Carnegie Mellon University
Heinz College

95-865 Unstructured Data Analytics

Lecture 5: PCA (cont'd), manifold learning

Slides by George H. Chen

Principal Component Analysis (PCA)

Demo

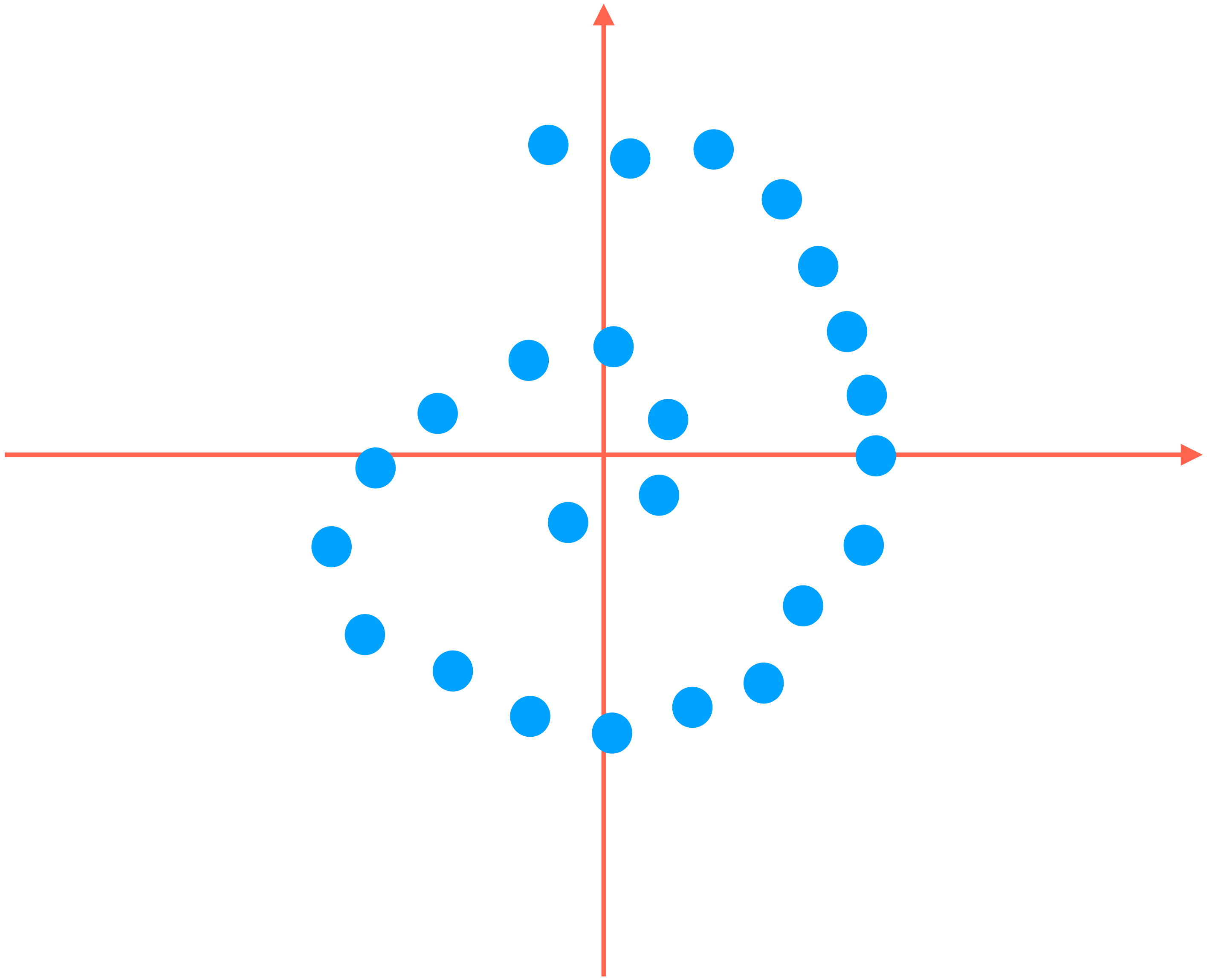
PCA Recap

- PCA reduces high-dimensional data to *k* dimensions
  - These *k* dimensions (the principal component directions) are the *k* orthogonal directions that explain the most variance in the data
- Fitting a PCA model means:
  - Figuring out the center of mass of the data we're fitting the model to
  - Figuring out "weights" for each principal component direction
    - We saw how to compute the PCA coordinates by taking an inner product (also called a dot product)
- After fitting a PCA model, we can also compute the fraction of variance explained by each principal component
- Reminder: a 3D PCA model contains the solution to a 2D PCA model as well as a 1D PCA model
  - More generally: if you have a *k*-dimensional PCA model, then we also have PCA models for number of dimensions from 1 up to *k*

When does PCA not work well?

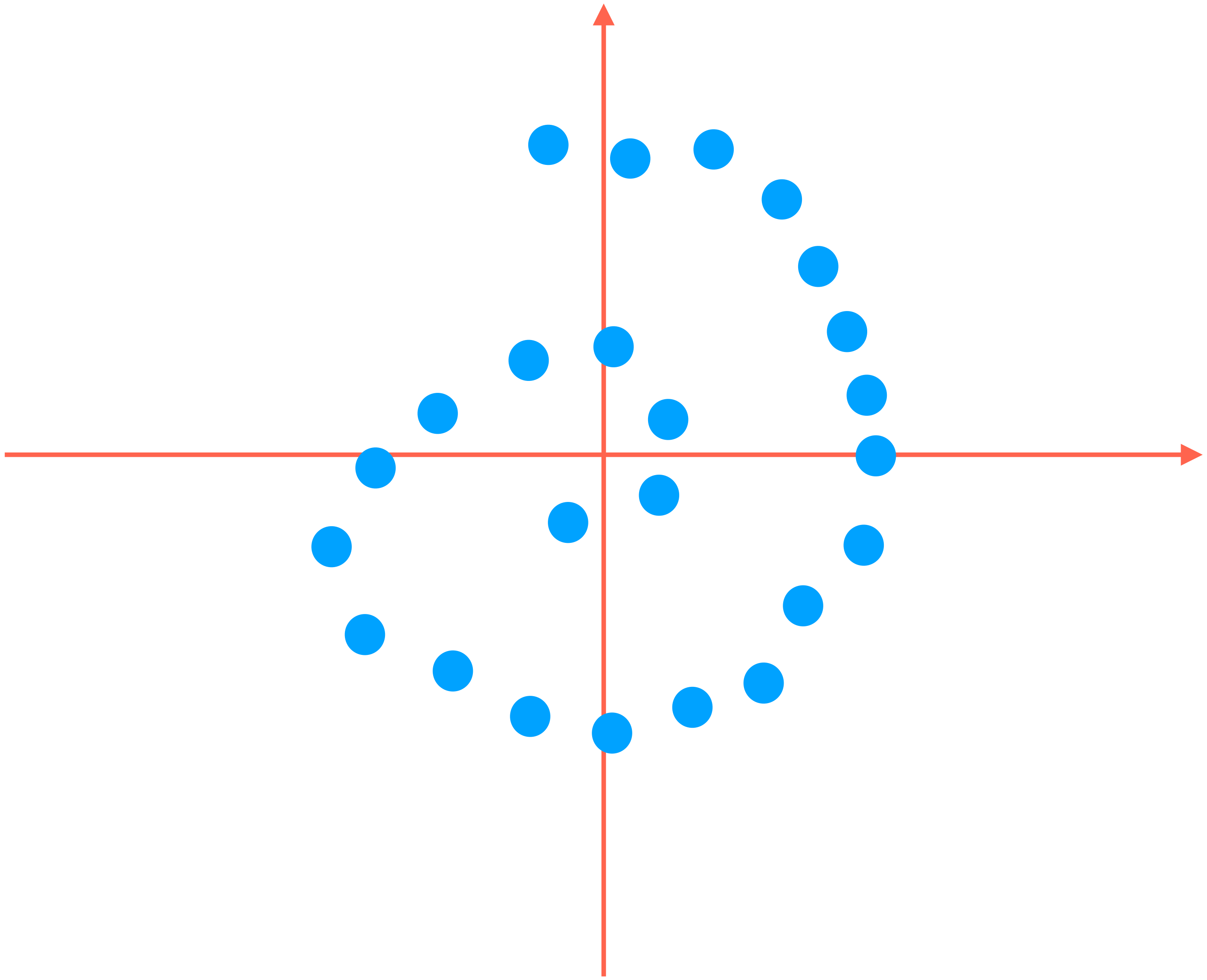
Image source: http://4.bp.blogspot.com/-USQEgoh1jCU/VfncdNOETcI/AAAAAAAAGp8/Hea8UtE_1c0/s1600/Blog%2B1%2BIMG_1821.jpg

2D Swiss Roll

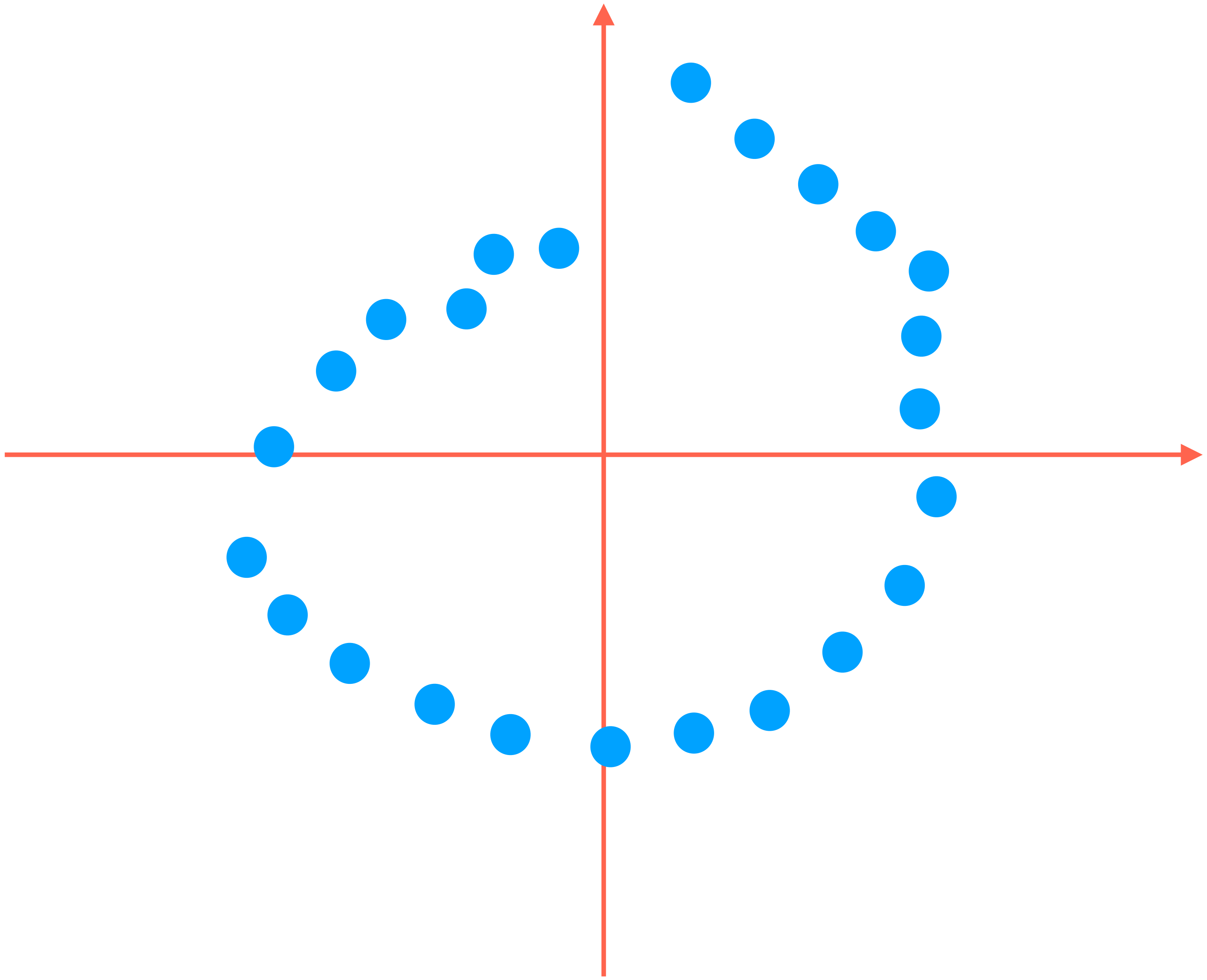


PCA would just flatten this thing and
lose the information that the data actually lives on a 1D line that has been curved!

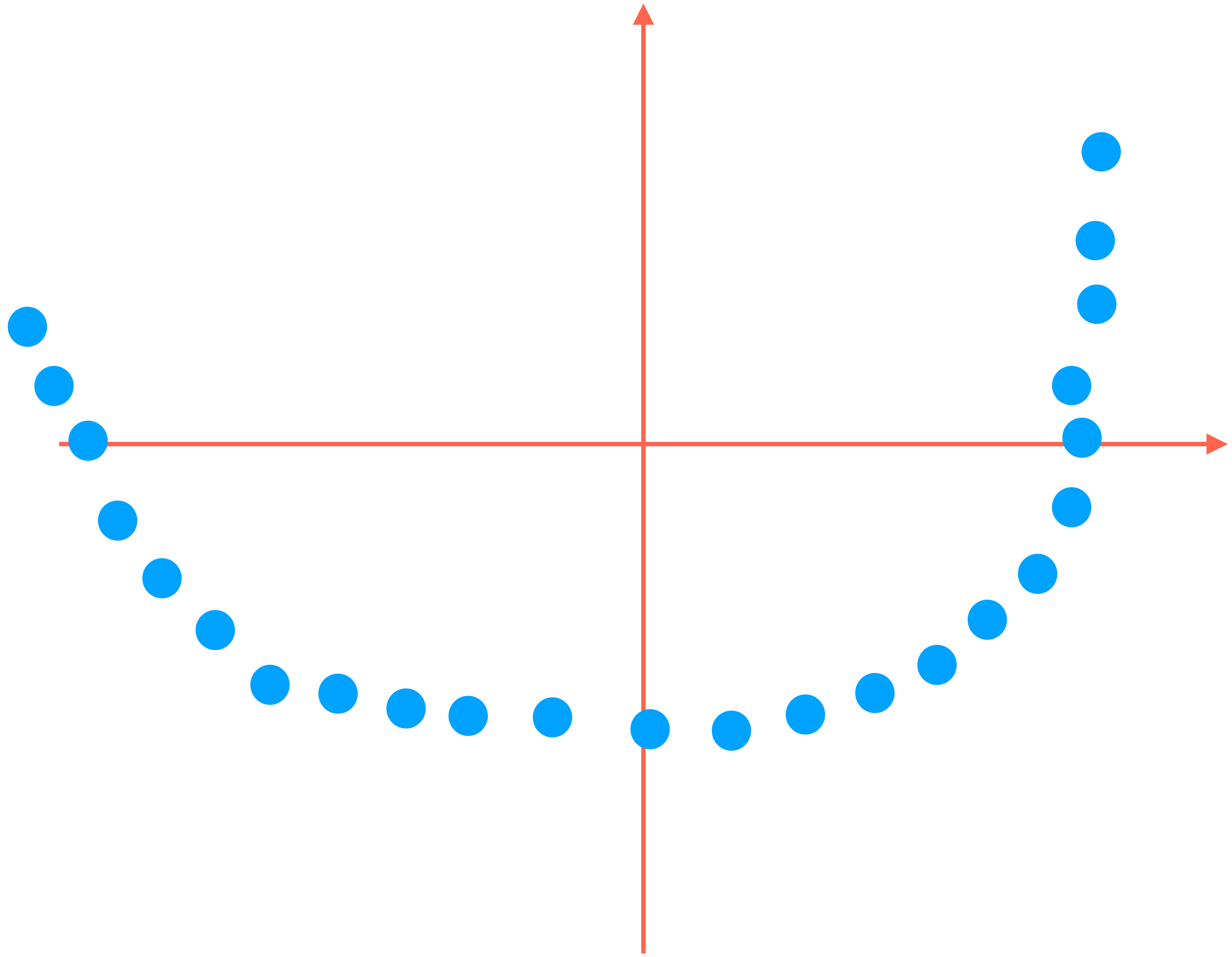
2D Swiss Roll



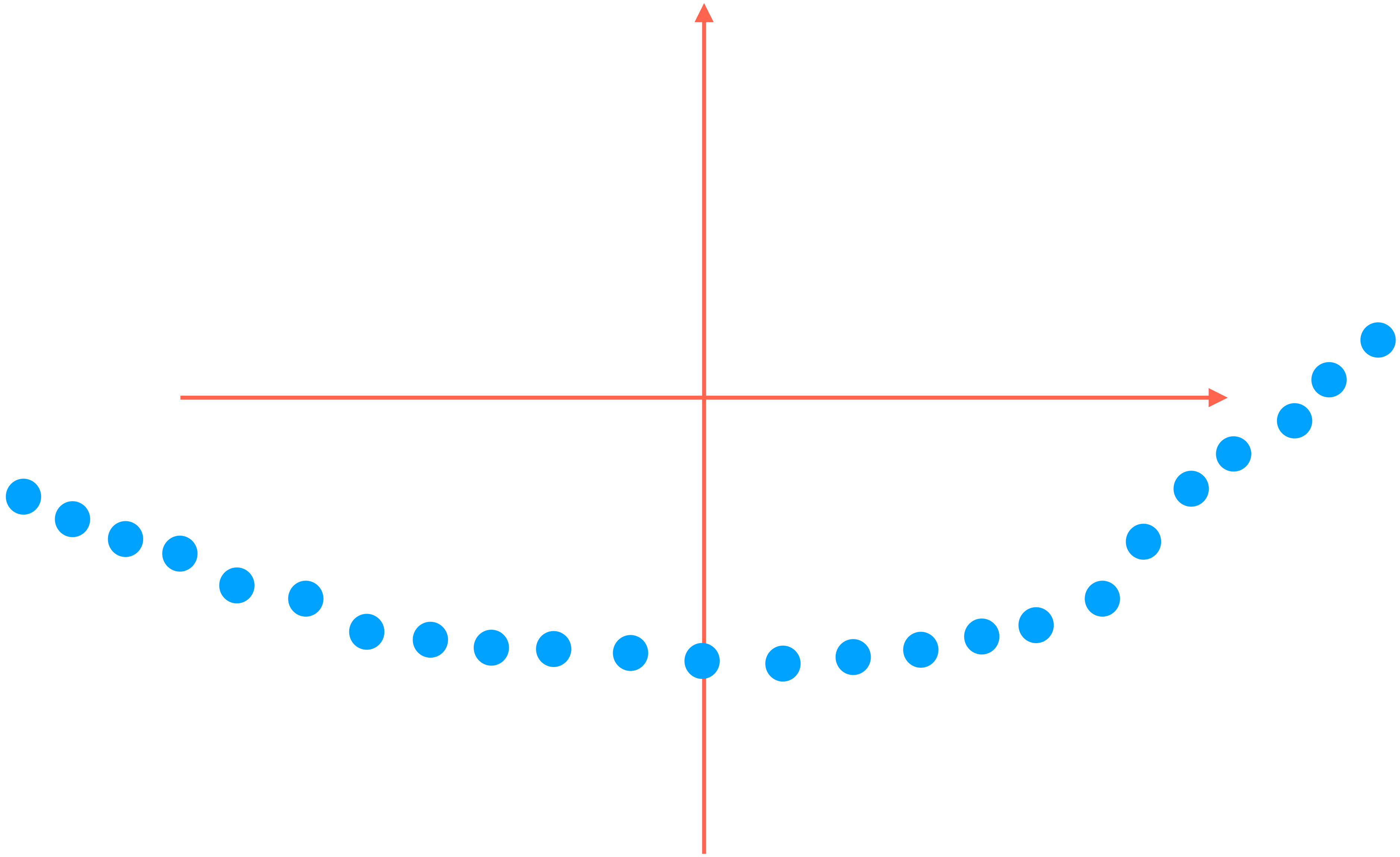
2D Swiss Roll



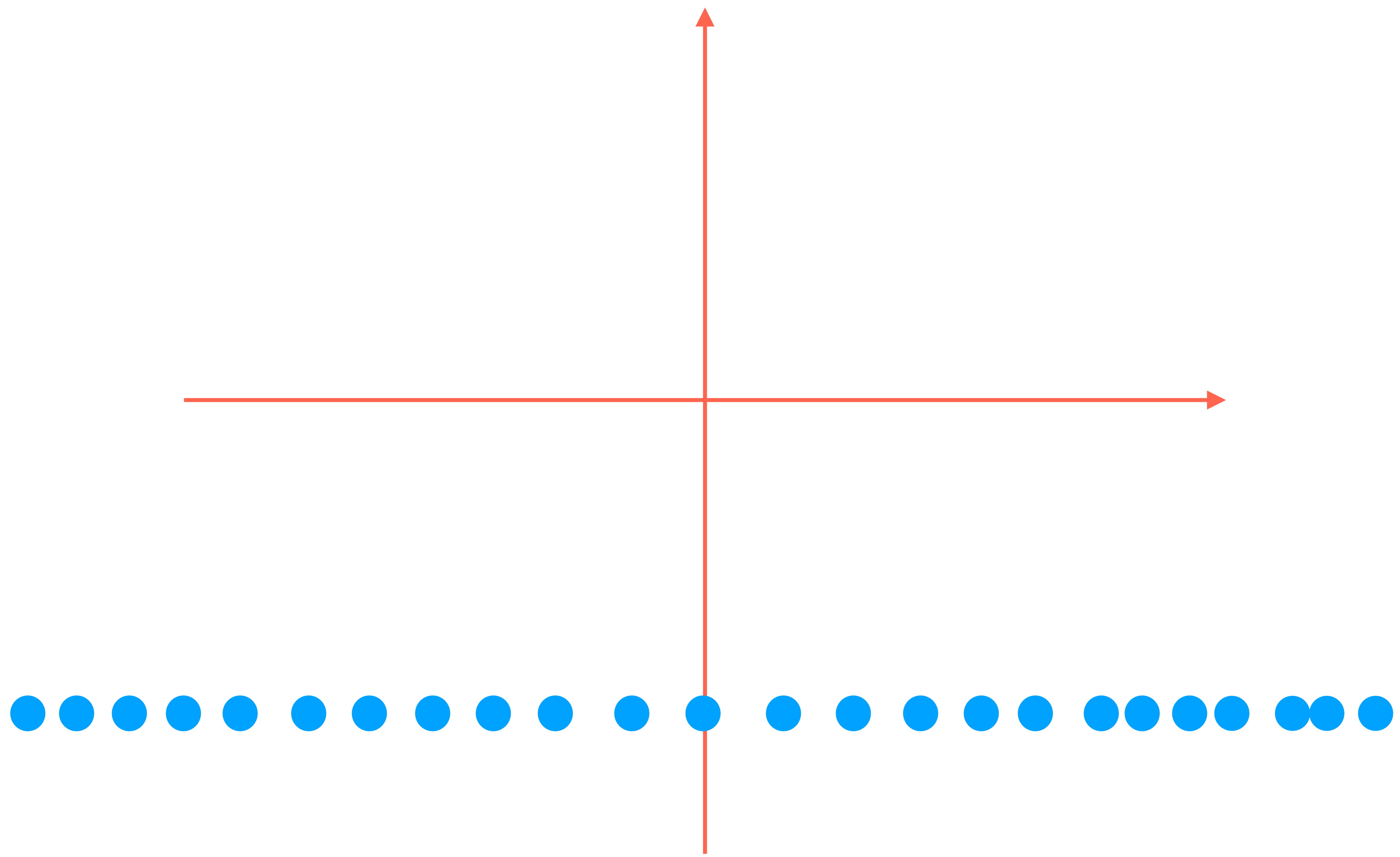
2D Swiss Roll



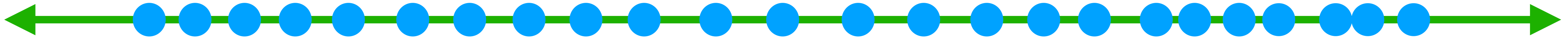
2D Swiss Roll



2D Swiss Roll

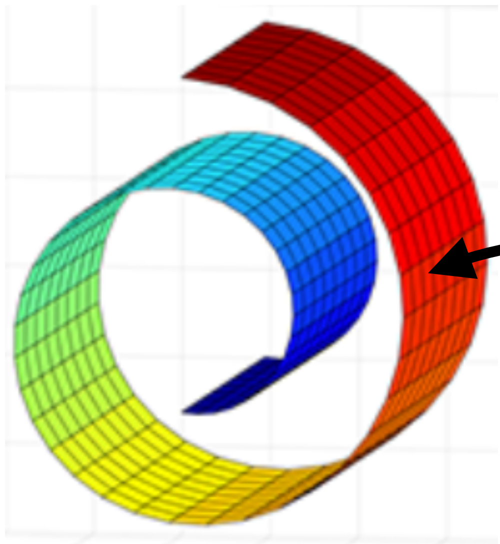


2D Swiss Roll



This is the desired result

Manifold Learning



The dataset here is clearly 3D

But when we zoom in a lot on any point, around the point it looks like a flat 2D sheet!

Another example: Earth is approximately a 3D sphere, but zooming a lot on any point, around the point it's approximately a 2D sheet

In general: if we have *d*-dimensional data where when you zoom in a lot, the data dimensionality is smaller than *d*, then the lower-dimensional object is called a **manifold**

- We have the data's high-dim. coordinates, but we want to find the low-dim. coordinates (on the manifold) ➜ this is manifold learning
- Manifold learning is *nonlinear* whereas PCA is linear (this will make more sense after we see code demos)

Image source: "Head Pose Estimation via Manifold Learning" (Wang et al 2017)

Do Data Actually Live on Manifolds?

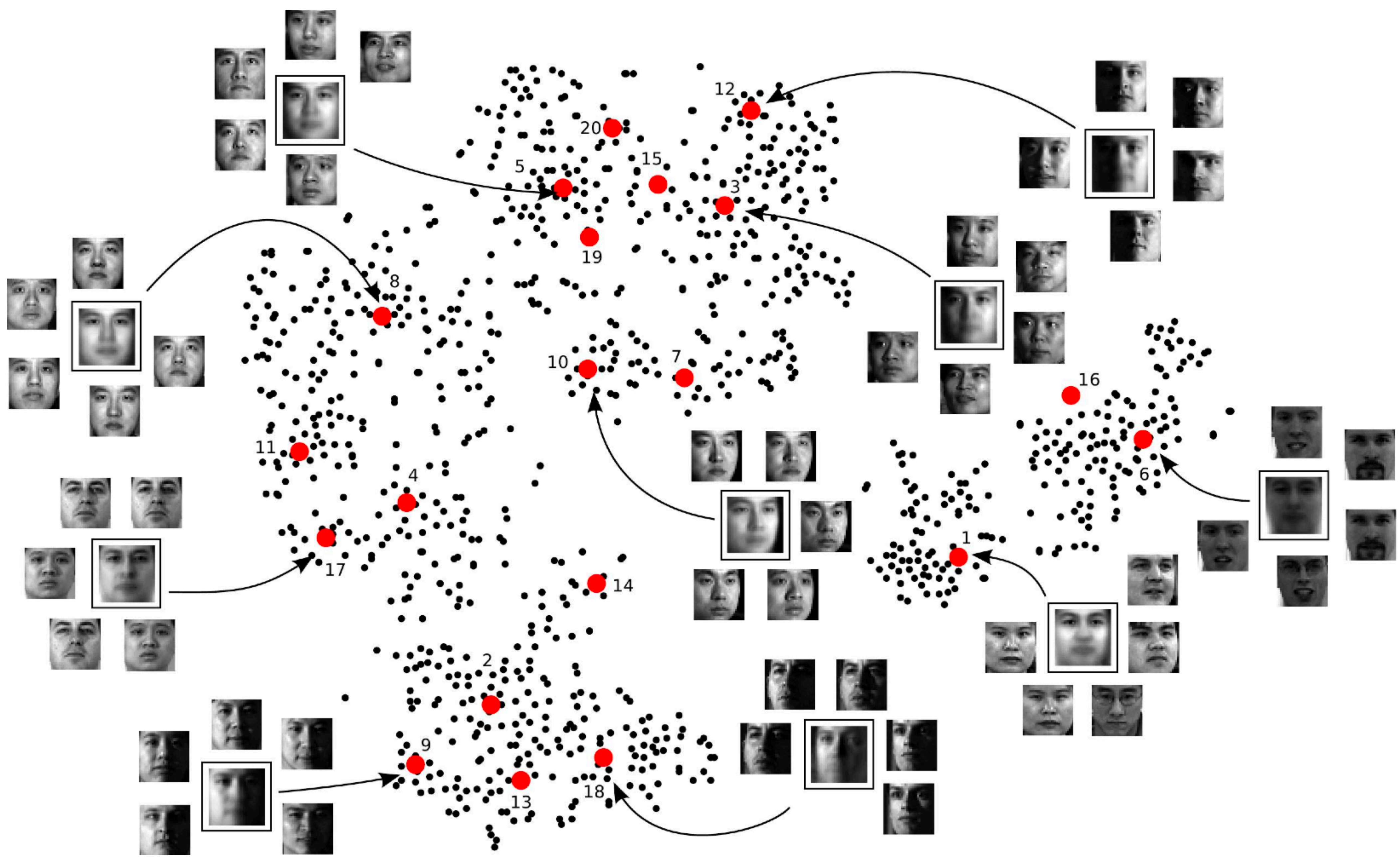


Image source: http://www.columbia.edu/~jwp2128/Images/faces.jpeg

Do Data Actually Live on Manifolds?

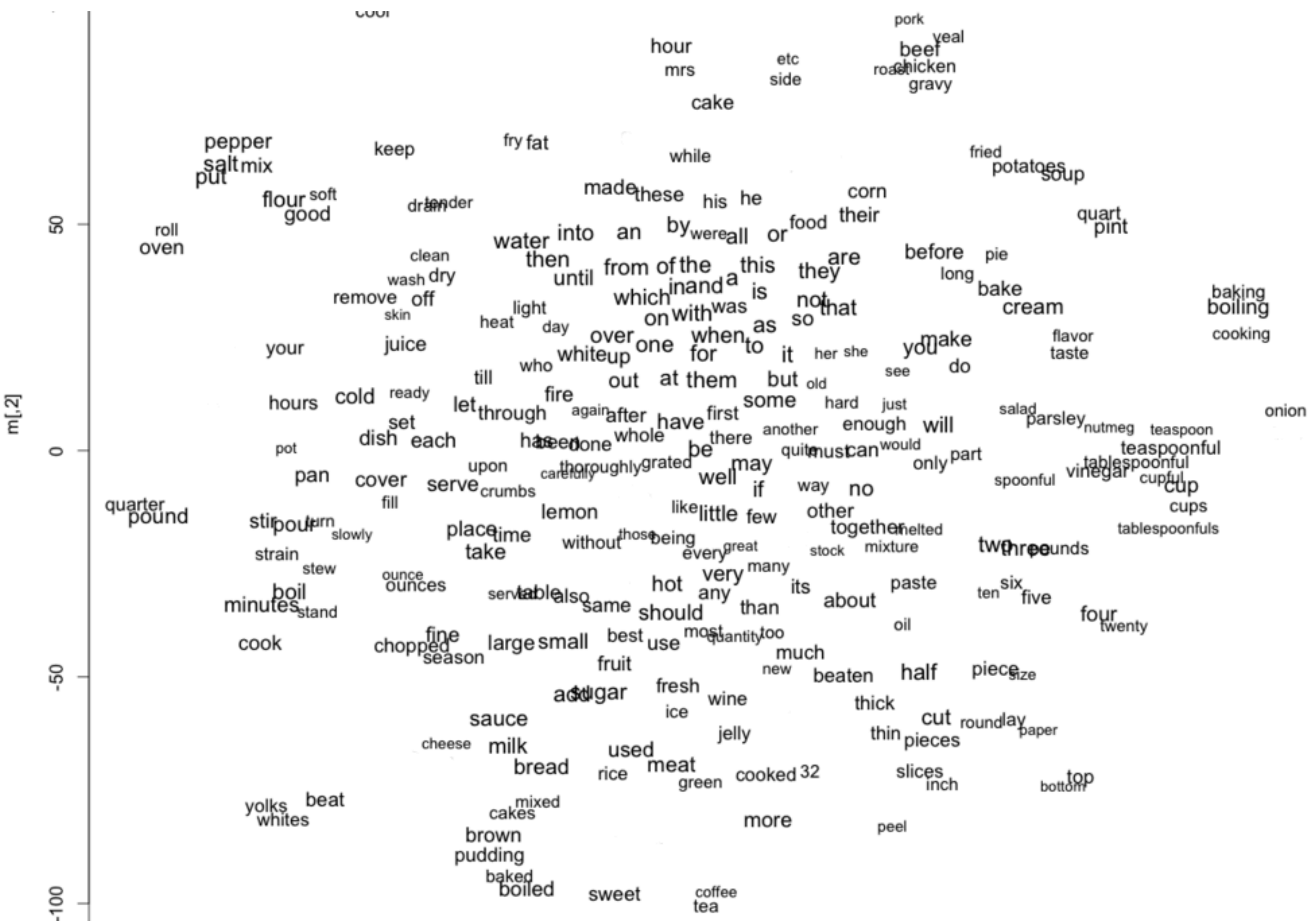
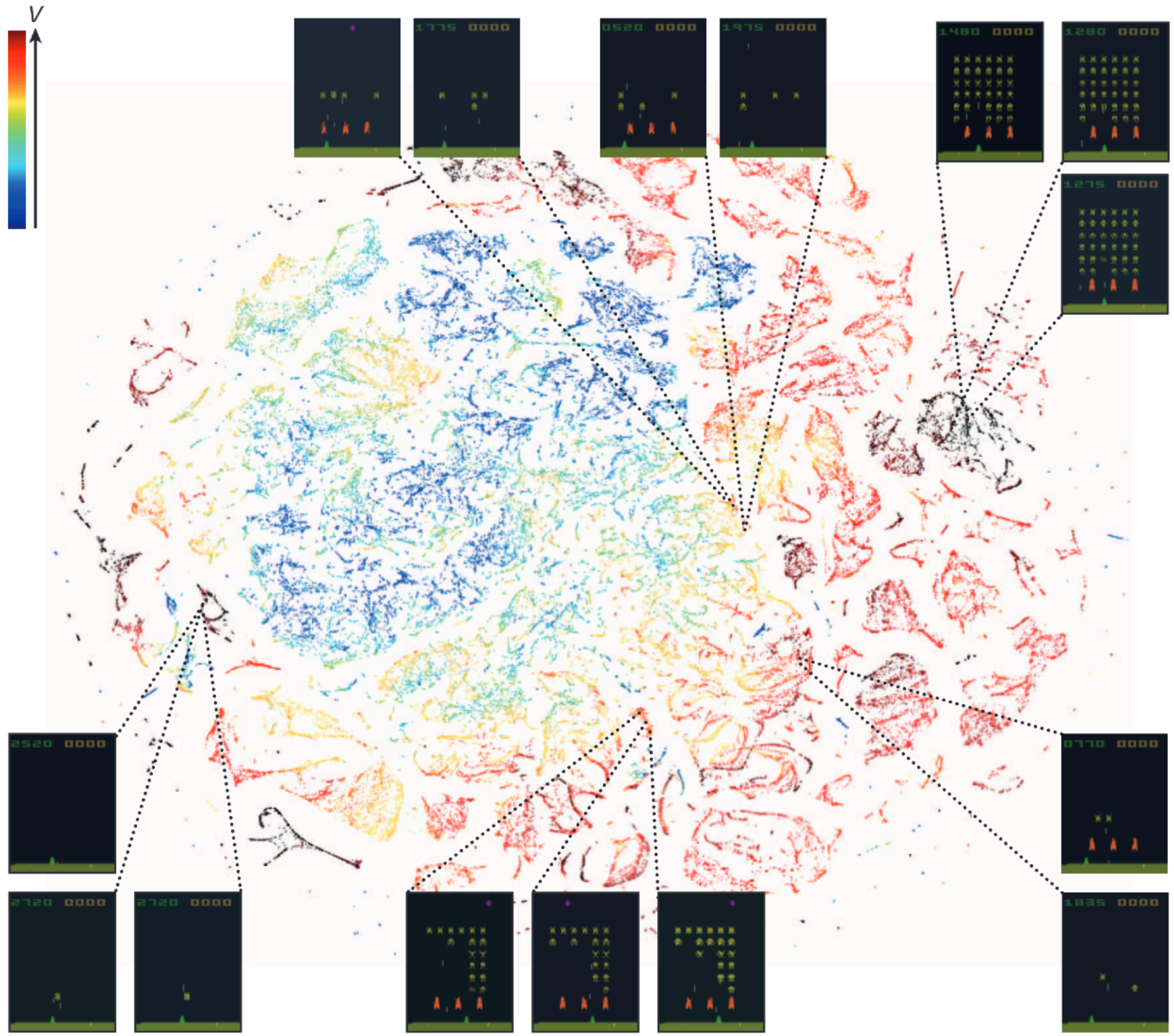


Image source: http://www.adityathakker.com/wp-content/uploads/2017/06/word-embeddings-994x675.png

Do Data Actually Live on Manifolds?



Mnih, Volodymyr, et al. Human-level control through deep reinforcement learning. Nature 2015.

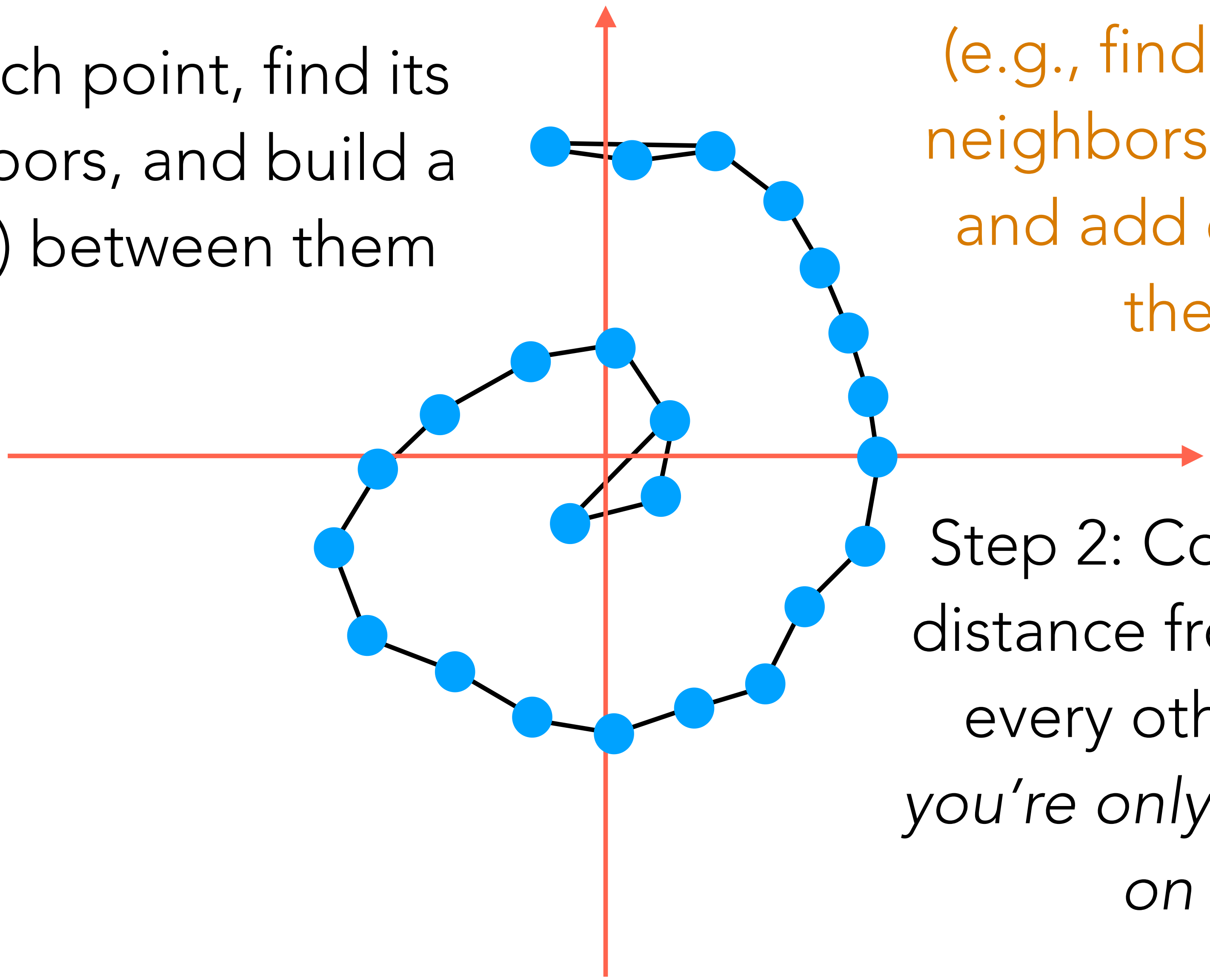
There are many manifold learning methods

We begin with one that’s easy to describe
(but it often doesn't work well in practice…)

Manifold Learning with Isomap

Step 1: For each point, find its nearest neighbors, and build a road (“edge”) between them

(e.g., find closest 2 neighbors per point and add edges to them)

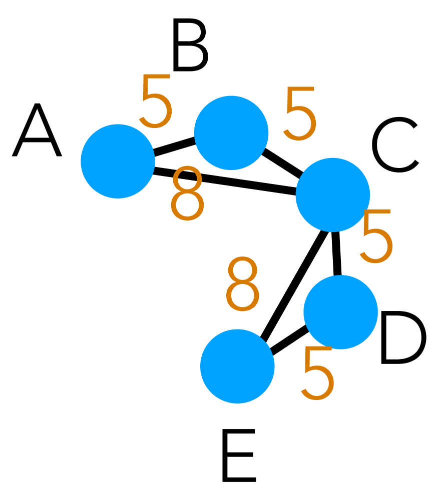


Step 2: Compute shortest distance from each point to every other point *where you’re only allowed to travel on the roads*

Step 3: It turns out that given all the distances between pairs of points, we can compute what the low-dimensional points should be (the algorithm for this is called *multidimensional scaling*)

Isomap Calculation Example

In orange: road lengths



2 nearest neighbors of A: B, C

2 nearest neighbors of B: A, C

2 nearest neighbors of C: B, D

2 nearest neighbors of D: C, E

2 nearest neighbors of E: C, D

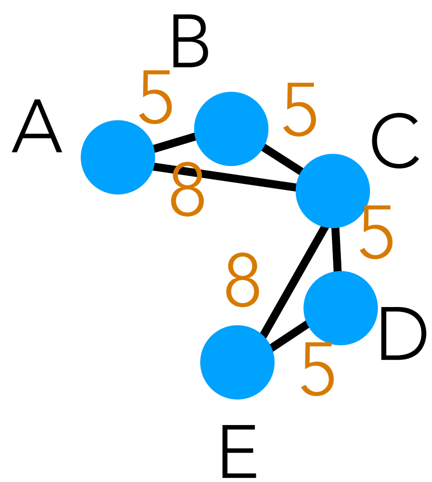
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

Shortest distances between every point to every other point *where we are only allowed to travel along the roads*

	A	B	C	D	E
A	0	5	8	13	16
B	5	0	5	10	13
C	8	5	0	5	8
D	13	10	5	0	5
E	16	13	8	5	0

Isomap Calculation Example

In orange: road lengths



2 nearest neighbors of A: B, C

2 nearest neighbors of B: A, C

2 nearest neighbors of C: B, D

2 nearest neighbors of D: C, E

2 nearest neighbors of E: C, D

Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

Shortest distances between every point to every other point *where we are only allowed to travel along the roads*

	A	B	C	D	E
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B	5	0	5	10	13
C	8	5	0	5	8
D	13	10	5	0	5
E	16	13	8	5	0

This matrix gets fed into *multidimensional scaling* to get 1D version of A, B, C, D, E

The solution is not unique!

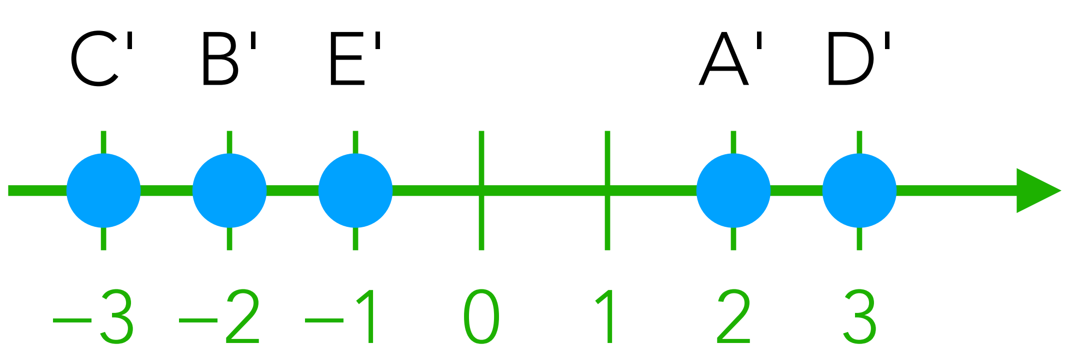
Multidimensional Scaling (MDS)

High-dimensional land

	A	B	C	D	E
A	0	5	8	13	16
B	5	0	5	10	13
C	8	5	0	5	8
D	13	10	5	0	5
E	16	13	8	5	0

Low-dimensional land

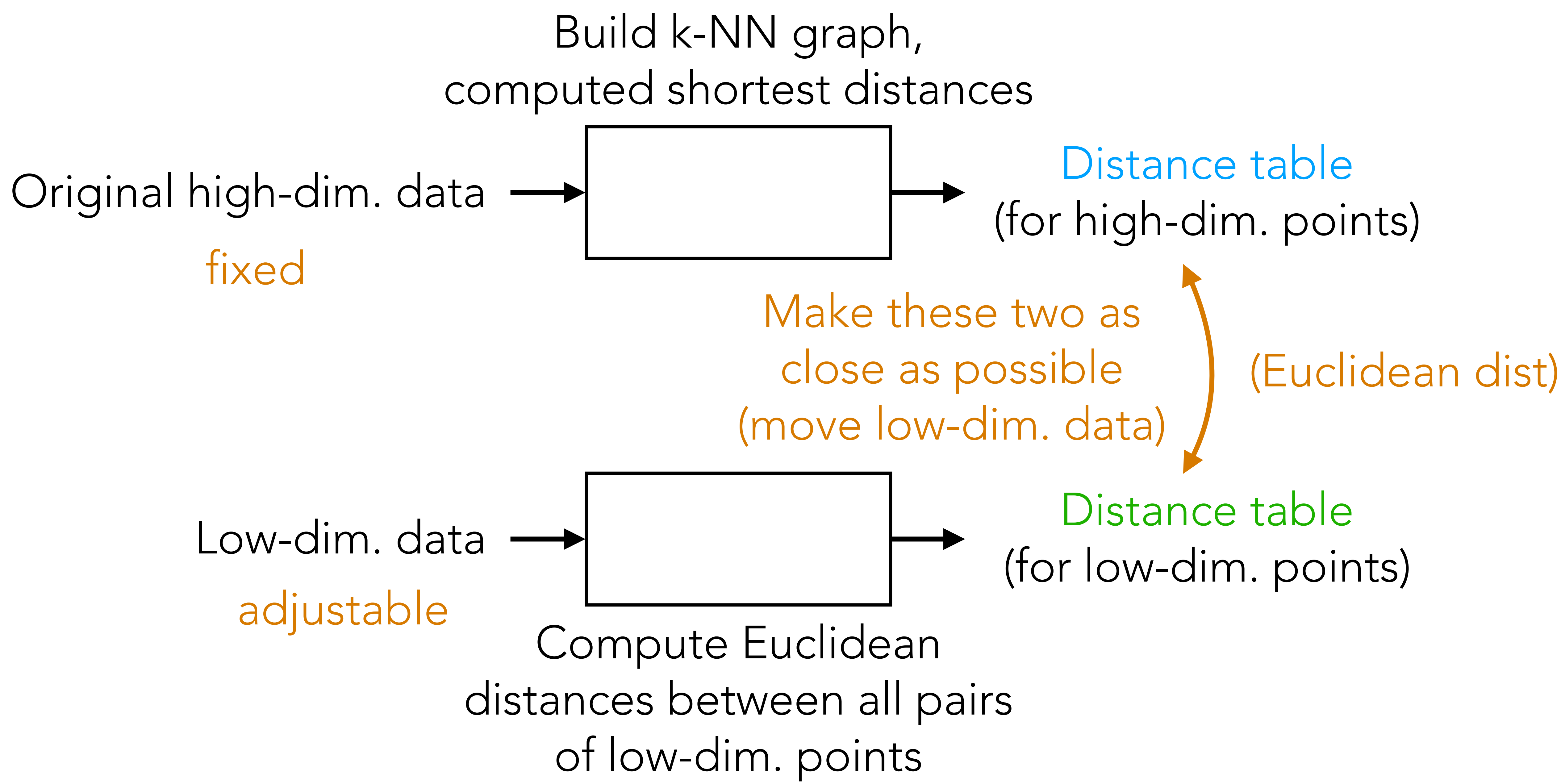
Suppose we have a guess for where the low-dimensional points are



	A'	B'	C'	D'	E'
A'	0	4	5	1	3
B'	4	0	1	5	1
C'	5	1	0	6	2
D'	1	5	6	0	4
E'	3	1	2	4	0

MDS moves the low-dim. points to make the 2 tables as close as possible

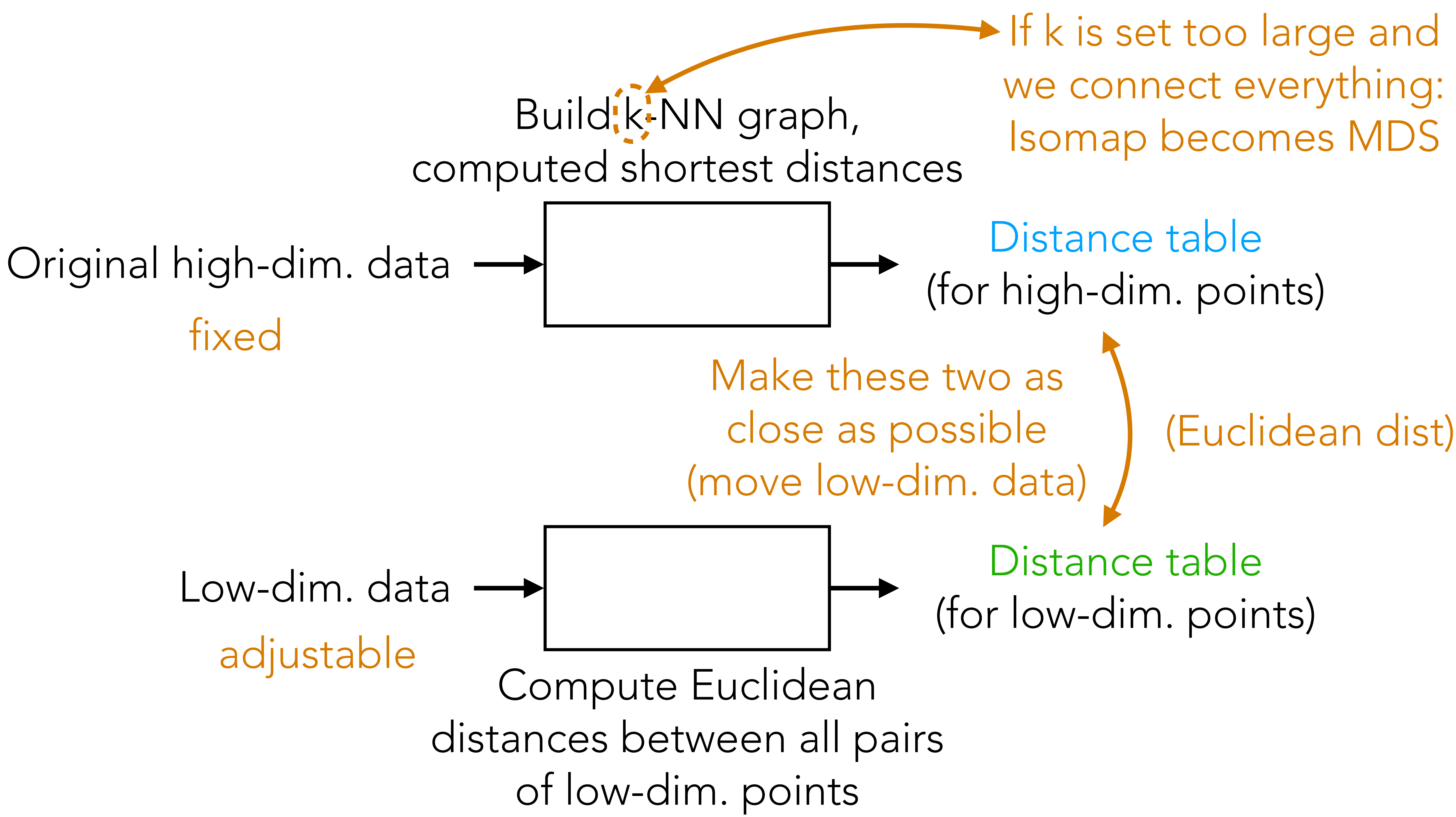
Isomap


Build k-NN graph,
computed shortest distances
Original high-dim. data
fixed
Distance table
(for high-dim. points)
Make these two as
close as possible
(move low-dim. data)
(Euclidean dist)
Distance table
(for low-dim. points)
Low-dim. data
adjustable
Compute Euclidean
distances between all pairs
of low-dim. points

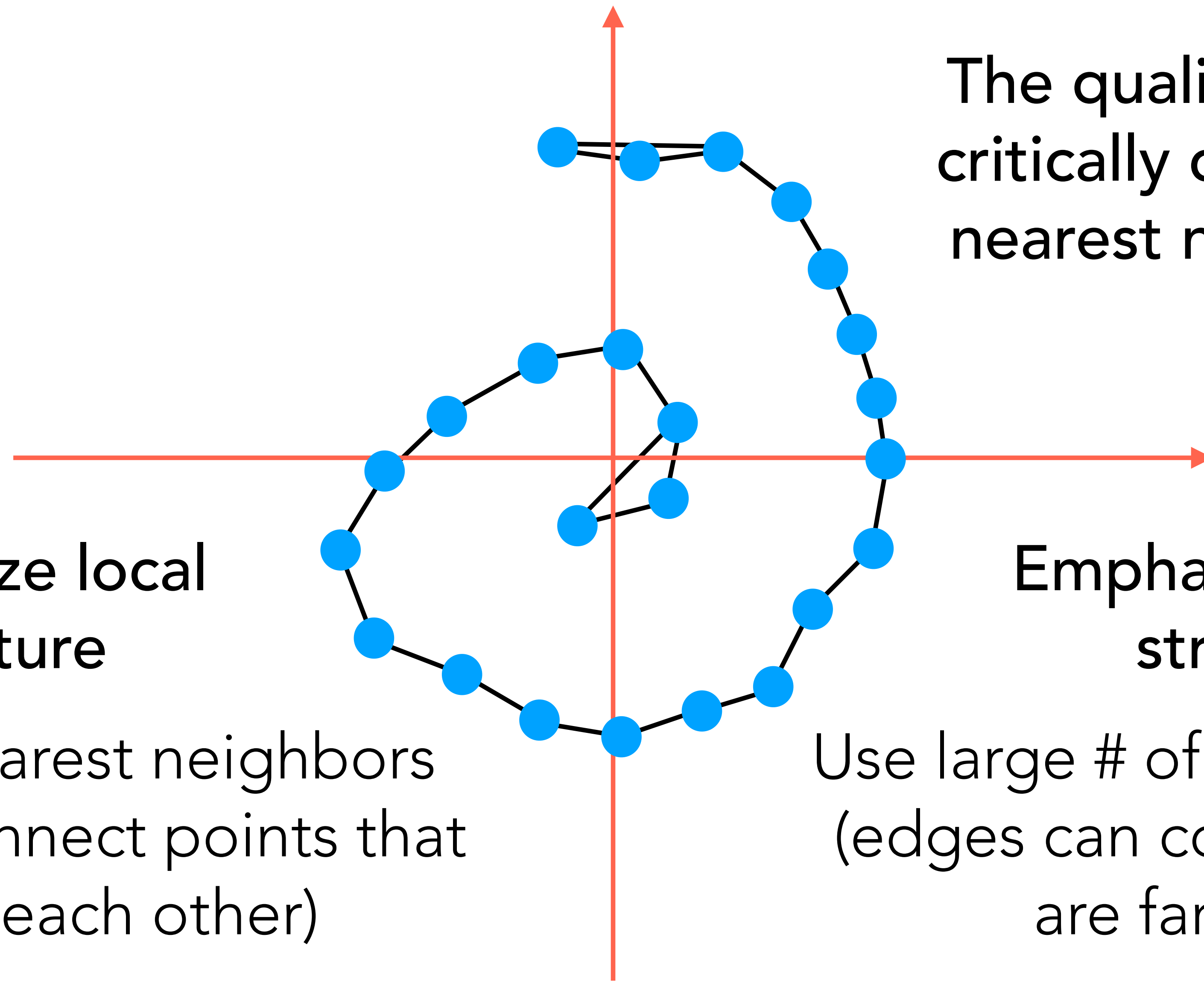
Isomap Calculation Example

Demo

Isomap


If k is set too large and we connect everything: Isomap becomes MDS
Build k-NN graph, computed shortest distances
Original high-dim. data
fixed
Distance table
(for high-dim. points)
Make these two as close as possible (move low-dim. data)
(Euclidean dist)
Low-dim. data
adjustable
Distance table
(for low-dim. points)
Compute Euclidean distances between all pairs of low-dim. points

Some Observations on Isomap



The quality of the result critically depends on the nearest neighbor graph

Emphasize local structure

Use small # of nearest neighbors (edges tend to connect points that are closer to each other)

There might not be enough edges

Emphasize global structure

Use large # of nearest neighbors (edges can connect points that are farther apart)

Might connect points that shouldn't be connected

In general: try different parameters for nearest neighbor graph construction when using Isomap + visualize

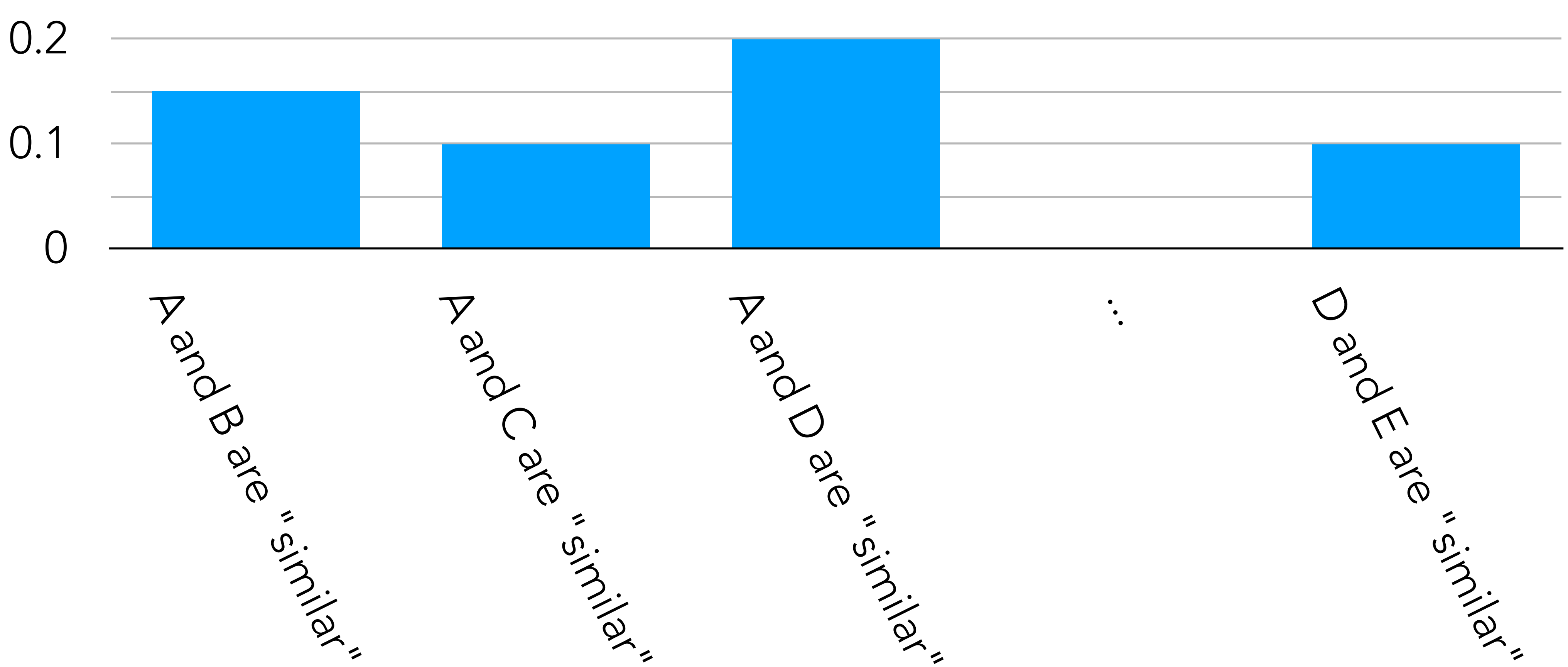
t-SNE
(t-distributed stochastic neighbor embedding)

High-level t-SNE Idea

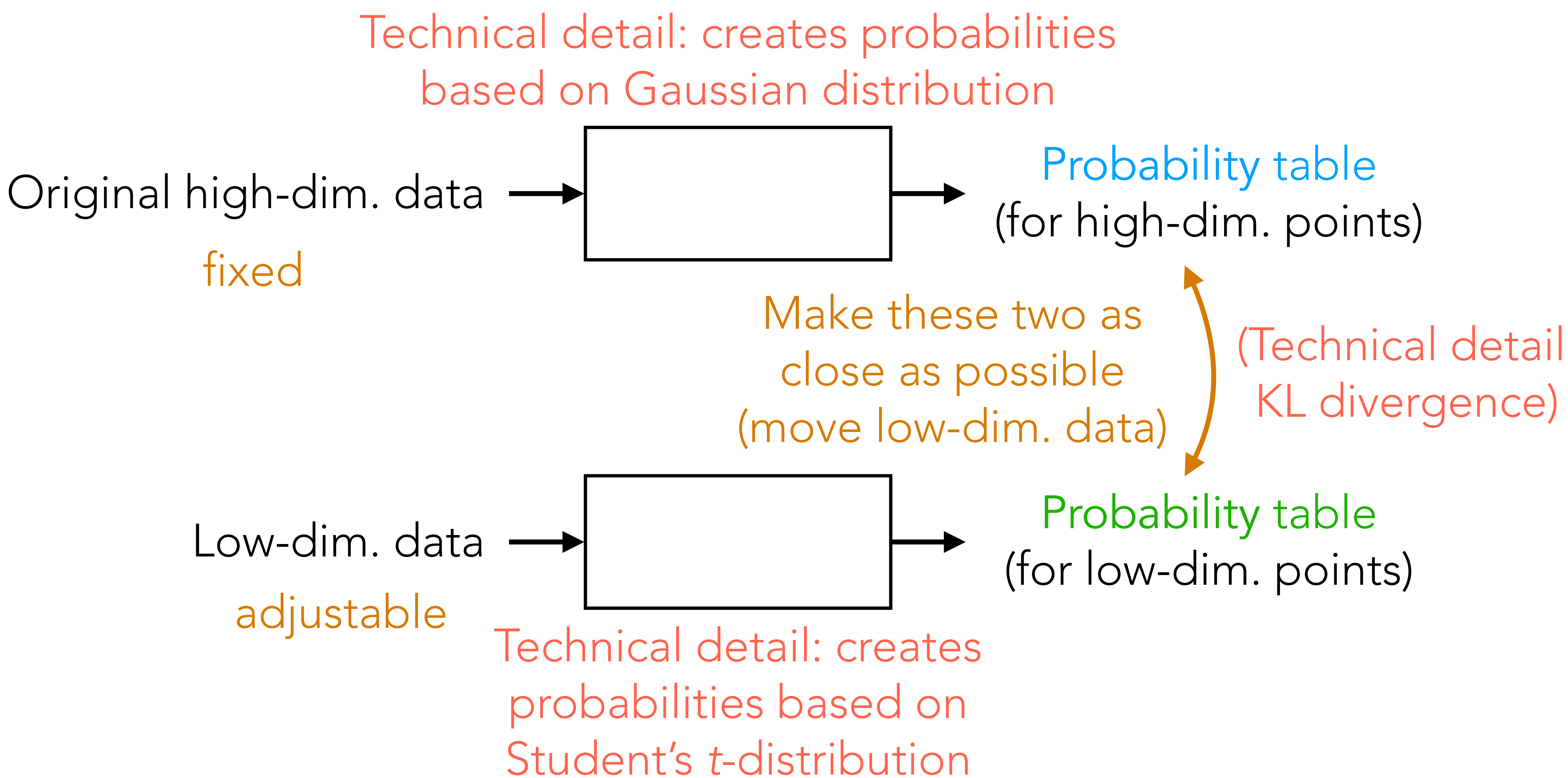
- Don't use deterministic definition of which points are neighbors

	A	B	C	D	E
A	0	5	8	13	16
B	5	0	5	10	13
C	8	5	0	5	8
D	13	10	5	0	5
E	16	13	8	5	0

- Use probabilistic notation instead



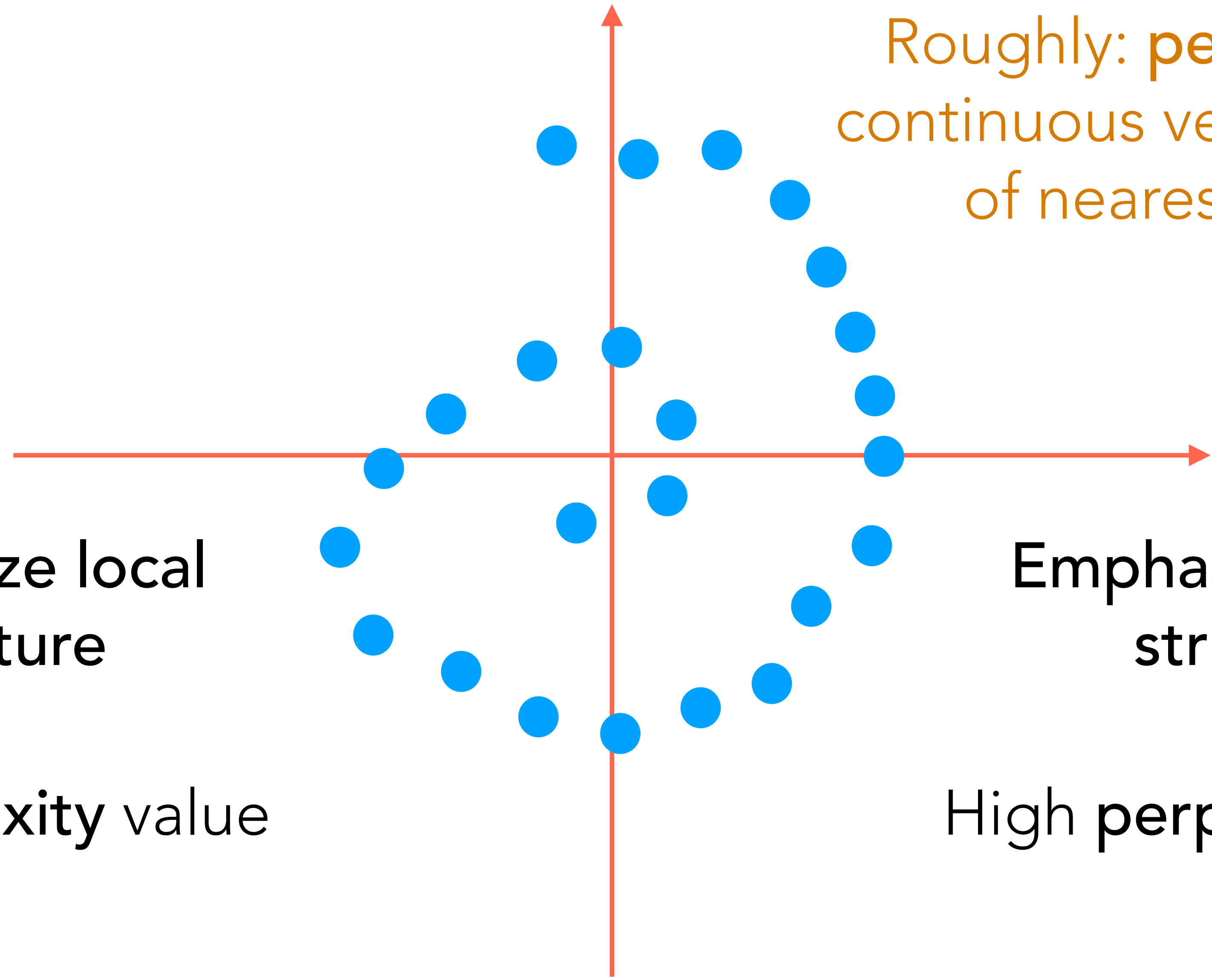
t-SNE



Technical details are in separate slides (posted on webpage)

t-SNE Parameters…

Roughly: **perplexity** is like a continuous version of “number of nearest neighbors”



Emphasize local structure

Low **perplexity** value

Emphasize global structure

High **perplexity** value

Also: play with # iterations, learning rate

how many times to try to improve guess of low-dim. representation

each time we try to improve low-dim. representation, how much we can change it

In practice, often people initialize with PCA

Manifold Learning with t-SNE

Demo