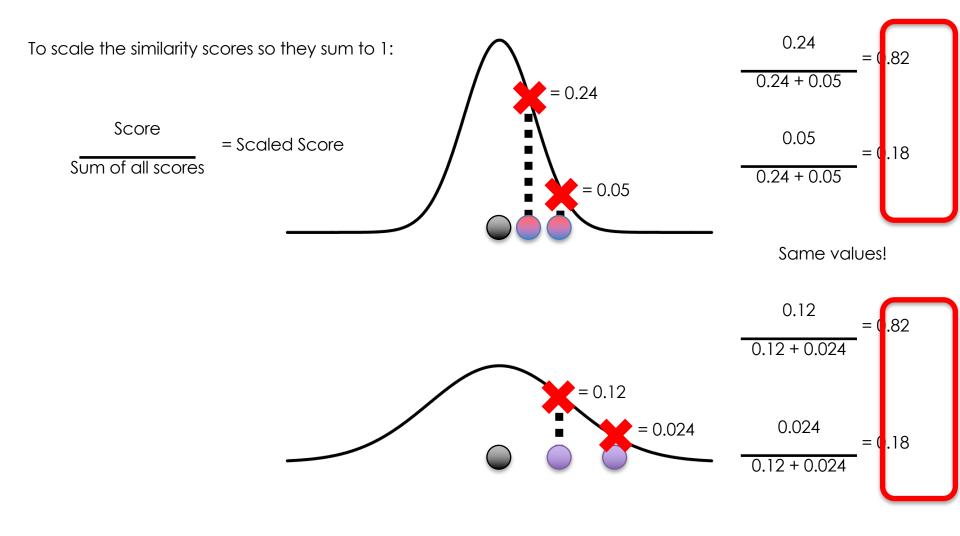








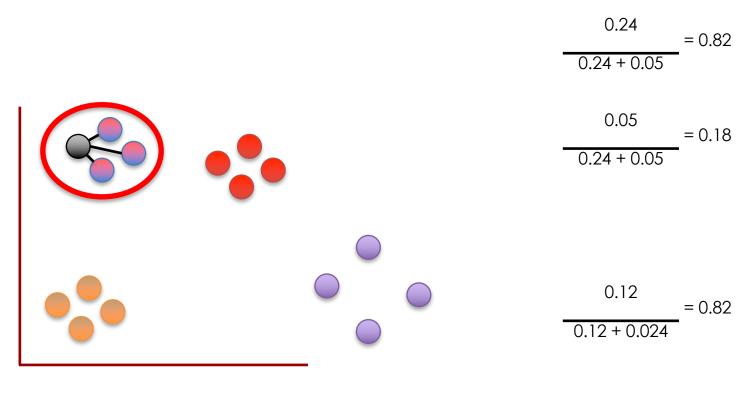








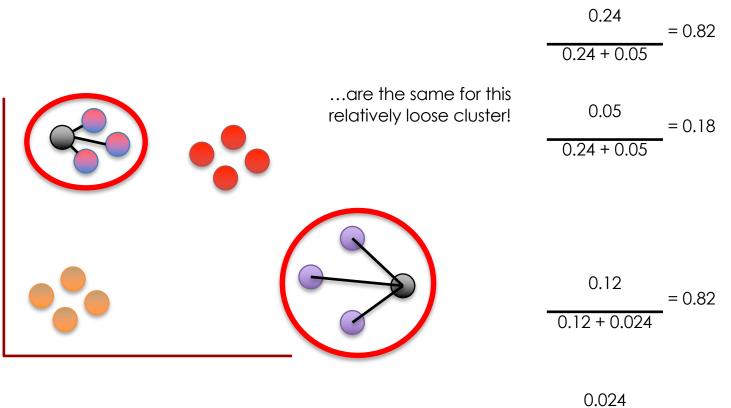
That implies that the scaled similarity scores for this relatively tight cluster...



0.024 = 0.18

COSMIC DAWN GENTER

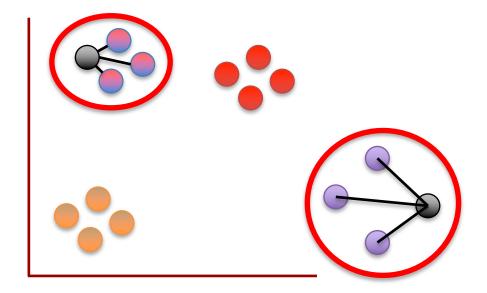
That implies that the scaled similarity scores for this relatively tight cluster...



= 0.18

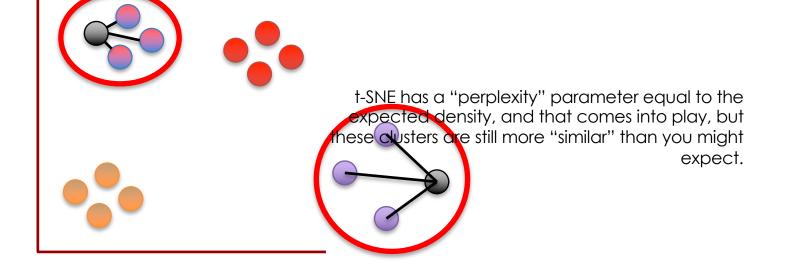


The reality is a little more complicated, but only slightly.



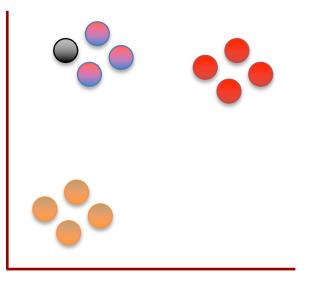


The reality is a little more complicated, but only slightly.



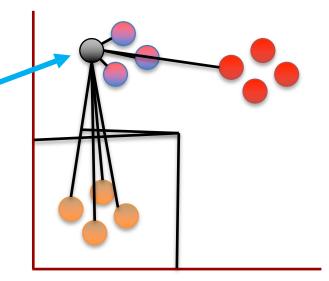


Now back to the original scatter plot...

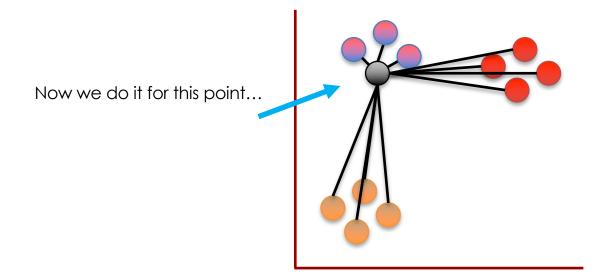




We've calculated similarity scores for this point.

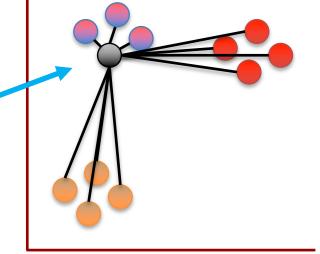






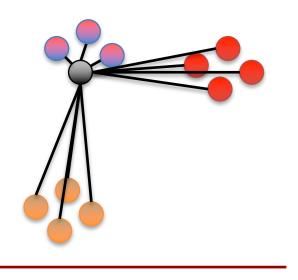








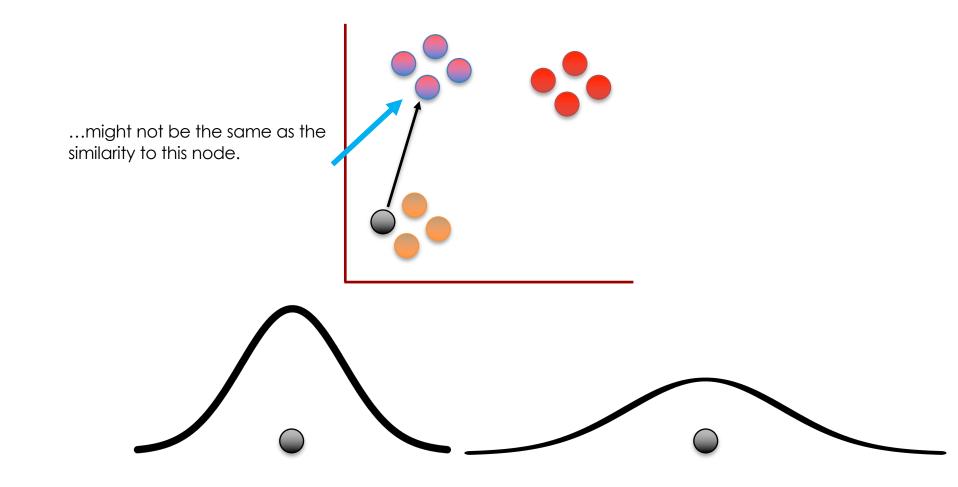
One last thing and the scatter plot will be all set with similarity scores!!!



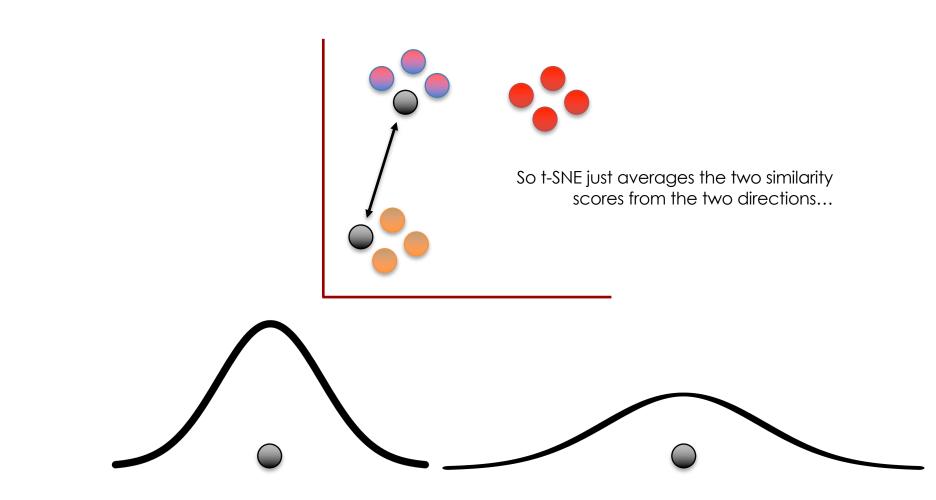


Because the width of the distribution is based on the density of the surrounding data points, the similarity score to this node...

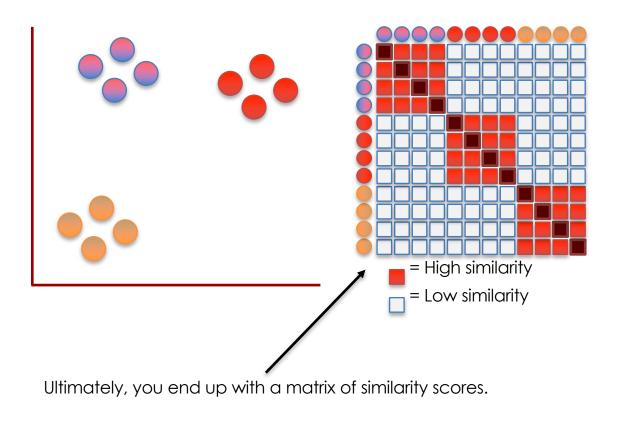




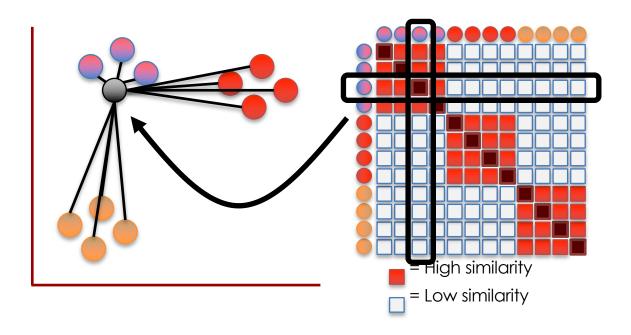






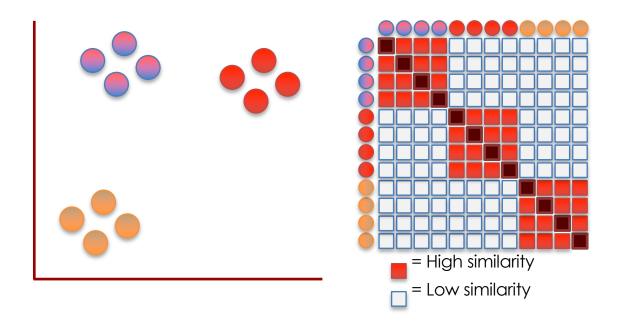






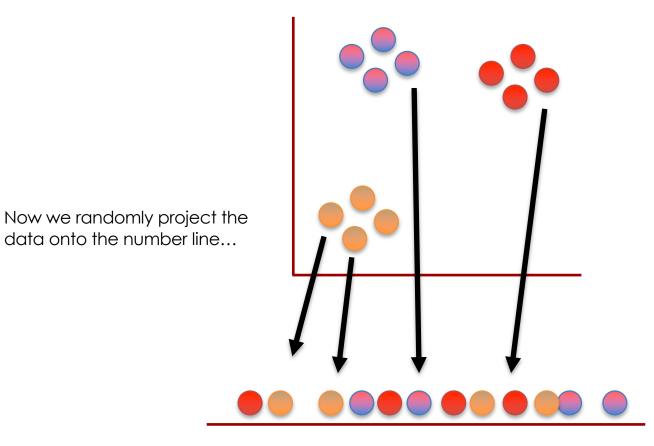




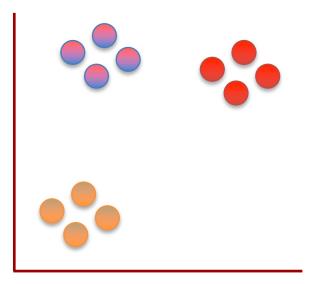


Hooray!!! We're done doing calculating similarity scores for the scatter plot!





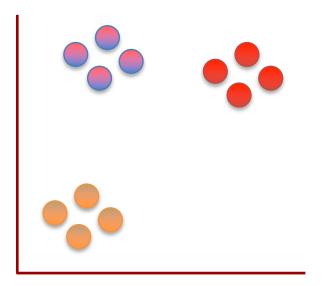
COSMIC DAWN CENTER



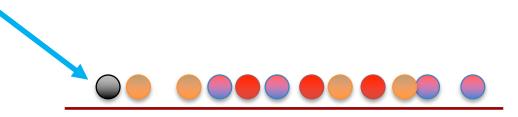
Now we randomly project the data onto the number line...

... and calculate similarity scores for the points on the number line.

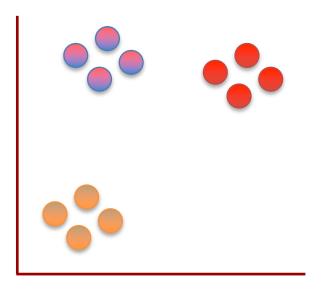




Just like before, that means picking a point...



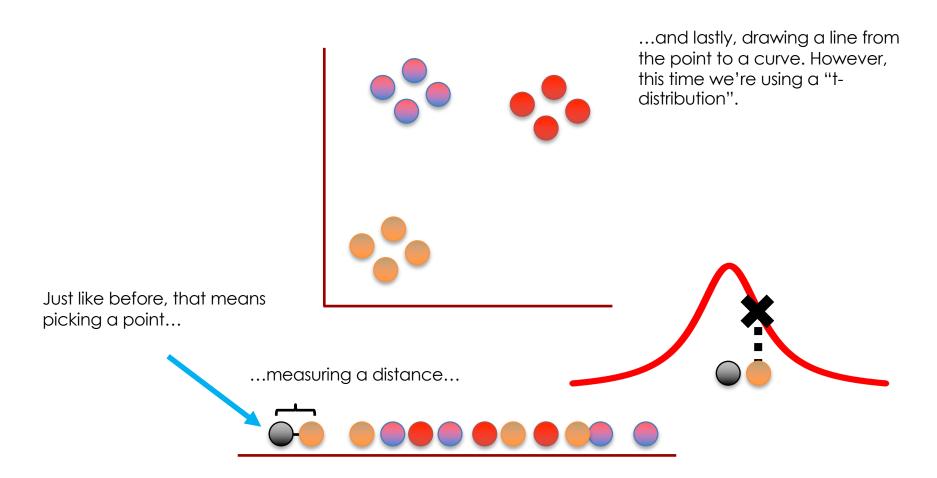




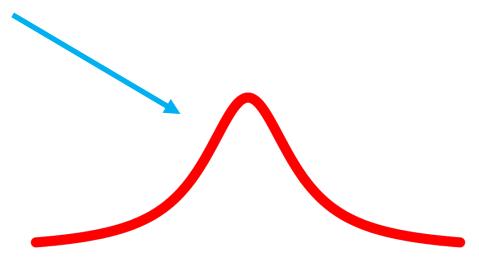
Just like before, that means picking a point...

...measuring a distance...



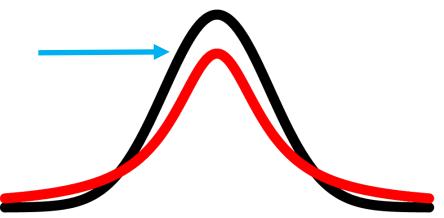








...is a lot like a normal distribution





...is a lot like a normal distribution... ...except the "t" isn't as tall in the middle...



... is a lot like a normal distribution...

...except the "t" isn't as tall in the middle...

... and the tails are taller on the ends.



... is a lot like a normal distribution...

...except the "t" isn't as tall in the middle...

... and the tails are taller on the ends.

The "t-distribution" is the "t" in t-SNE.



... is a lot like a normal distribution...

...except the "t" isn't as tall in the middle...

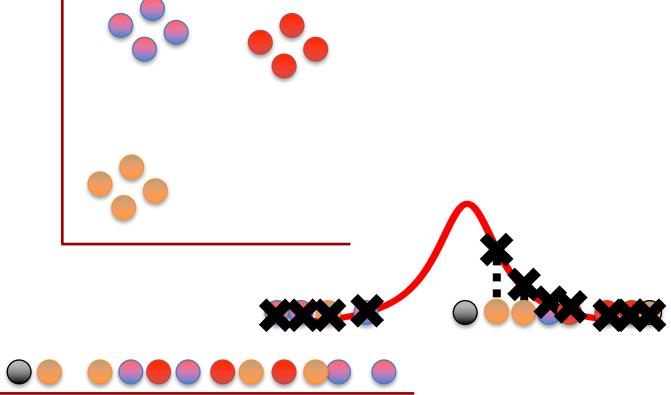
... and the tails are taller on the ends.

The "t-distribution" is the "t" in t-SNE.

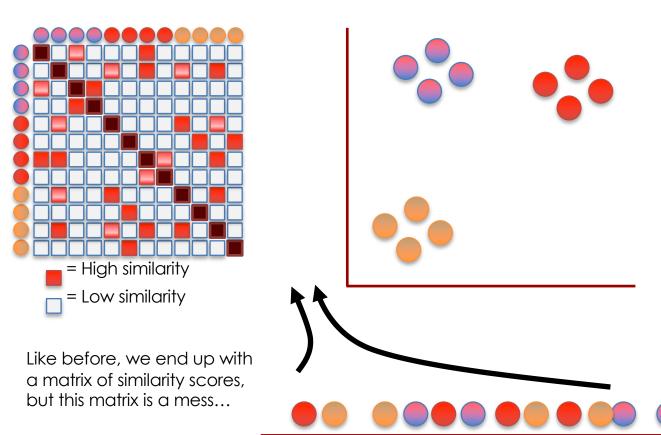
We'll talk about why the t-distribution is used in a bit...



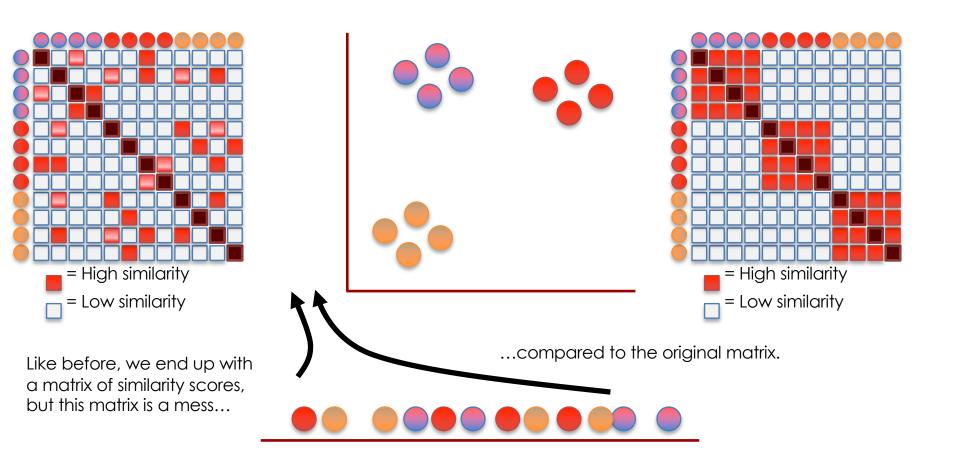
So, using a t-distribution, we calculate "unscaled" similarity scores for all the points and then scale them like before.



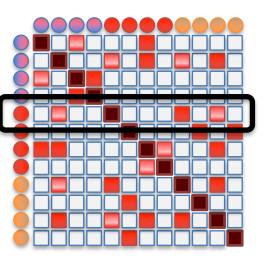


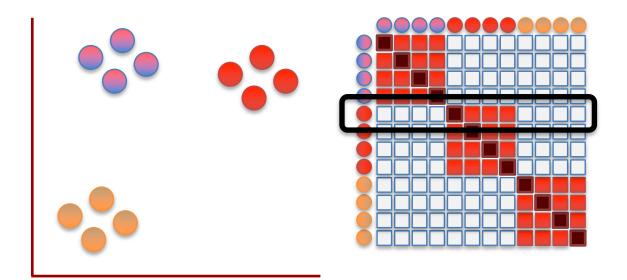








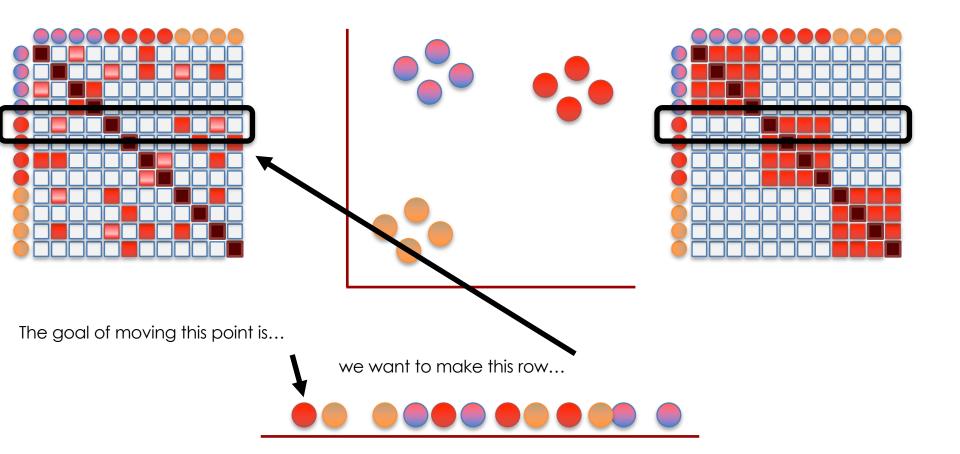




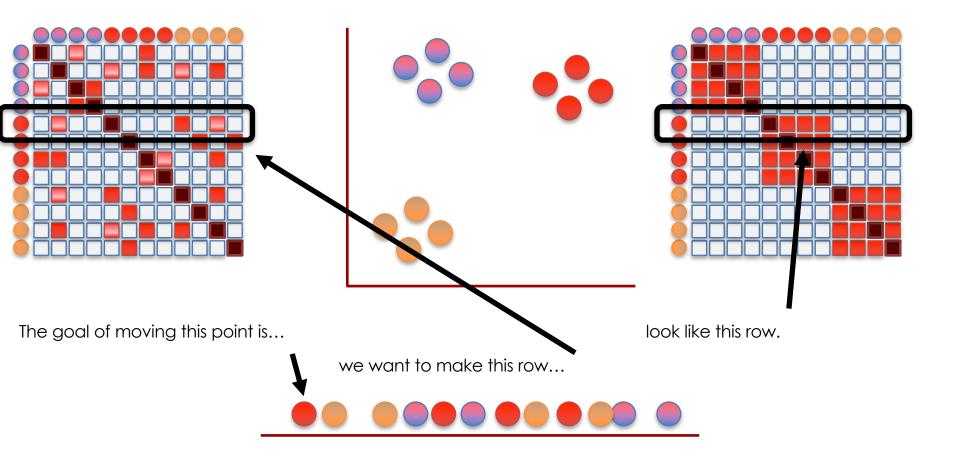
The goal of moving this point is...



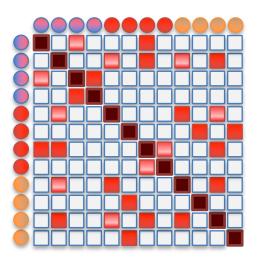


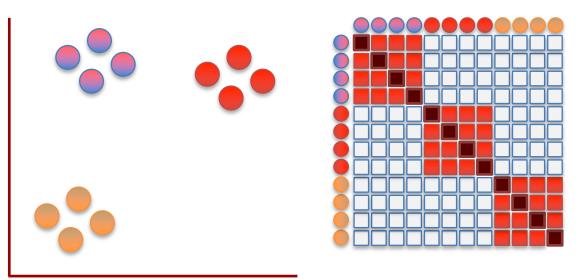








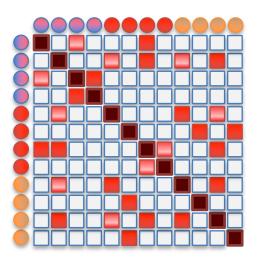


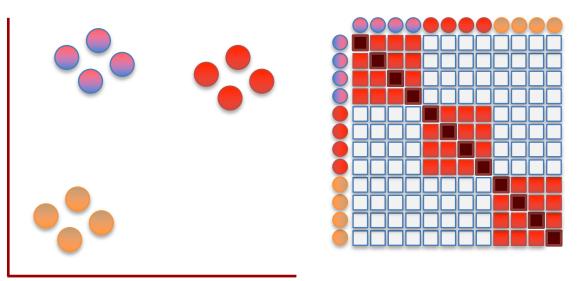


t-SNE moves the points a little bit at a time, and each step it chooses a direction that makes the matrix on the left more like the matrix on the right.







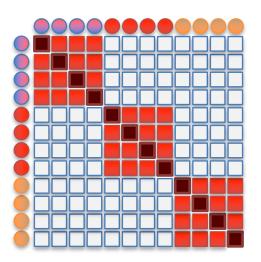


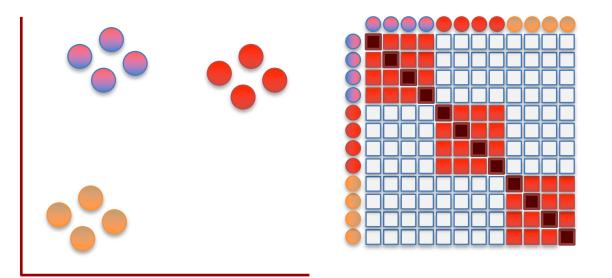
t-SNE moves the points a little bit at a time, and each step it chooses a direction that makes the matrix on the left more like the matrix on the right.



It uses small steps, because it's a little bit like a chess game and can't be solved all at once. Instead, it goes one move at at time.



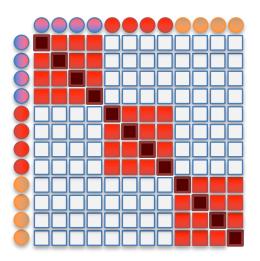


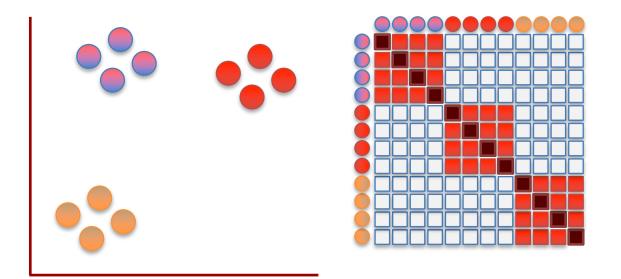


BAM!!!





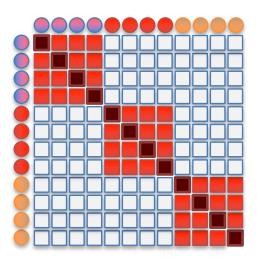


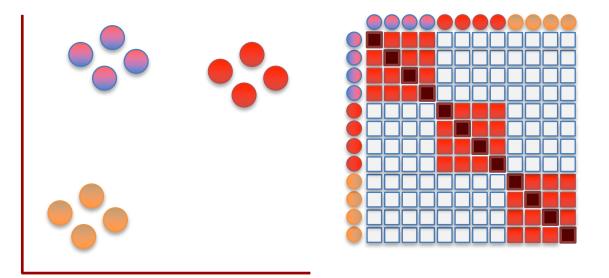


Now to finally tell you why the "t-distribution" is used...





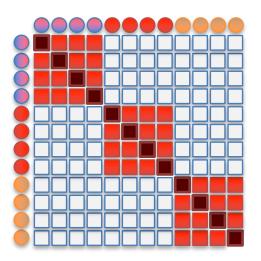


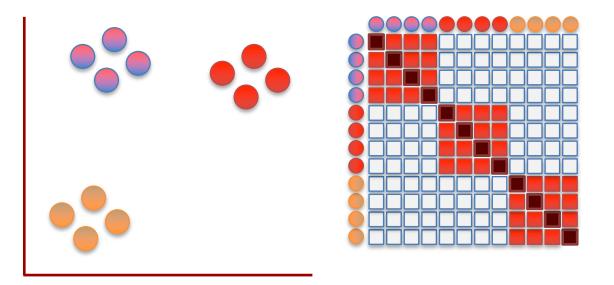


Originally, the "SNE" algorithm used a normal distribution throughout and the clusters clumped up in the middle and were harder to see.





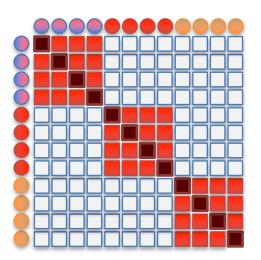


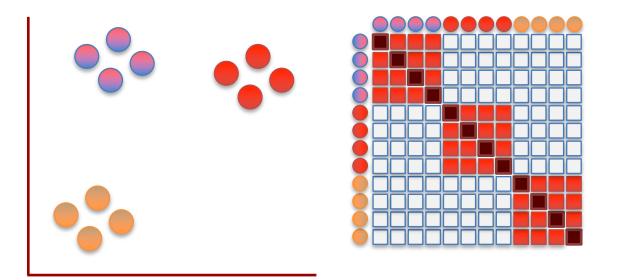


The t-distribution forces some space between the points.









Triple Bam!!!





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$$p_{j|i} = \frac{\exp\left(-||x_i - x_j||^2 / 2\sigma_i^2\right)}{\sum_{k \neq i} \exp\left(-||x_i - x_k||^2 / 2\sigma_i^2\right)}, \quad p_{ij} = \frac{p_{i|j} + p_{j|i}}{2N} \quad (1)$$

$$-\sum_{j} p_{j|i} \log_2 p_{j|i}$$
Perplexity = 2 (2)
$$q_{ij} = \frac{\left(1 + ||y_i - y_j||^2\right)^{-1}}{\sum_{k \neq l} \left(1 + ||y_k - y_l||^2\right)^{-1}} \quad (3)$$

$$KL(P_i||Q_i) = \sum_{i} \sum_{j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}, \quad \frac{\partial KL}{\partial y_i} = 4 \sum_{j} (p_{ij} - q_{ij})(y_i - y_j) \left(1 + ||y_i - y_j||^2\right)^{-1} \quad (4)$$



N. Oskolkov, towardsdatascience.com

Defines distance probability as Gaussian

$$p_{j|i} = \frac{\exp\left(-||x_{i} - x_{j}||^{2}/2\sigma_{i}^{2}\right)}{\sum_{k \neq i} \exp\left(-||x_{i} - x_{k}||^{2}/2\sigma_{i}^{2}\right)}, \quad p_{ij} = \frac{p_{i|j} + p_{j|i}}{2N} \quad (1)$$

$$-\sum_{j} p_{j|i} \log_{2} p_{j|i}$$
Perplexity = 2 (2)
$$q_{ij} = \frac{\left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1}}{\sum_{k \neq l} \left(1 + ||y_{k} - y_{l}||^{2}\right)^{-1}} \quad (3)$$

$$P_{i}||Q_{i}\rangle = \sum_{i} \sum_{j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}, \quad \frac{\partial KL}{\partial y_{i}} = 4 \sum_{j} (p_{ij} - q_{ij})(y_{i} - y_{j})\left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1} \quad (4)$$



KL(

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Determines optimal σ

$$-\sum_{j} p_{j|i} \log_{2} p_{j|i}$$
Perplexity = 2
$$q_{ij} = \frac{\left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1}}{\sum_{k \neq l} \left(1 + ||y_{k} - y_{l}||^{2}\right)^{-1}} \qquad (3)$$

$$KL(P_{i}||Q_{i}) = \sum_{i} \sum_{j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}, \qquad \frac{\partial KL}{\partial y_{i}} = 4 \sum_{j} (p_{ij} - q_{ij})(y_{i} - y_{j}) \left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1} \qquad (4)$$



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Defines distance probability as Gaussian

$$p_{j|i} = \frac{\exp\left(-||x_{i} - x_{j}||^{2}/2\sigma_{i}^{2}\right)}{\sum_{k \neq i} \exp\left(-||x_{i} - x_{k}||^{2}/2\sigma_{i}^{2}\right)}, \qquad p_{ij} = \frac{p_{i|j} + p_{j|i}}{2N} \qquad (1)$$
Determines optimal σ , $-\sum_{j} p_{j|i} \log_{2} p_{j|i}$
global vs. local
Perplexity = 2 (2)
$$q_{ij} = \frac{\left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1}}{\sum_{k \neq l} \left(1 + ||y_{k} - y_{l}||^{2}\right)^{-1}} \qquad (3)$$

$$KL(P_{i}||Q_{i}) = \sum_{i} \sum_{j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}, \qquad \frac{\partial KL}{\partial y_{i}} = 4 \sum_{j} (p_{ij} - q_{ij})(y_{i} - y_{j}) \left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1} \qquad (4)$$



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Defines distance probability as Gaussian

$$p_{j|i} = \frac{\exp\left(-||x_{i} - x_{j}||^{2}/2\sigma_{i}^{2}\right)}{\sum_{k \neq i} \exp\left(-||x_{i} - x_{k}||^{2}/2\sigma_{i}^{2}\right)}, \quad p_{ij} = \frac{p_{i|j} + p_{j|i}}{2N} \quad (1)$$
Determines optimal σ ,
global vs. local

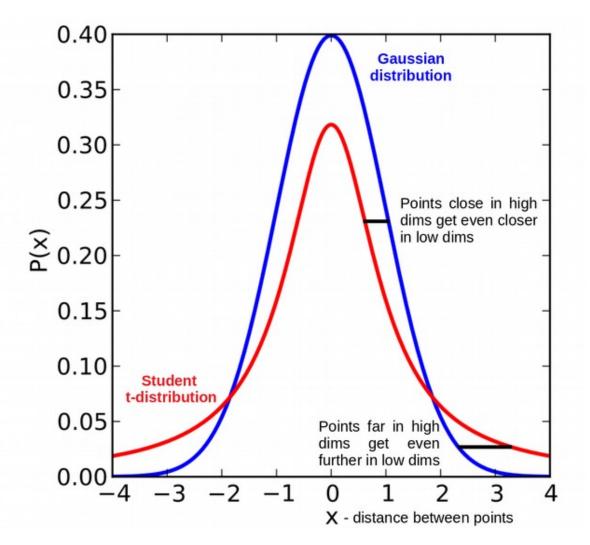
$$Perplexity = 2 \quad (2)$$

$$q_{ij} = \frac{\left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1}}{\sum_{k \neq l} \left(1 + ||y_{k} - y_{l}||^{2}\right)^{-1}} \quad (3)$$

$$KL(P_{i}||Q_{i}) = \sum_{i} \sum_{j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}, \quad \frac{\partial KL}{\partial y_{i}} = 4 \sum_{j} (p_{ij} - q_{ij})(y_{i} - y_{j}) \left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1} \quad (4)$$



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Defines distance probability as Gaussian

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Determines optimal σ ,
global vs. local

$$Perplexity = 2 \quad (2)$$

$$q_{ij} = \frac{\left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1}}{\sum_{k \neq l} \left(1 + ||y_{k} - y_{l}||^{2}\right)^{-1}} \quad (3)$$

$$KL(P_{i}||Q_{i}) = \sum_{i} \sum_{j} p_{j|i} \log \frac{p_{j|i}}{q_{j|i}}, \quad \frac{\partial KL}{\partial y_{i}} = 4 \sum_{j} (p_{ij} - q_{ij})(y_{i} - y_{j}) \left(1 + ||y_{i} - y_{j}||^{2}\right)^{-1} \quad (4)$$

Defines loss function for gradient descent



Problem 1: Preprocessing/Standardization

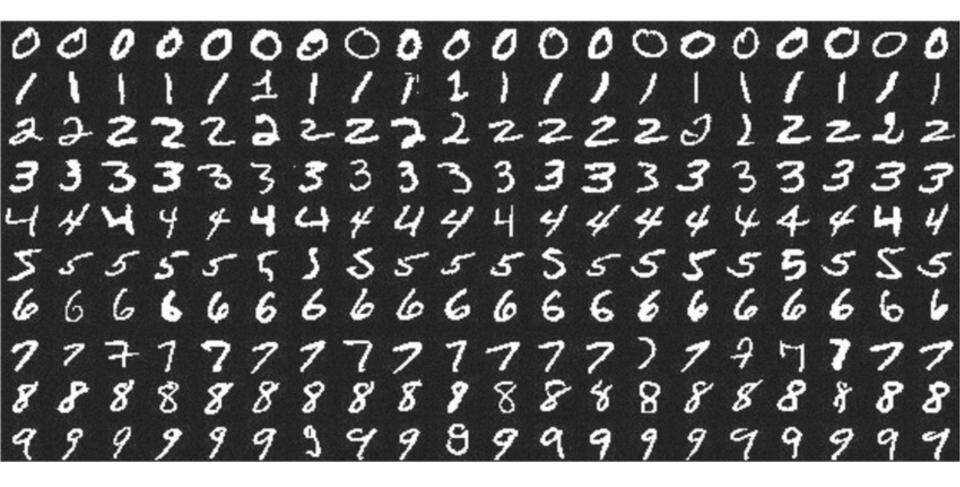
MNIST, raw data

	-					•			_			•				
	1															
1	7	1	7	1	7	7	1	7	7	1	7	1	1	1	2	
3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	12
r	a	ຊ	2	a	Ŷ	Ŷ	2	3	Ŷ	a	ิจ	R	a	3	a	1
9	9	9	9	9	q	9	9	9	9	9	9	9	9	9	9	9
6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6	6
	8															
ч	4	4	٤	イ	۷	ч	4	4	4	4	4	4	4	4	4	4



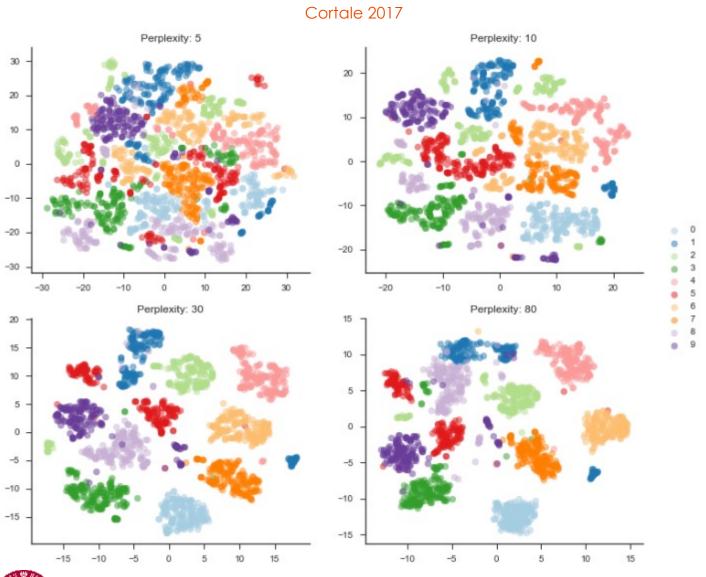
Problem 2 (or 1.5): Distance Metrics

MNIST





Problem 3: Hyperparameters



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DAWN



• t-SNE is slow and scales poorly



• t-SNE is slow and scales poorly

Difficult tradeoff between global and local structure



• t-SNE is slow and scales poorly

Difficult tradeoff between global and local structure

• Lack of mathematical formalism



• t-SNE is slow and scales poorly

Barnes-Hut approximation!

Difficult tradeoff between global and local structure

• Lack of mathematical formalism



• t-SNE is slow and scales poorly

Barnes-Hut approximation!

Barnes-Hut approximation ONLY IN 2D OR 3D!

Difficult tradeoff between global and local structure

• Lack of mathematical formalism



UMAP

UMAP builds on using **Riemannian manifolds!** Within differential geometry, this allows the definition of angles, hyper-area, and curvature in high dimensionality.

Abstract

UMAP (Uniform Manifold Approximation and Projection) is a novel manifold learning technique for dimension reduction. UMAP is constructed from a theoretical framework based in Riemannian geometry and algebraic topology. The result is a practical scalable algorithm that is applicable to real world data. The UMAP algorithm is competitive with t-SNE for visualization quality, and arguably preserves more of the global structure with superior run time performance. Furthermore, UMAP has no computational restrictions on embedding dimension, making it viable as a general purpose dimension reduction technique for machine learning.

UMAP paper, arXiv 1802.03426, Sep. 2020



UMAP

As in the t-SNE case, UMAP tries to find a metric in both the original (large) space X, and the lower dimension output space Y, which can be (topologically) matched:

At a high level, UMAP uses local manifold approximations and patches together their local fuzzy simplicial set representations to construct a topological representation of the high dimensional data. Given some low dimensional representation of the data, a similar process can be used to construct an equivalent topological representation. UMAP then optimizes the layout of the data representation in the low dimensional space, to minimize the cross-entropy between the two topological representations.

UMAP paper, arXiv 1802.03426, Sep. 2020

However, the metrics in X and Y used by UMAP and t-SNE differ:

For t-SNE these metrics are as follows:

$$v_{j|i} = \exp(-\|x_i - x_j\|_2^2 / 2\sigma_i^2)$$

For UMAP they are:

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$$v_{j|i} = \exp[(-d\left(x_i, x_j\right) -
ho_i)/\sigma_i]$$

$$w_{ij} = \left(1 + \|y_i - y_j\|_2^2\right)^{-1}$$

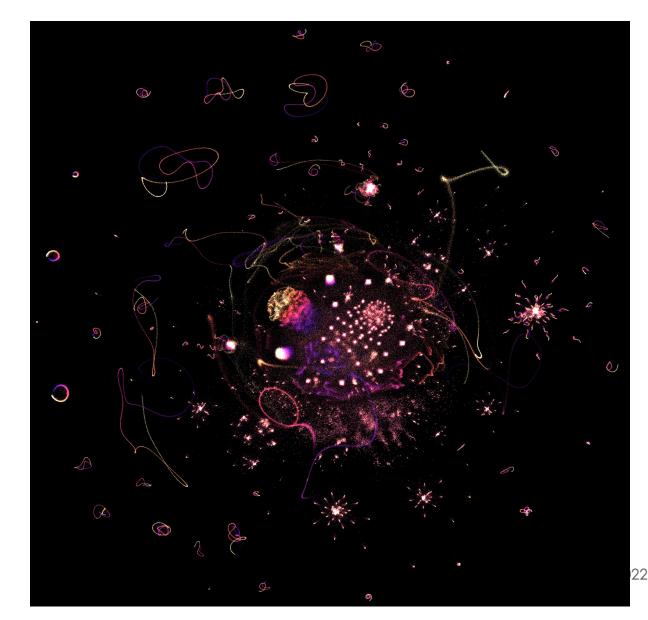
$$w_{ij} = \left(1 + a \|y_i - y_j\|_2^{2b}\right)^{-1}$$

First million integers in UMAP

Prime factorising the first million integers, and drawing them (artfully) gives the following image.

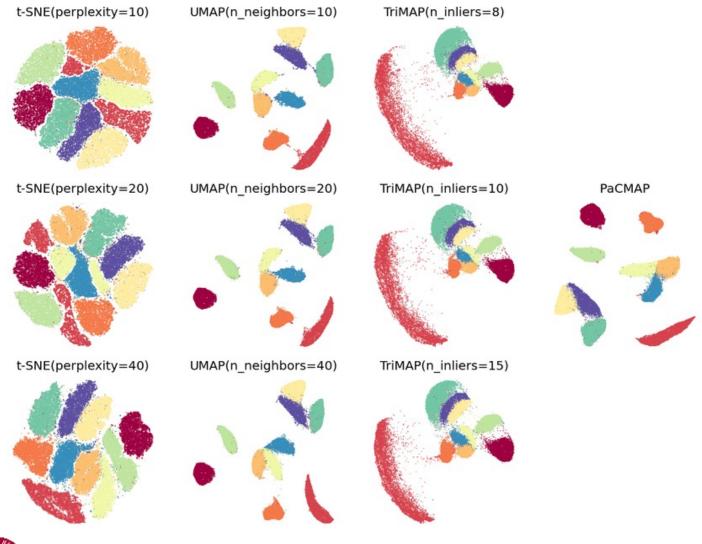
I find it quite visually pleasing, and a cool interplay between mathematics, ML, and art.





Group "similar" things together

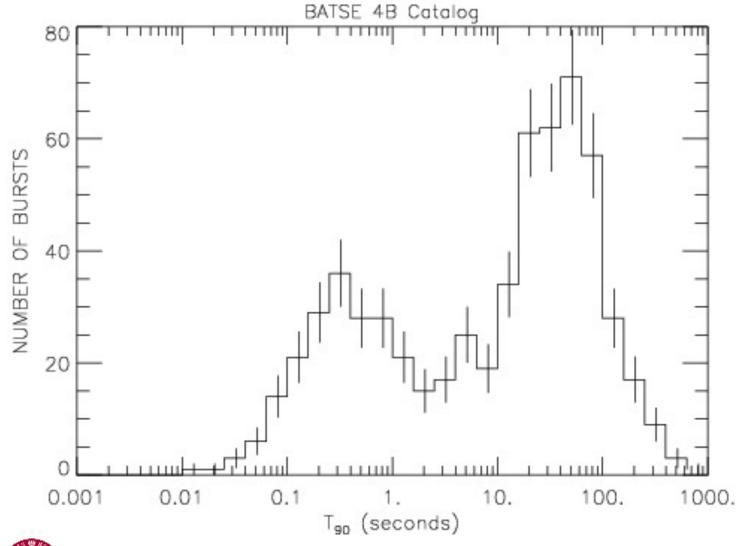
Wang et al. 2020



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Task: Separate Short and Long GRBs

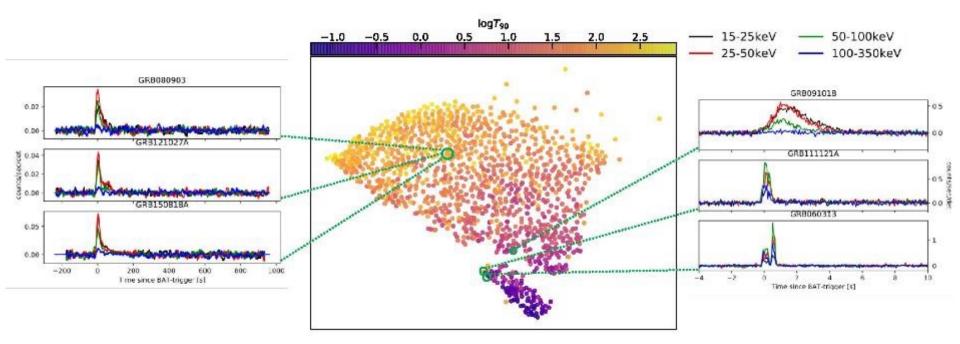
R. Mallozzi, updated Aug 2018 at https://gammaray.msfc.nasa.gov/batse/grb/duration/



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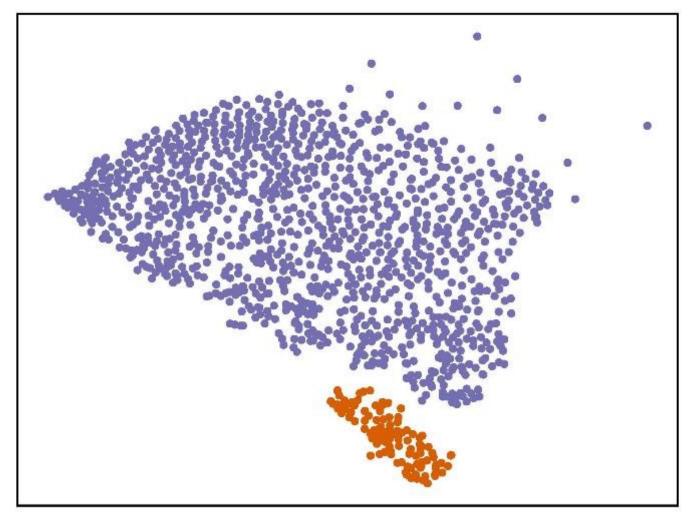
DAWN

Kragh Jespersen et al. 2020



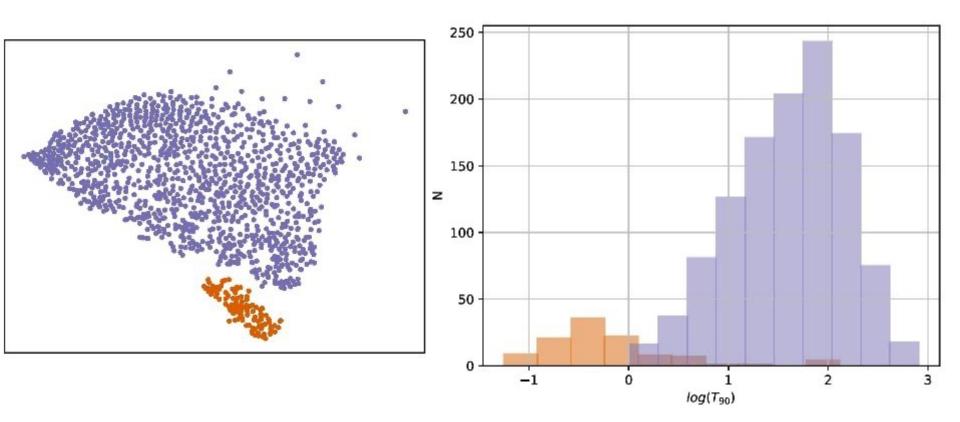


Kraah Jespersen et al. 2020



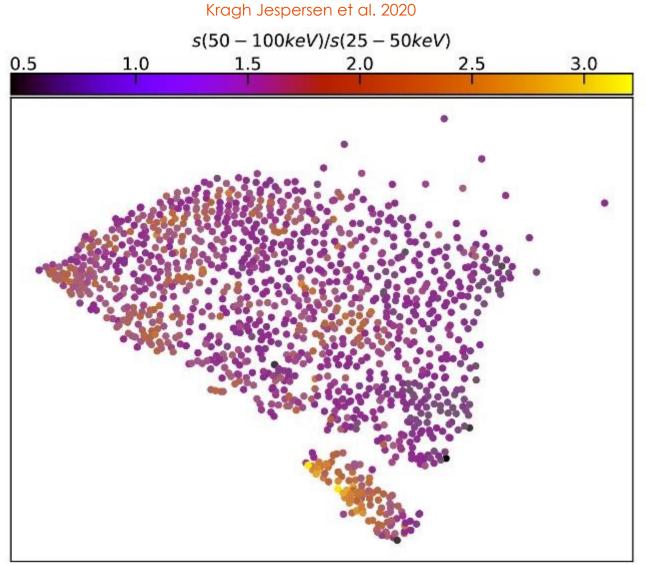


Kragh Jespersen et al. 2020





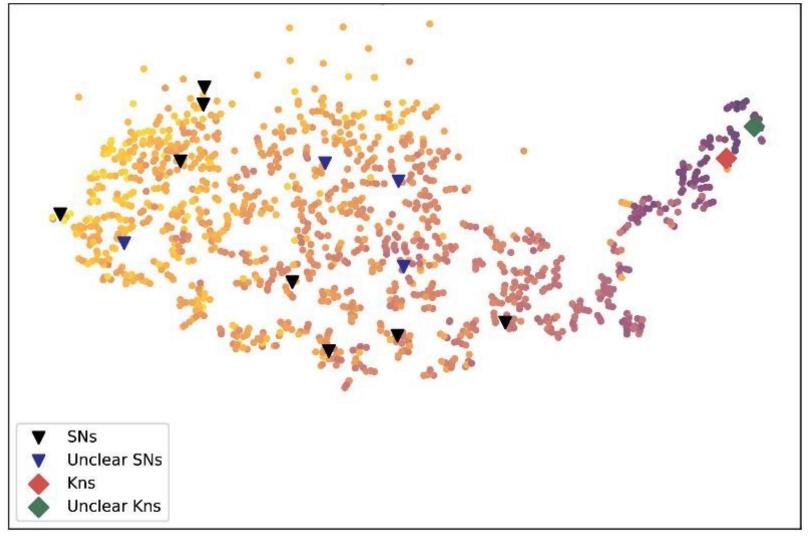
Hardness distribution





Possible subgroupings?

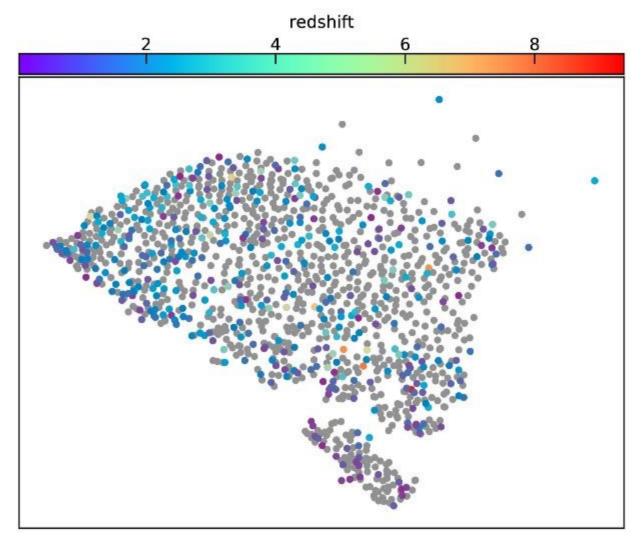
Kragh Jespersen et al. 2020





Redshift distribution

Kragh Jespersen et al. 2020





Kragh Jespersen et al. 2020

