Carnegie Mellon University
Heinz College

Unstructured Data Analysis

Lecture 5: Manifold learning

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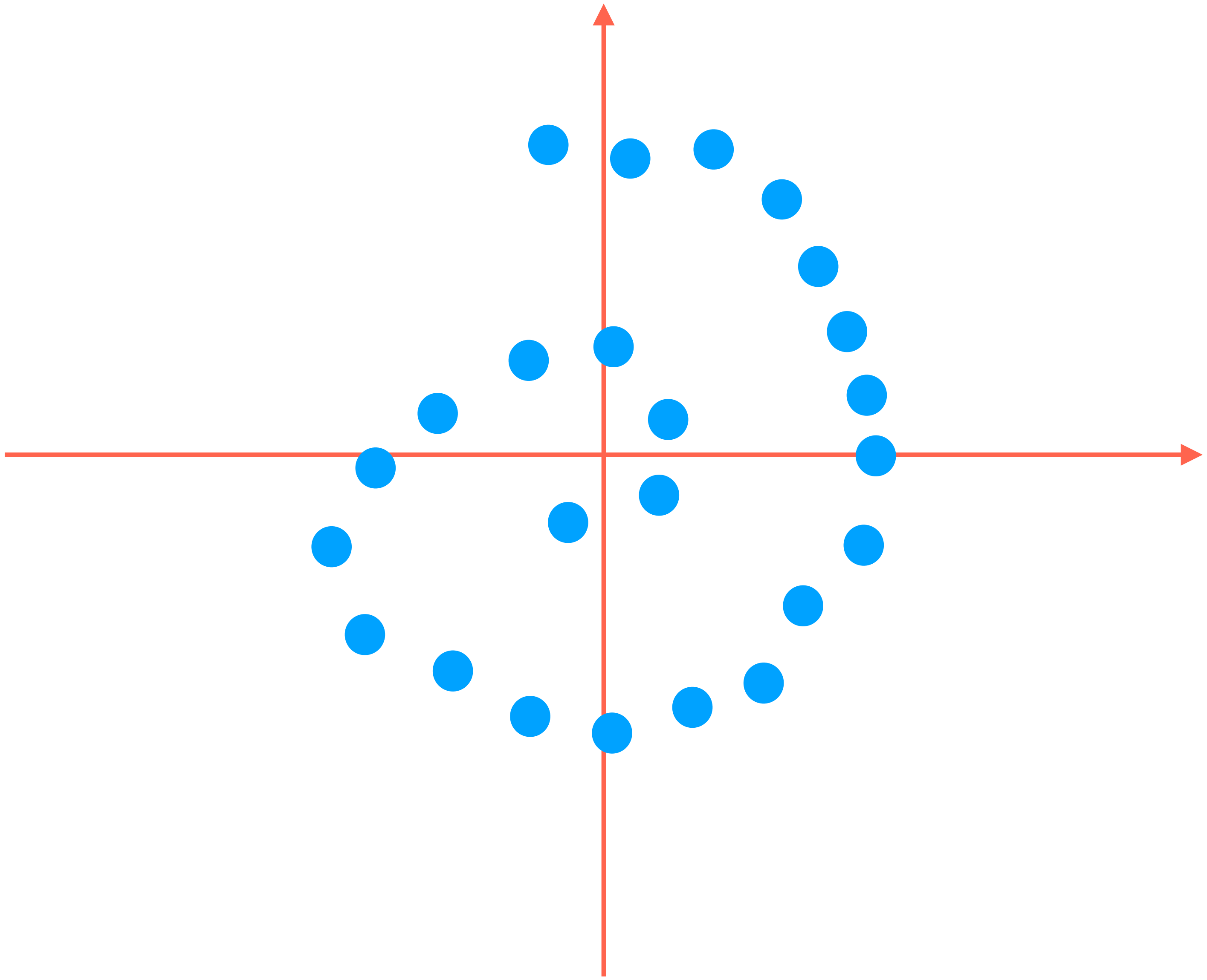
A Note on Design Choices

- Should I lowercase? Should I lemmatize? How do I count co-occurrences (at the sentence level? paragraph level? document level?), … *lots of design choices!*
    - When you do data analysis for a company/organization, often there is an **infinite number of design choices**
    - There usually will not be someone that tells you what is the “correct” way to choose all of these design choices
    - *You* have to make these decisions!
- **If you’re not sure about what to use, try multiple options and see for yourself how the output changes and whether this affects conclusions that are drawn from the analysis!**
    - It’s good for you to figure out what design choices lead to significant changes and what do not

PCA reorients data so axes explain variance in “decreasing order”
➔ can “flatten” (*project*) data onto a few axes that captures most variance

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!

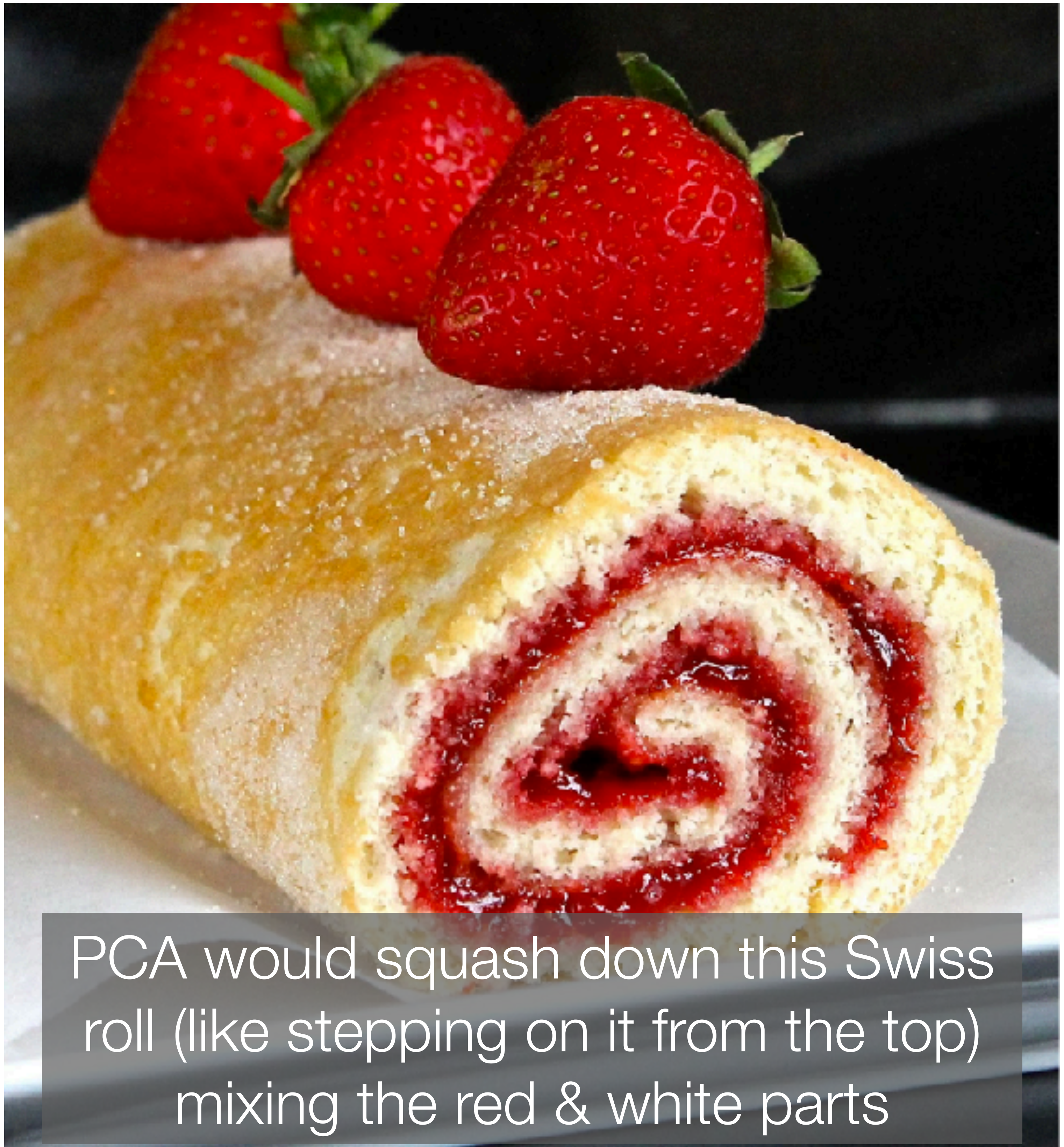
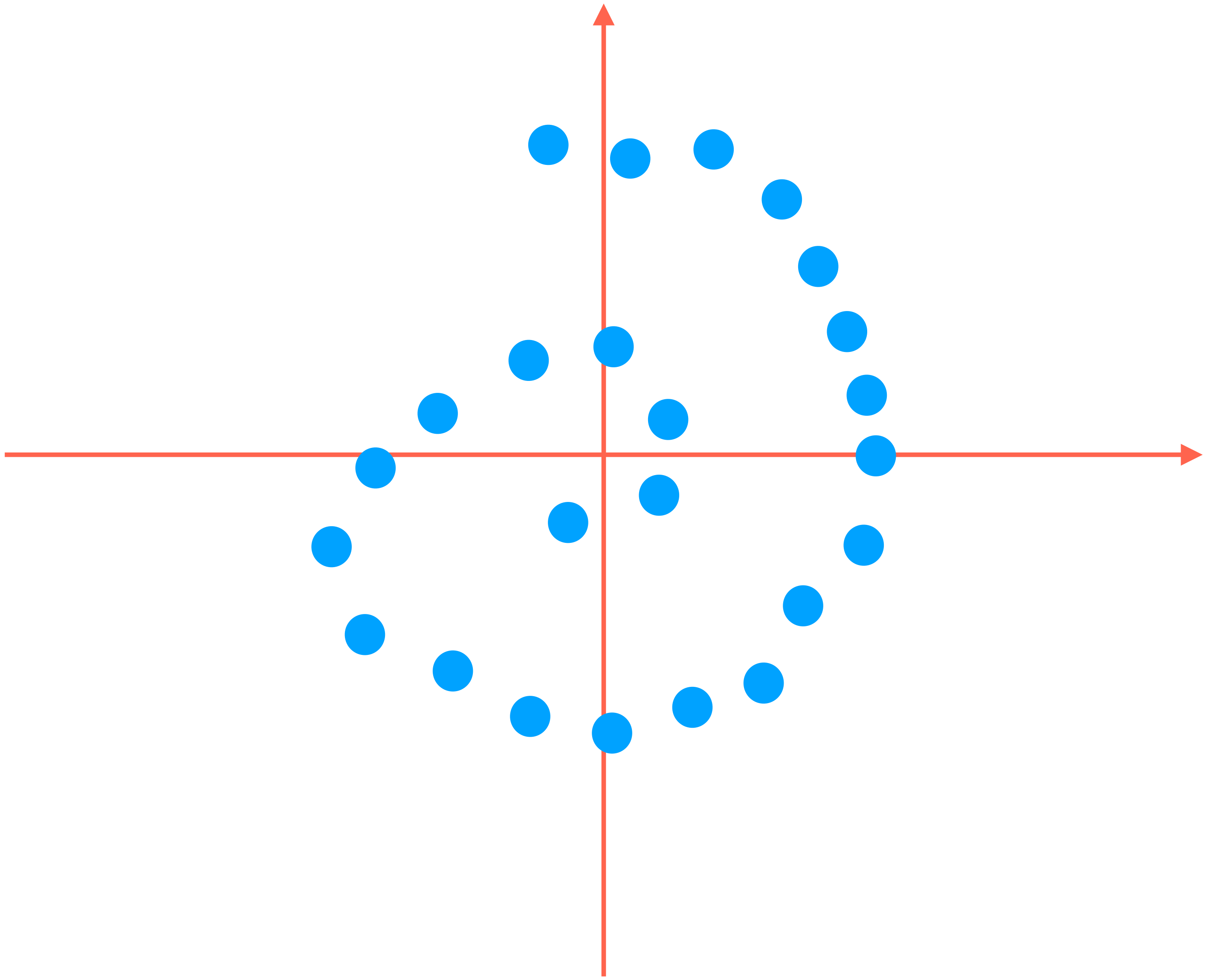
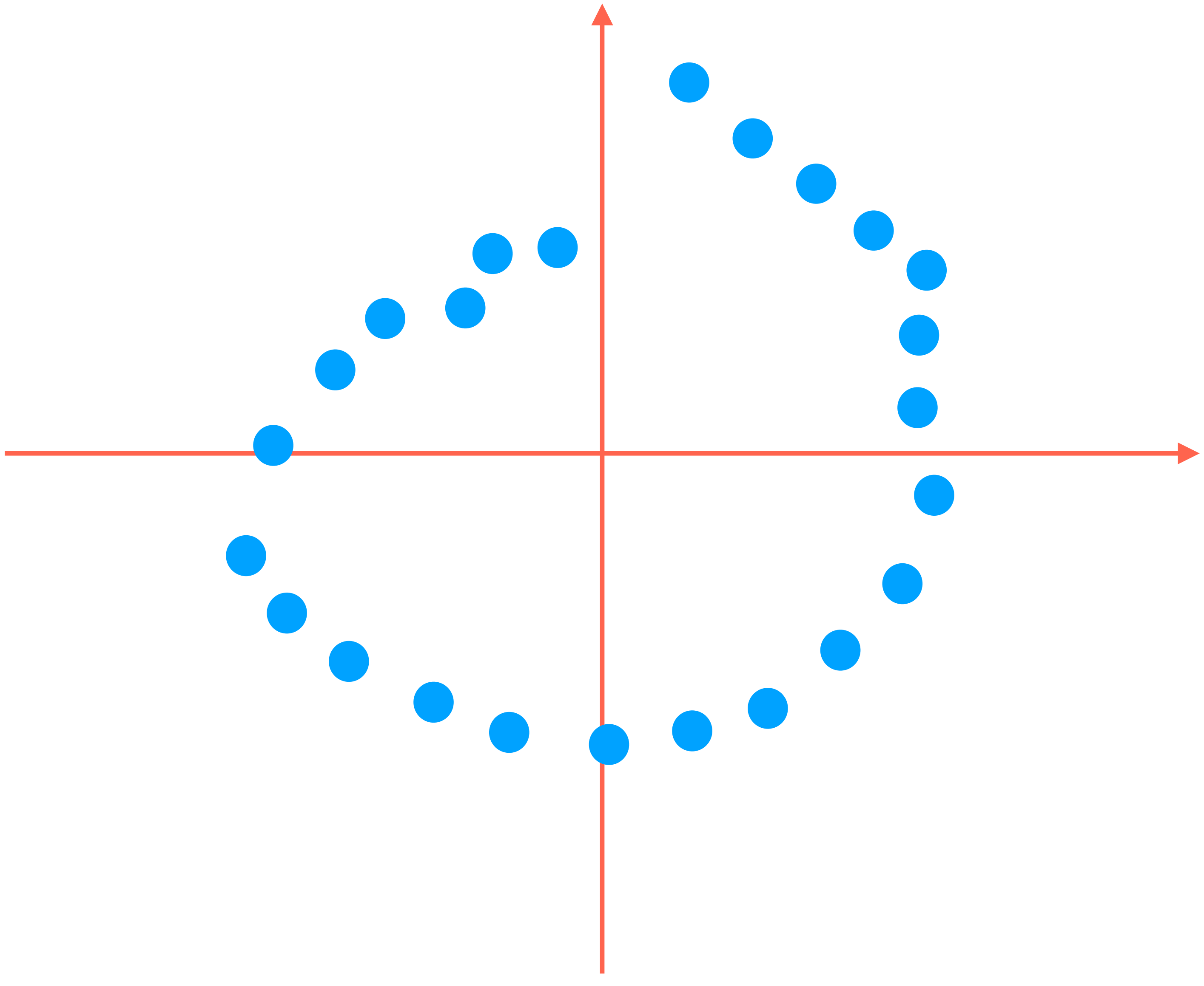


Image source: http://4.bp.blogspot.com/-USQEgoh1jCU/VfncdNOETcI/AAAAAAAAGp8/Hea8UtE_1c0/s1600/Blog%2B1%2BIMG_1821.jpg

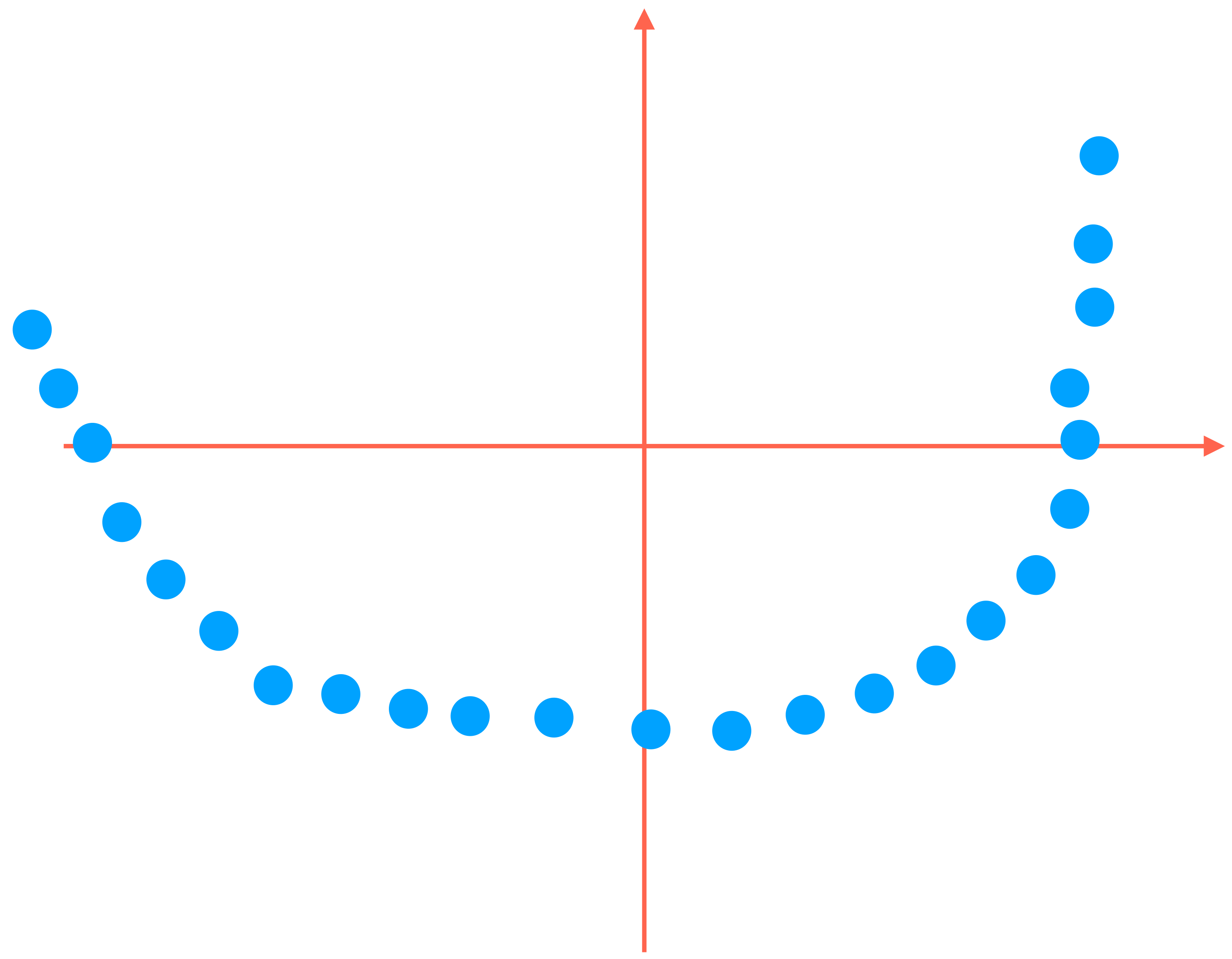
2D Swiss Roll



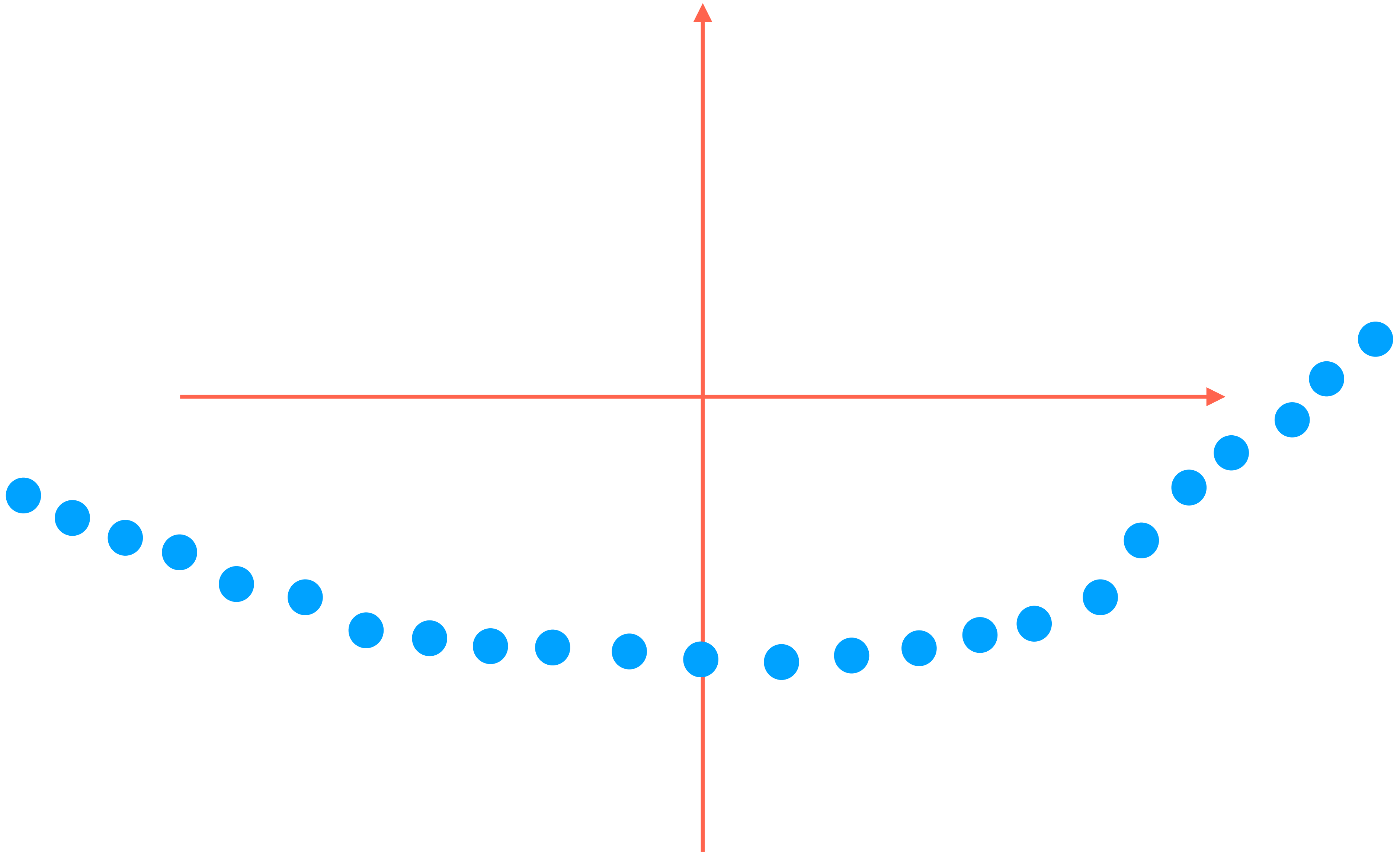
2D Swiss Roll



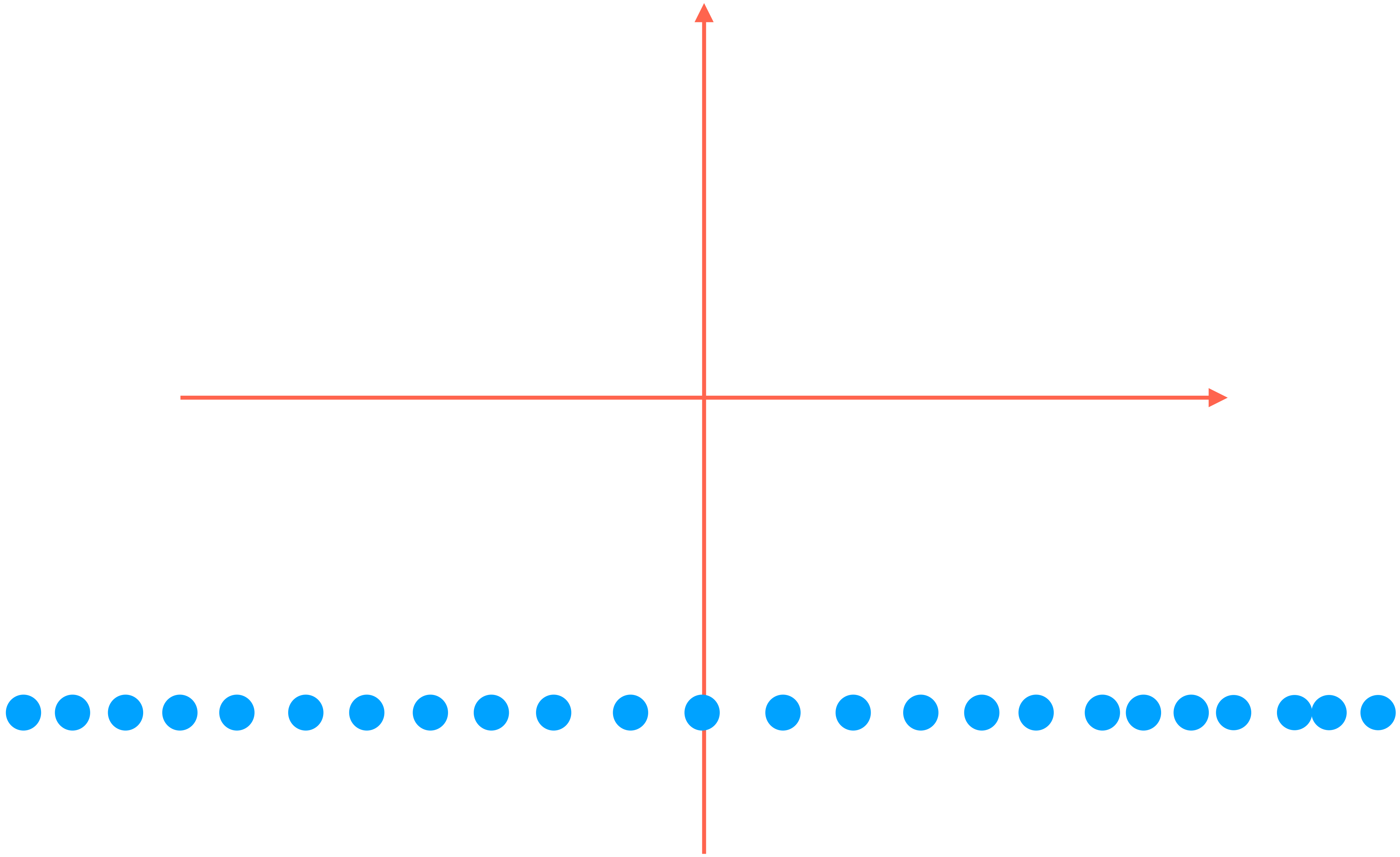
2D Swiss Roll



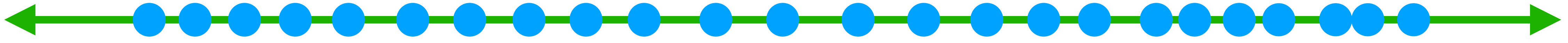
2D Swiss Roll



2D Swiss Roll



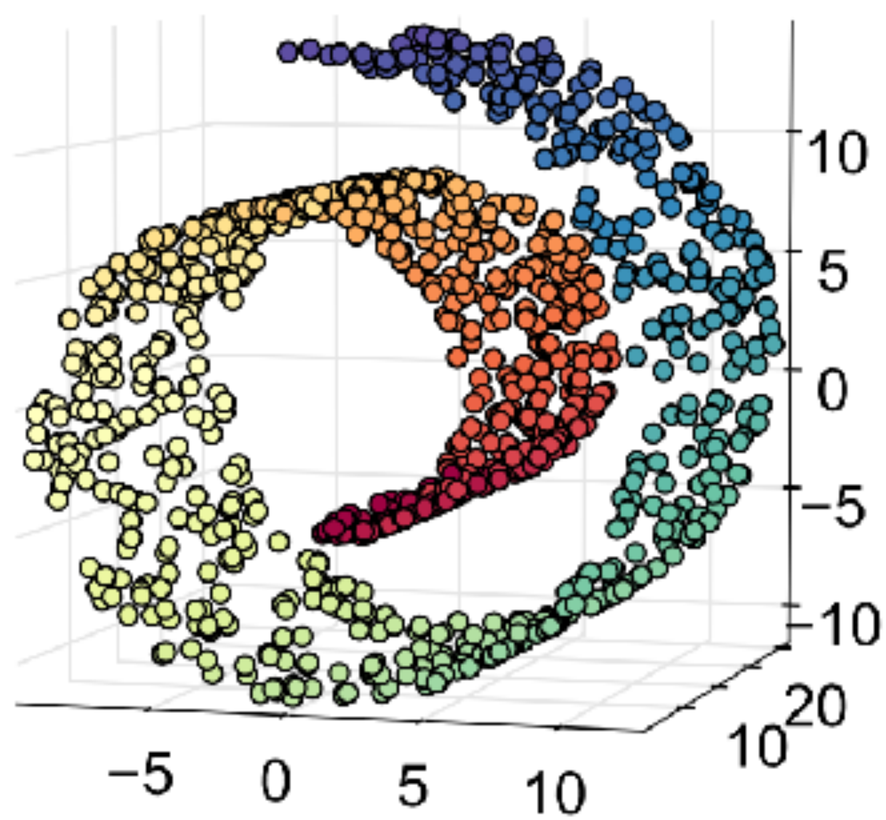
2D Swiss Roll



This is the desired result

Manifold Learning

- Nonlinear dimensionality reduction (in contrast to PCA which is linear)
- Find low-dimensional “manifold” that the data live on



Basic idea of a manifold:

1. Zoom in on any point (say, *x*)

2. The points near *x* look like they’re in a lower-dimensional Euclidean space (e.g., a 2D plane in Swiss roll)

Do Data Actually Live on Manifolds?

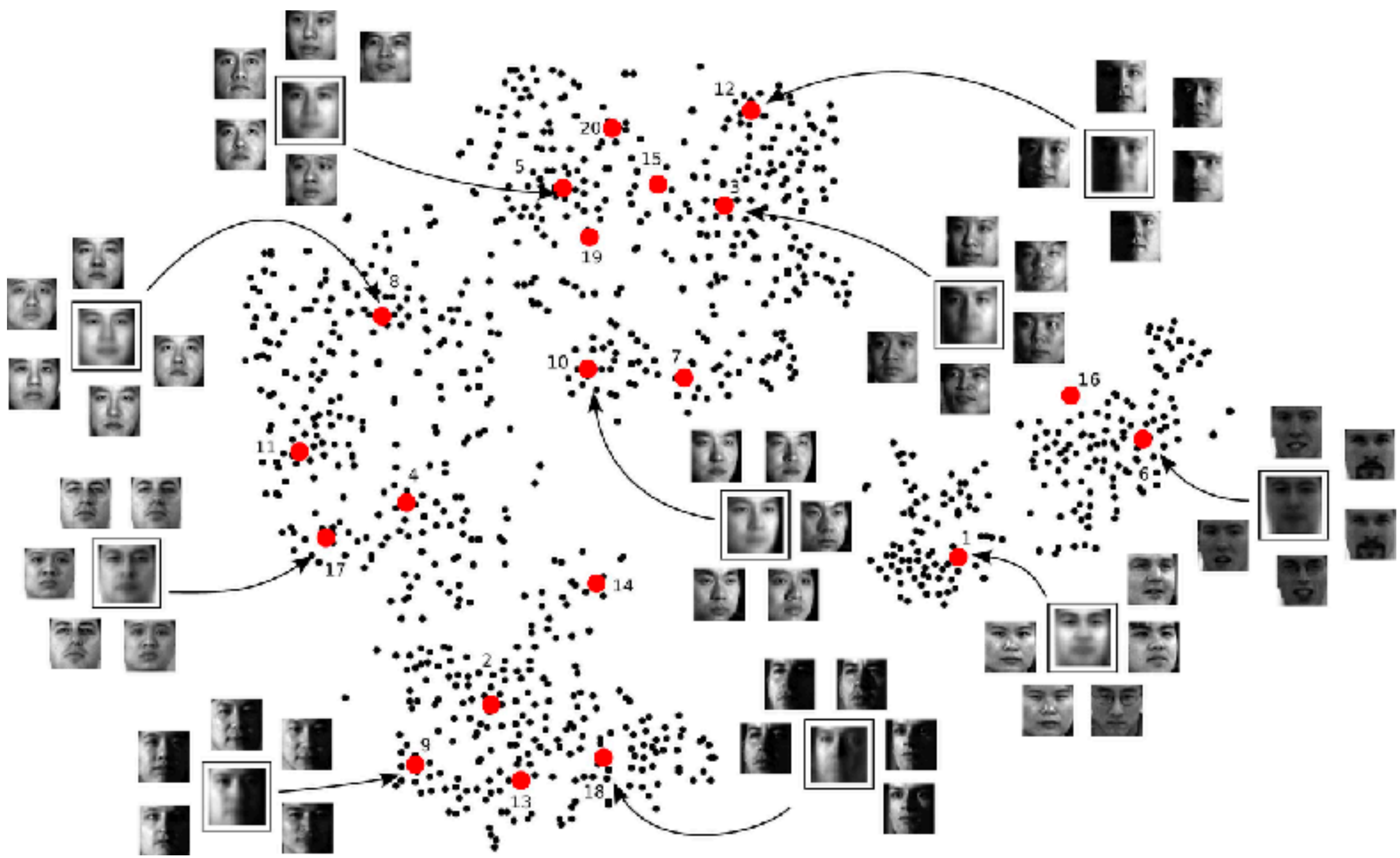
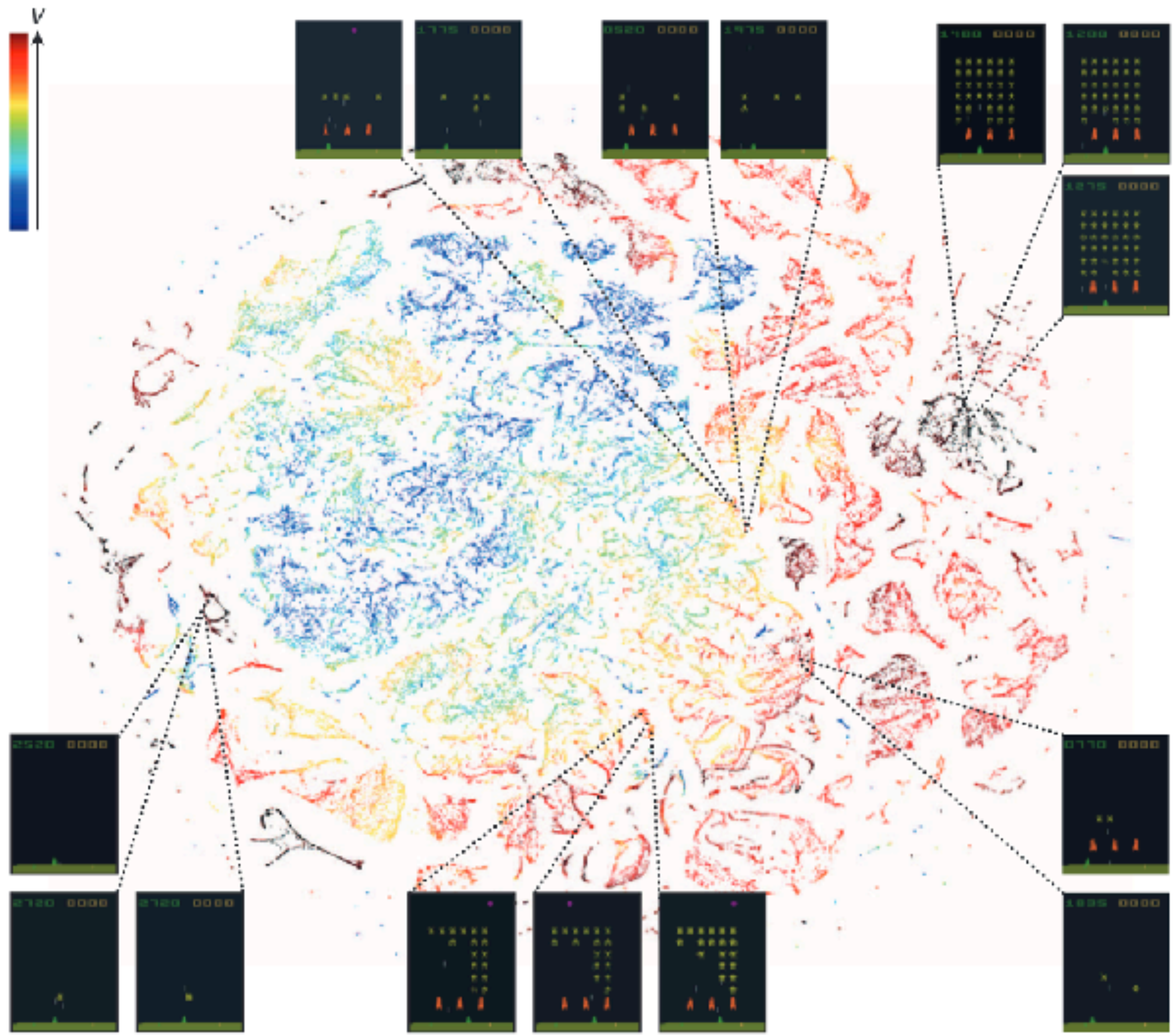


Image source: http://www.columbia.edu/~jwp2128/Images/faces.jpeg

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?

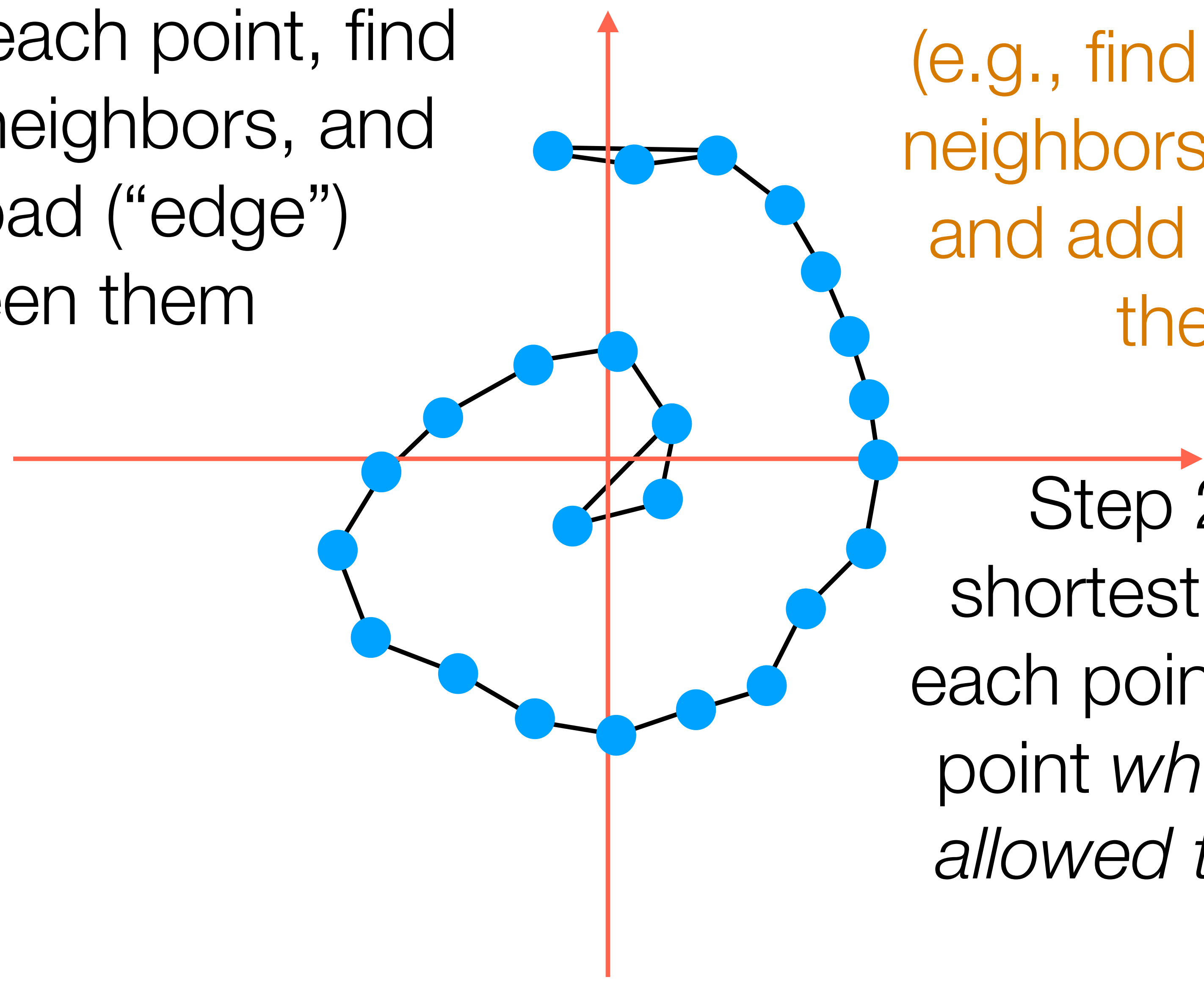


Mnih, Volodymyr, et al. Human-level control through deep reinforcement learning. Nature 2015.

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)

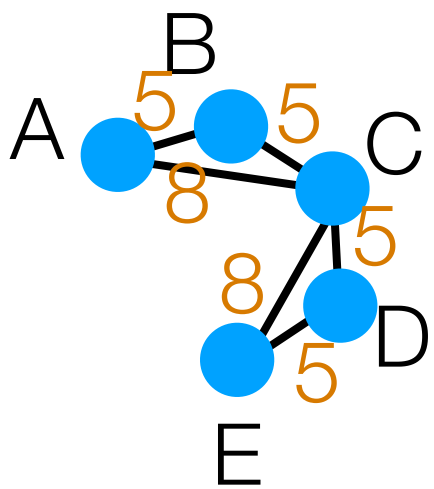


Step 2: Compute shortest distance from each point to every other point *where you’re only allowed to travel on the roads*

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

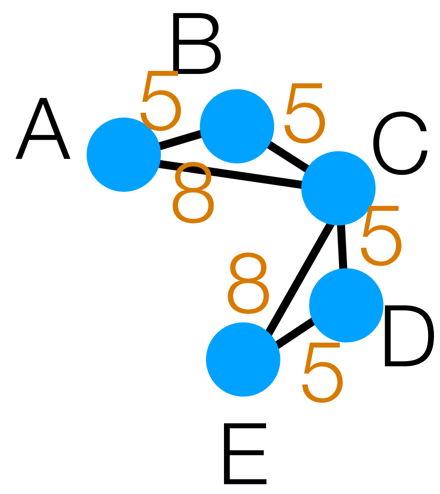
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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					
B					
C					
D					
E					

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

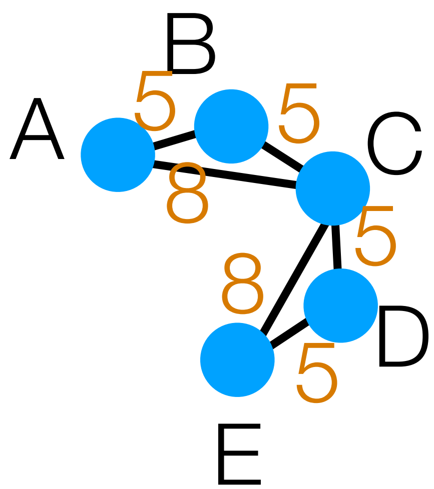
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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				
B		0			
C			0		
D				0	
E					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

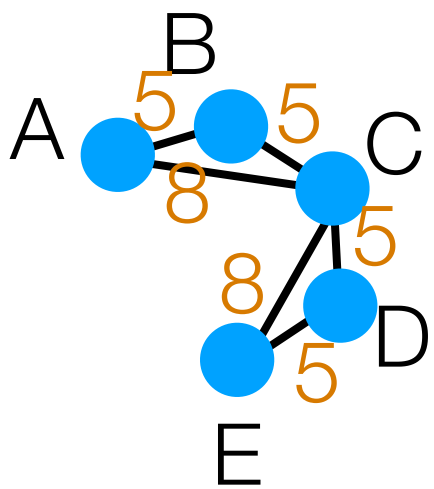
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

	A	B	C	D	E
A	0	5			
B		0	5		
C			0	5	
D				0	5
E					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

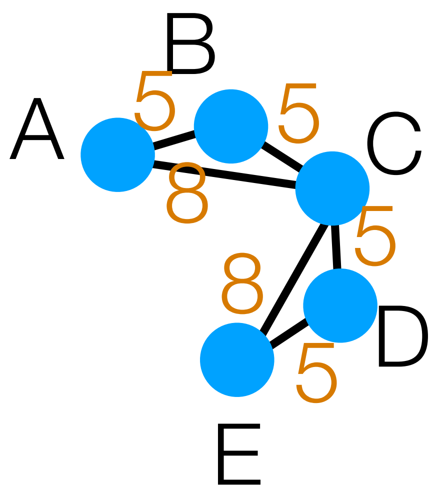
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

	A	B	C	D	E
A	0	5	8		
B		0	5		
C			0	5	
D				0	5
E					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

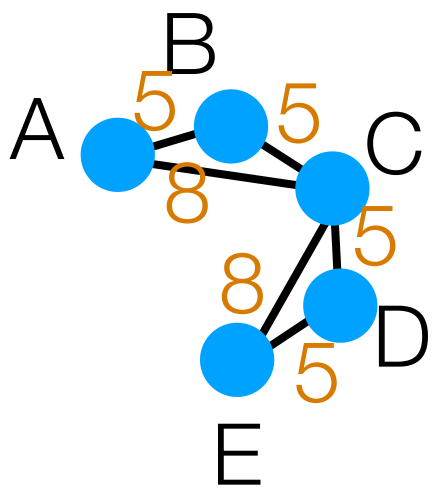
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

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

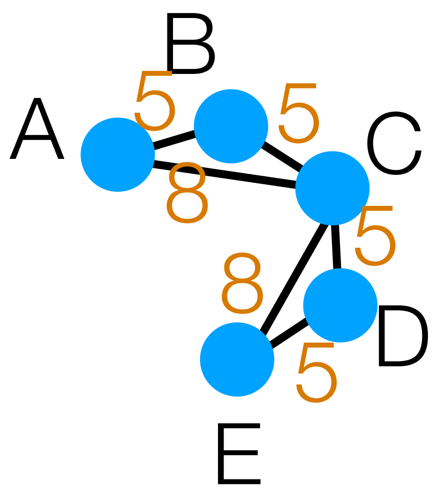
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

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

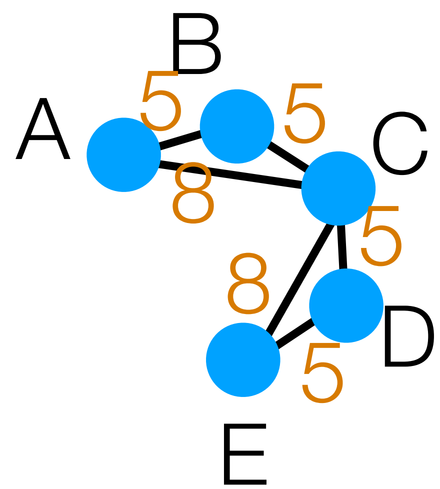
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

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

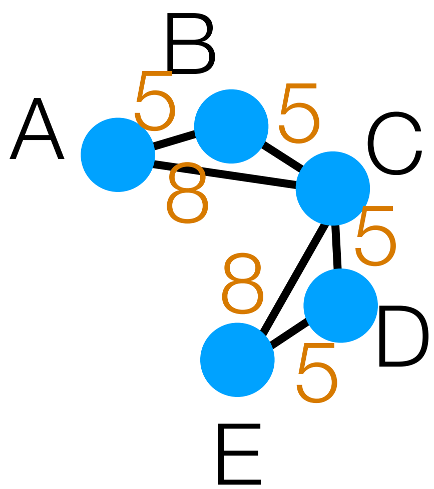
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

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

Isomap Calculation Example

In orange: road lengths



2 nearest neighbors of A: B, C

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2 nearest neighbors of D: C, E

2 nearest neighbors of E: C, D

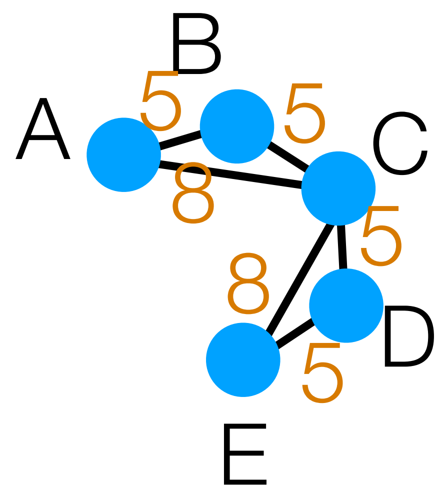
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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		0	5	10	13
C			0	5	8
D				0	5
E					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

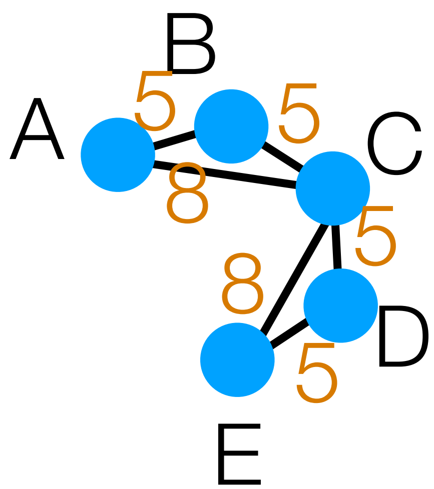
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

	A	B	C	D	E
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)

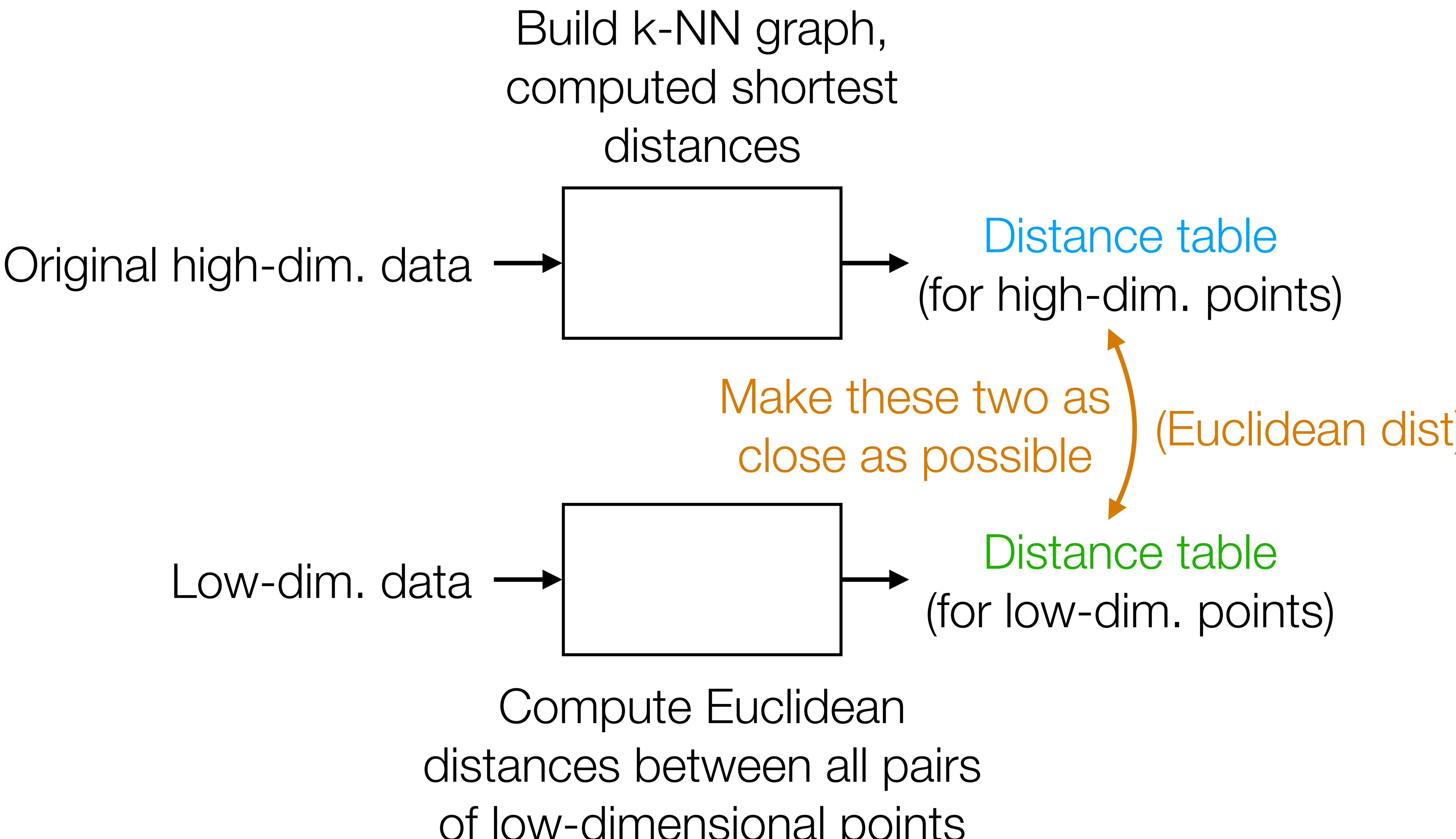
Shortest distances between every point to every other point *where we are only allowed to travel along the roads*

	A	B	C	D	E
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

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

The solution is not unique!

Isomap

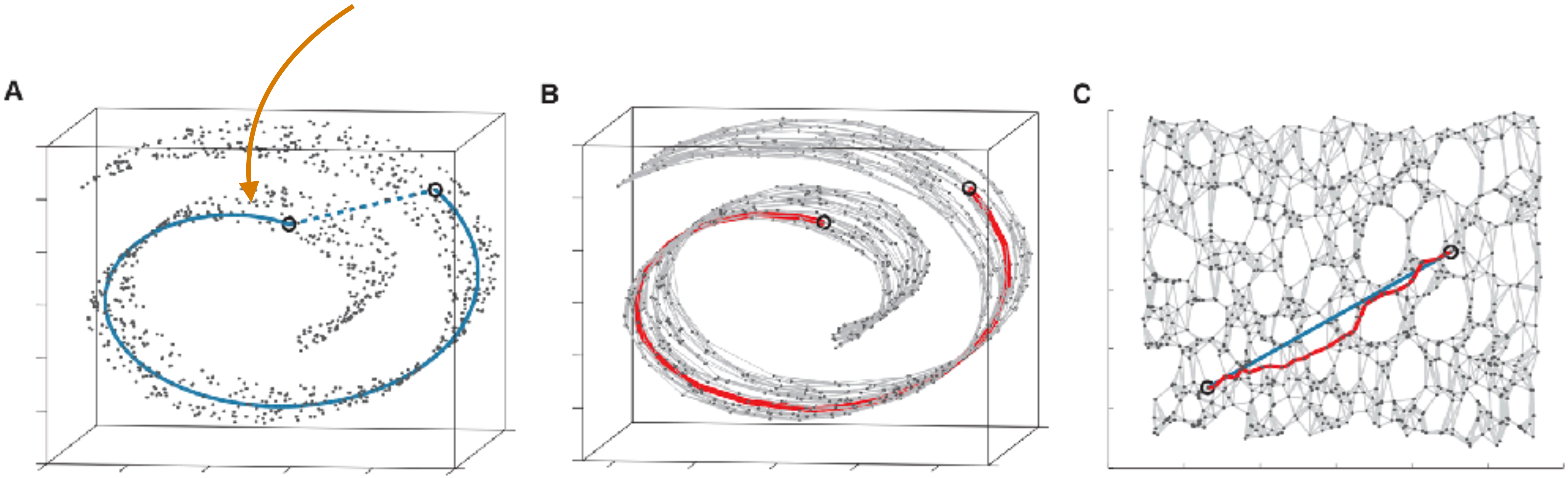

Build k-NN graph,
computed shortest
distances
Original high-dim. data
Distance table
(for high-dim. points)
Make these two as
close as possible
(Euclidean dist)
Low-dim. data
Distance table
(for low-dim. points)
Compute Euclidean
distances between all pairs
of low-dimensional points

Isomap Calculation Example

Demo

3D Swiss Roll Example

Key idea: true distance on manifold is the blue line

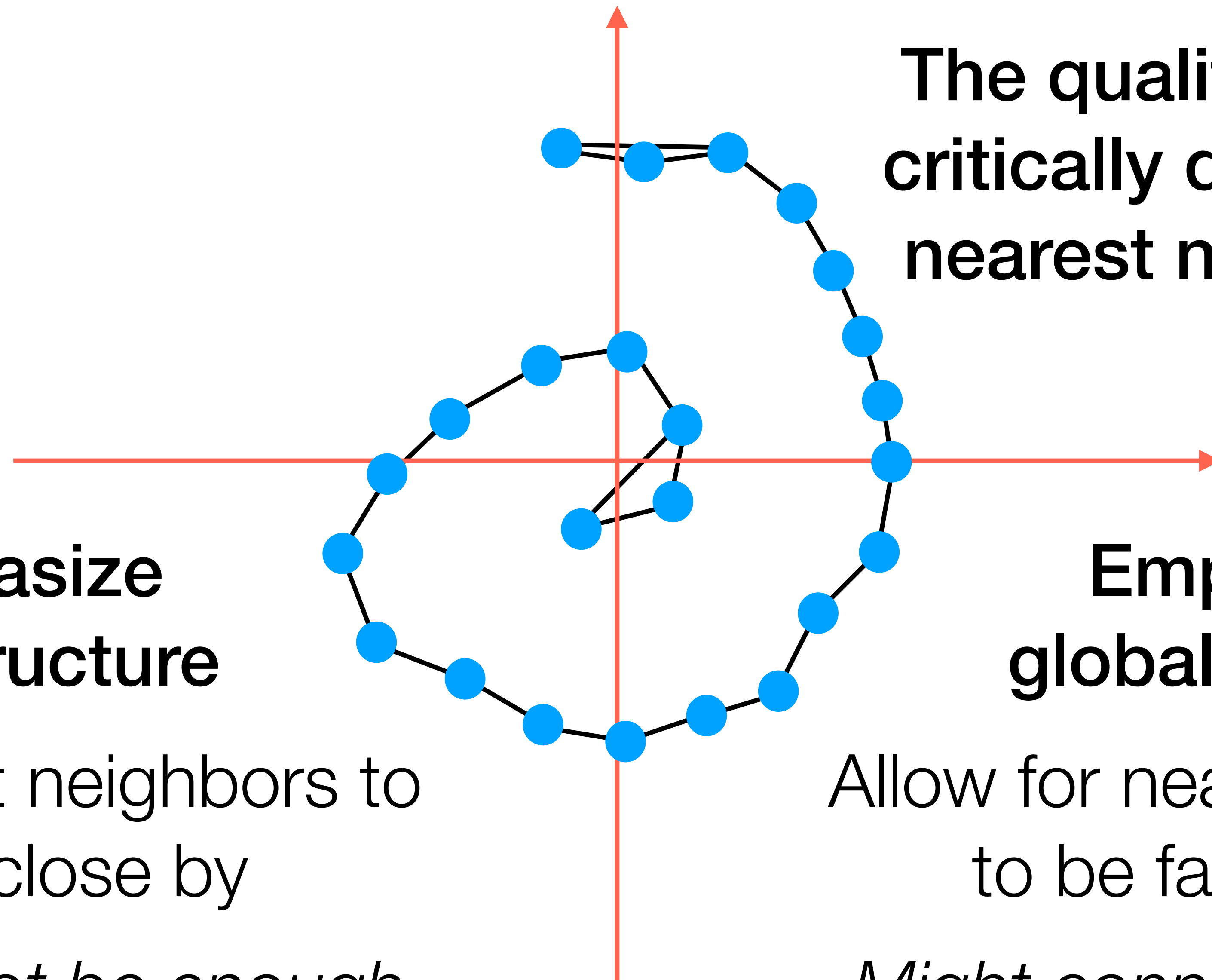


We're approximating the blue line with the red line
(poor choice of # nearest neighbors can make approximation bad)

Joshua B. Tenenbaum, Vin de Silva, John C. Langford. A Global Geometric Framework for Nonlinear Dimensionality Reduction. Science 2000.

Some Observations on Isomap

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



Emphasize local structure

Ask for nearest neighbors to be really close by

There might not be enough edges

Emphasize global structure

Allow for nearest neighbors to be farther away

Might connect points that shouldn't be connected

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