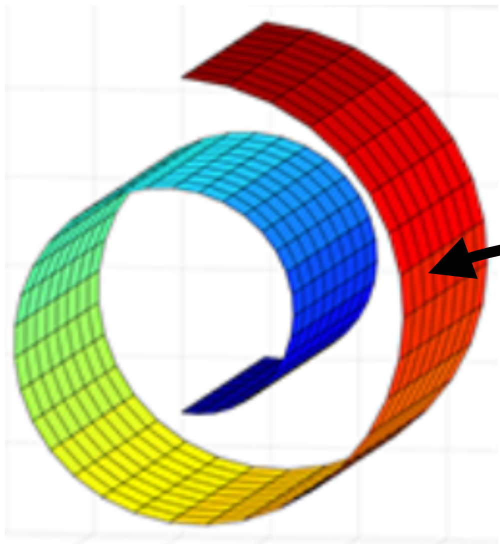
Carnegie Mellon University
Heinz College

Unstructured Data Analytics for Policy

Lecture 5: Manifold learning

George Chen

(Last Time) 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?

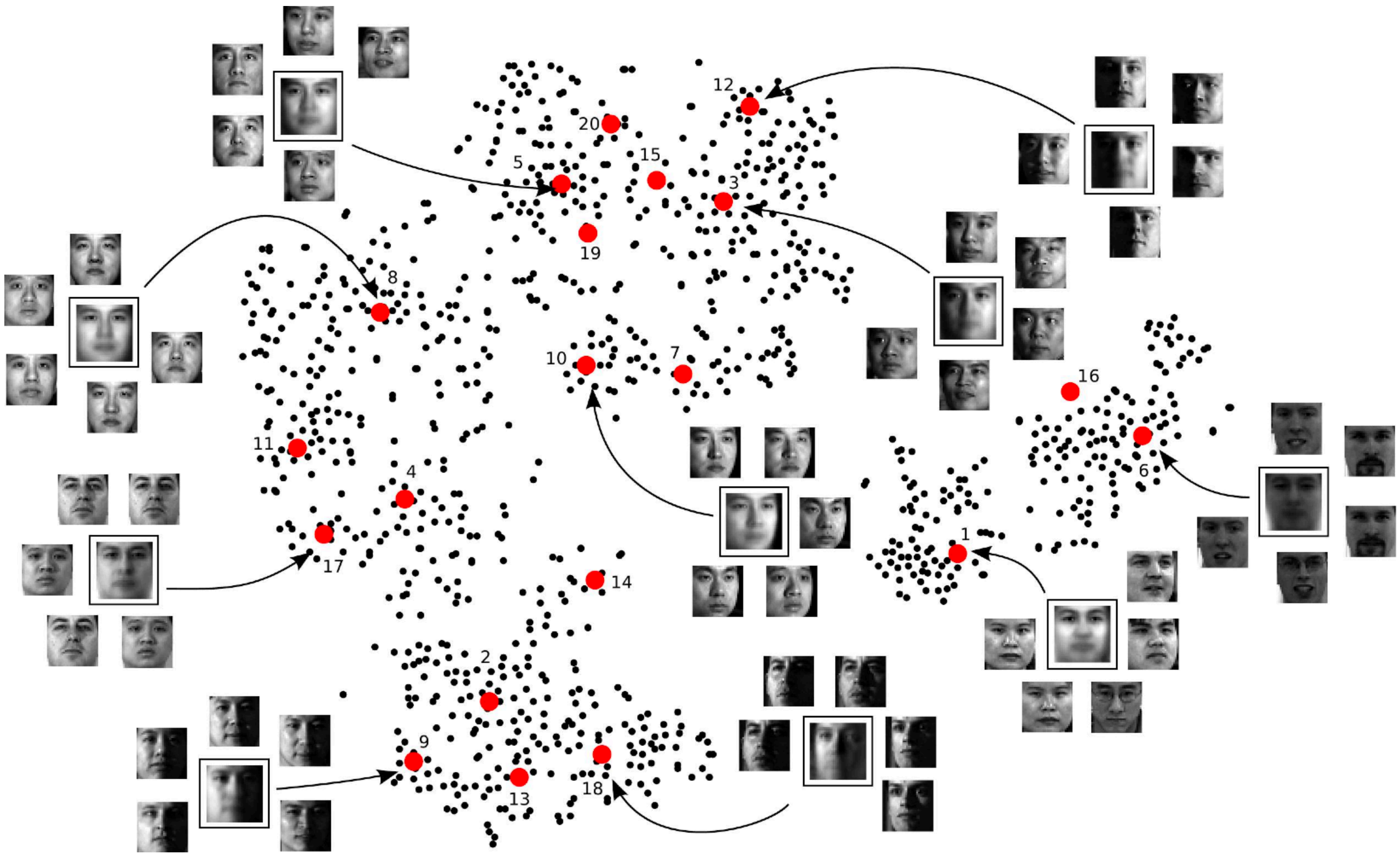


Image source: http://www.columbia.edu/~jwp2128/Images/faces.jpeg

Do Data Actually Live on Manifolds?

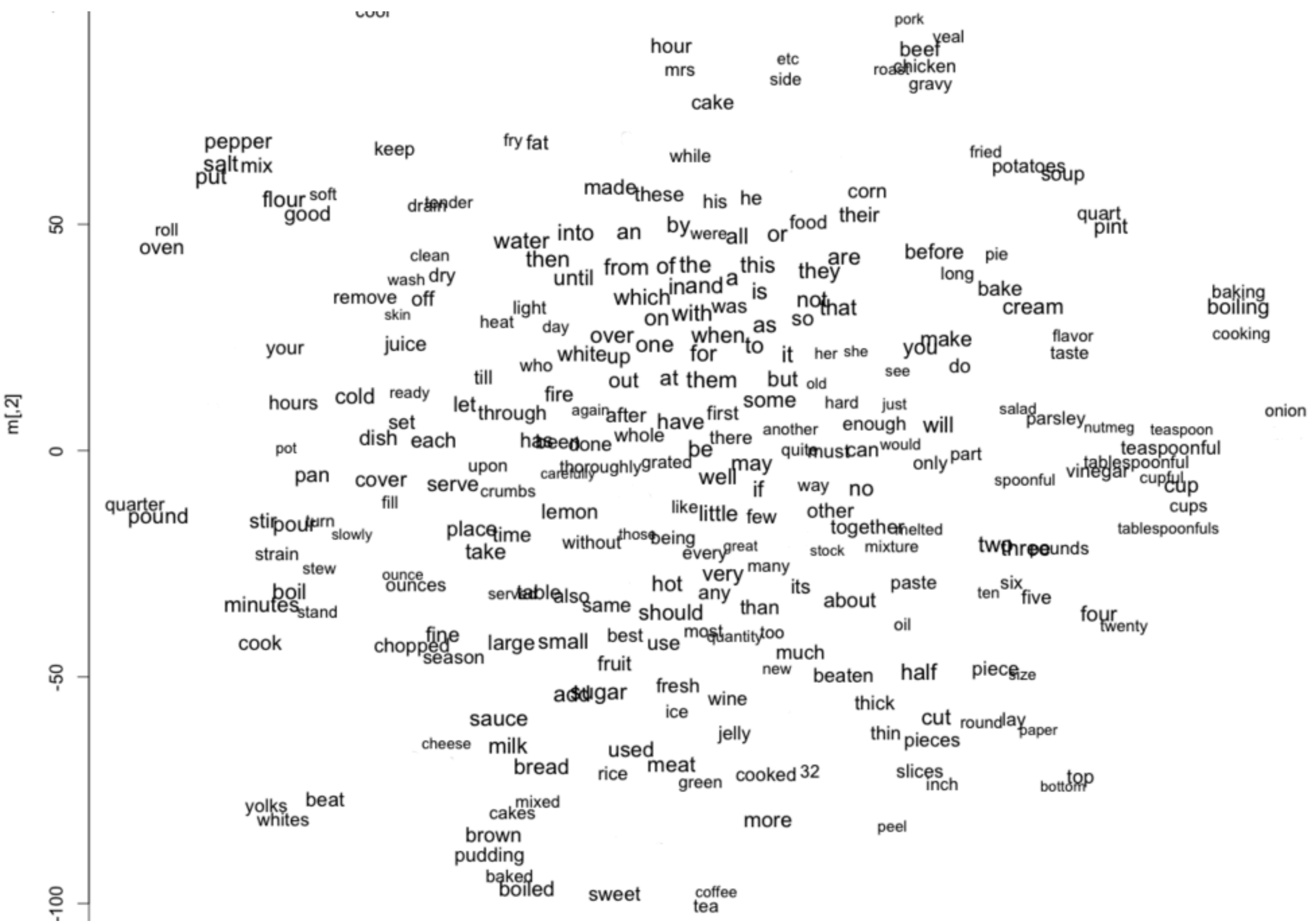
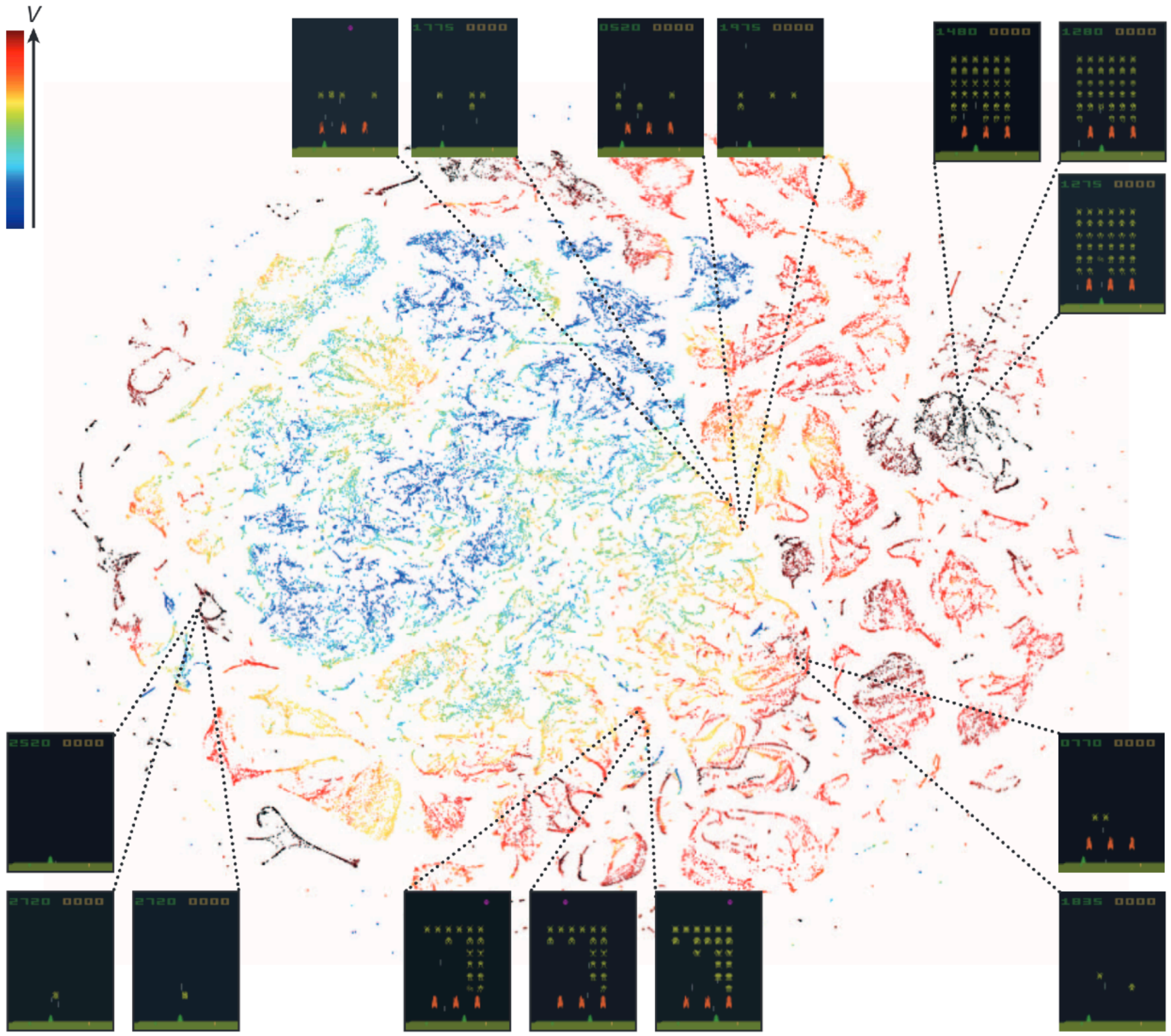


Image source: http://www.adityathakker.com/wp-content/uploads/2017/06/word-embeddings-994x675.png

Do Data Actually Live on Manifolds?



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

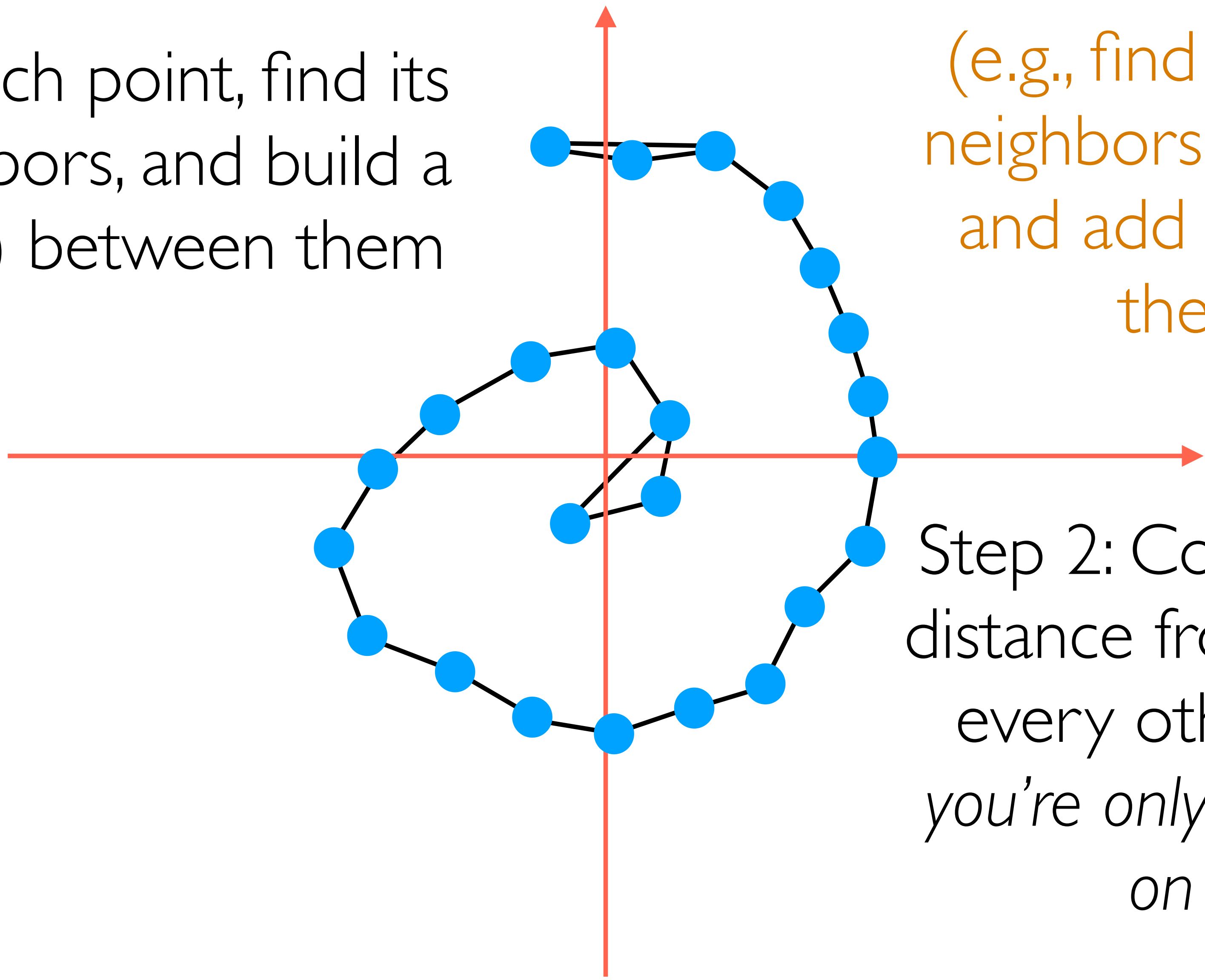
There are many manifold learning methods

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)

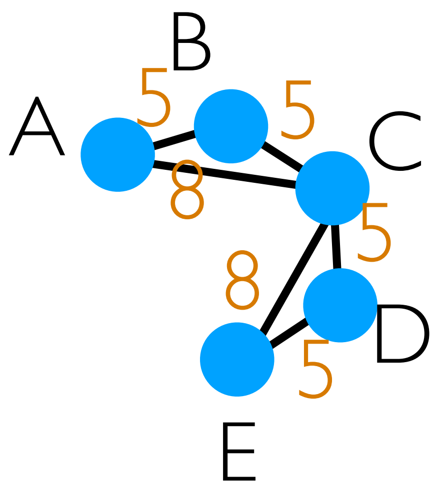


Step 2: Compute shortest distance from each point to every other point *where you're only allowed to travel on the roads*

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

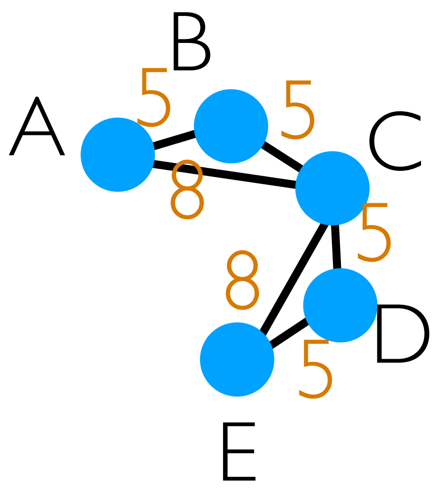
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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					
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

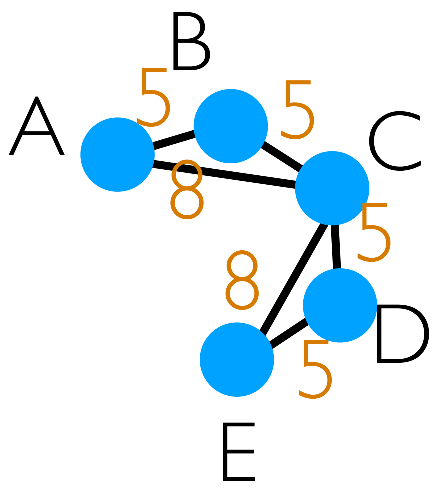
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

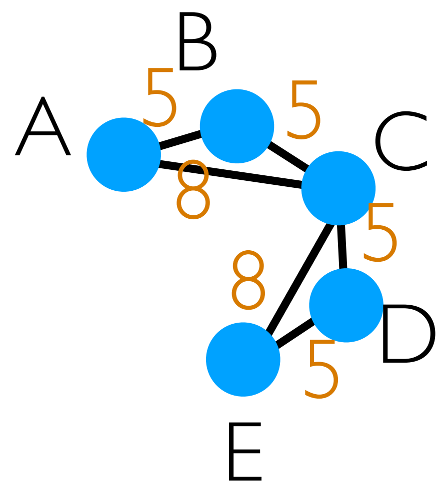
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

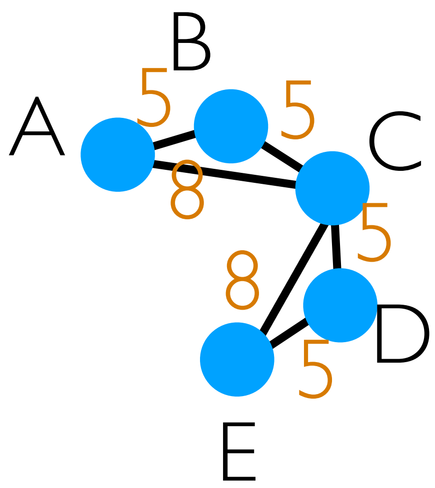
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

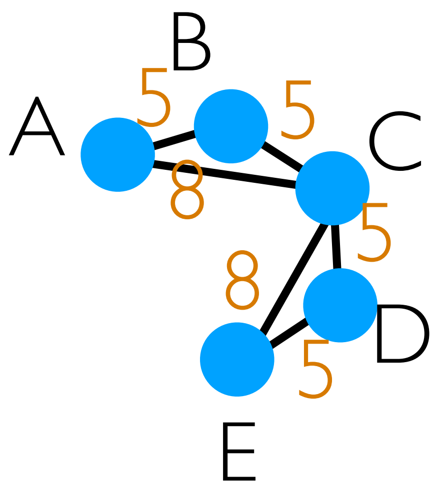
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

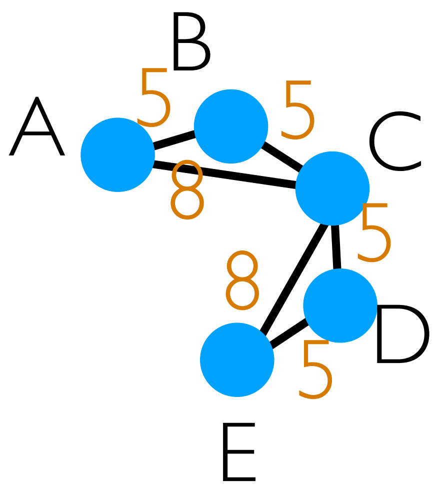
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

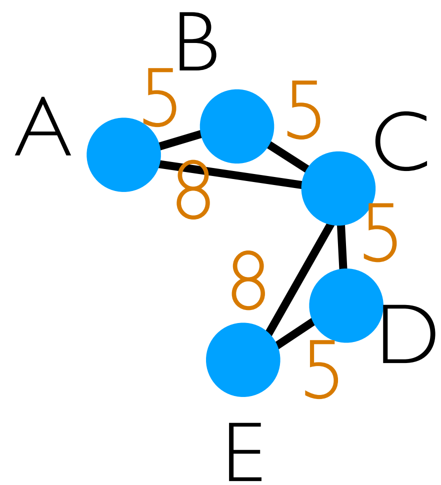
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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

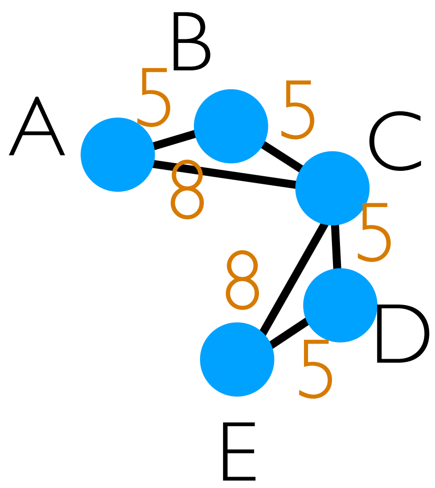
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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



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2 nearest neighbors of C: B, D

2 nearest neighbors of D: C, E

2 nearest neighbors of E: C, D

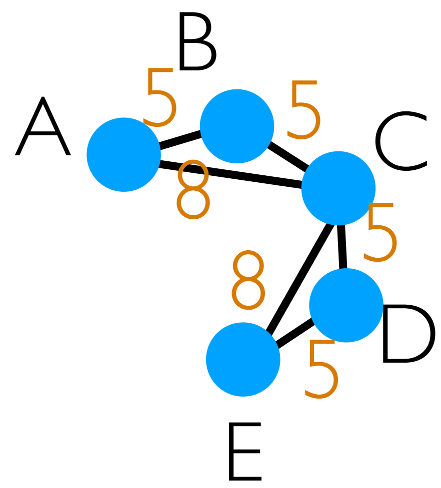
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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	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

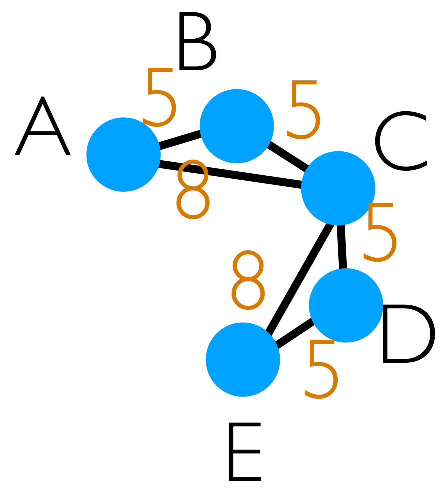
Build "symmetric 2-NN" graph (add edges for each point to its 2 nearest neighbors)

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!

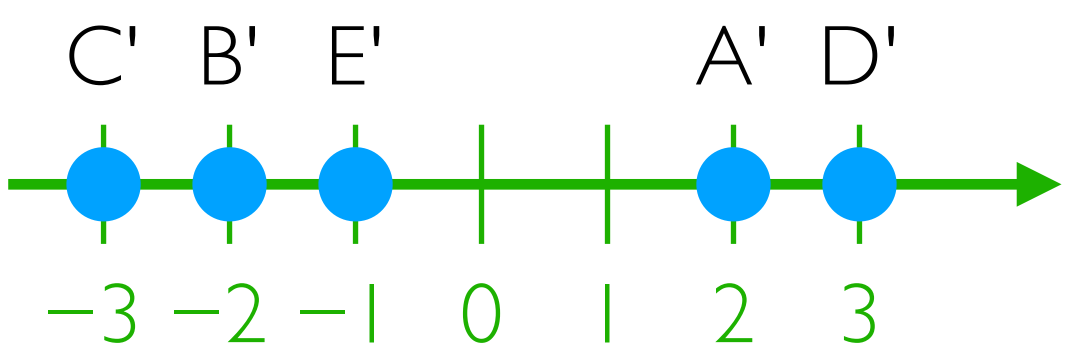
Multidimensional Scaling (MDS)

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'					
B'					
C'					
D'					
E'					

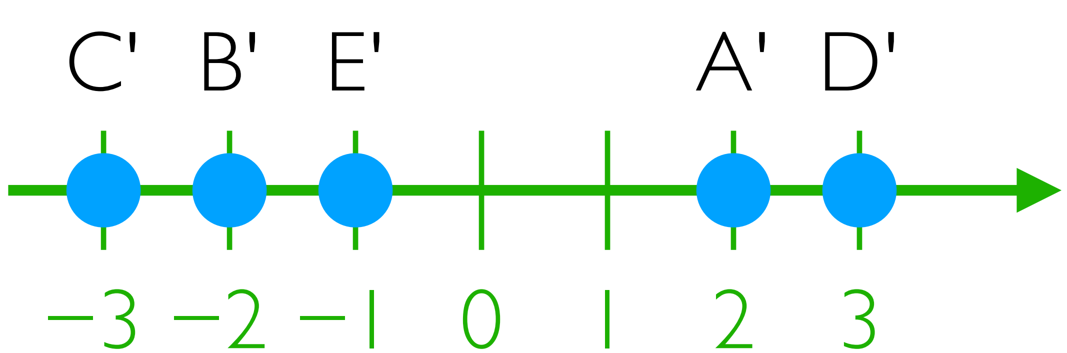
Multidimensional Scaling (MDS)

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				
B'		0			
C'			0		
D'				0	
E'					0

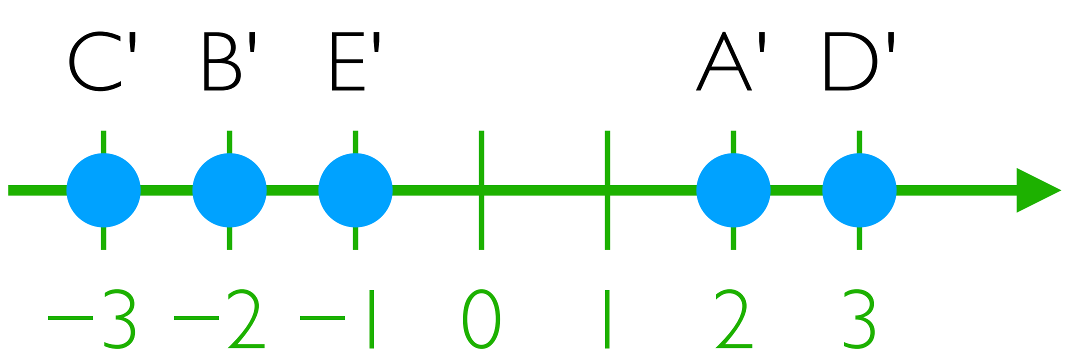
Multidimensional Scaling (MDS)

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			
B'		0			
C'			0		
D'				0	
E'					0

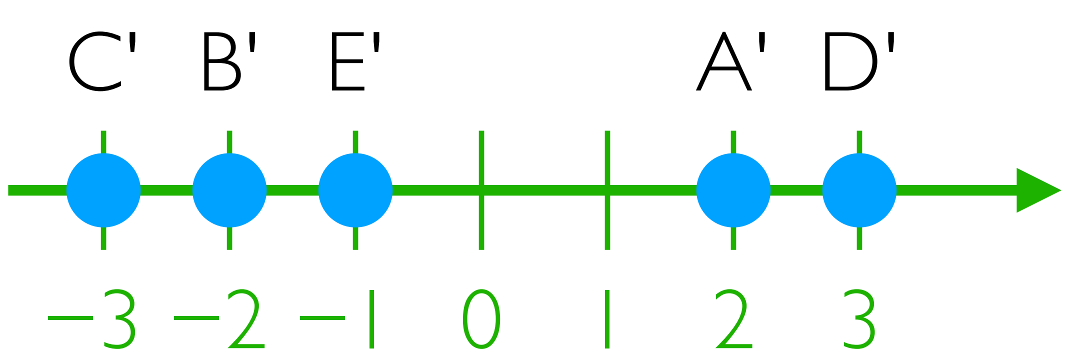
Multidimensional Scaling (MDS)

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		
B'		0			
C'			0		
D'				0	
E'					0

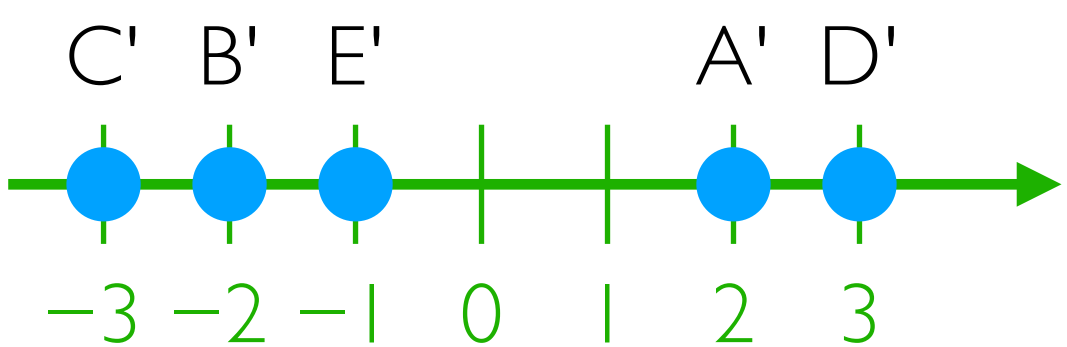
Multidimensional Scaling (MDS)

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	
B'		0			
C'			0		
D'				0	
E'					0

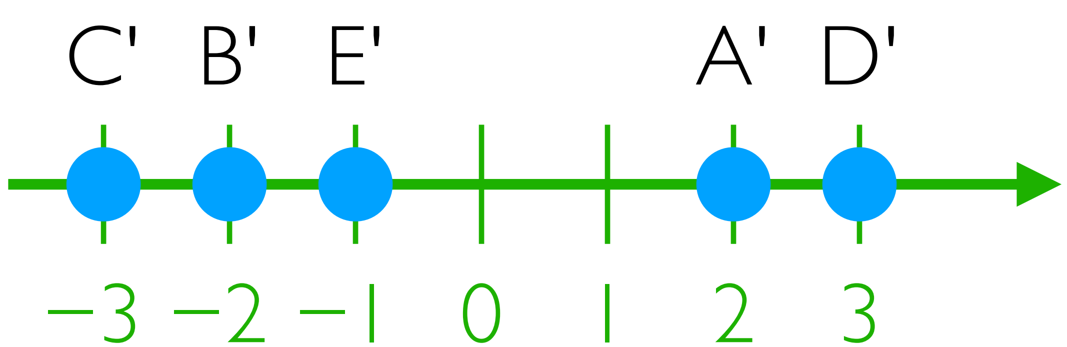
Multidimensional Scaling (MDS)

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'		0			
C'			0		
D'				0	
E'					0

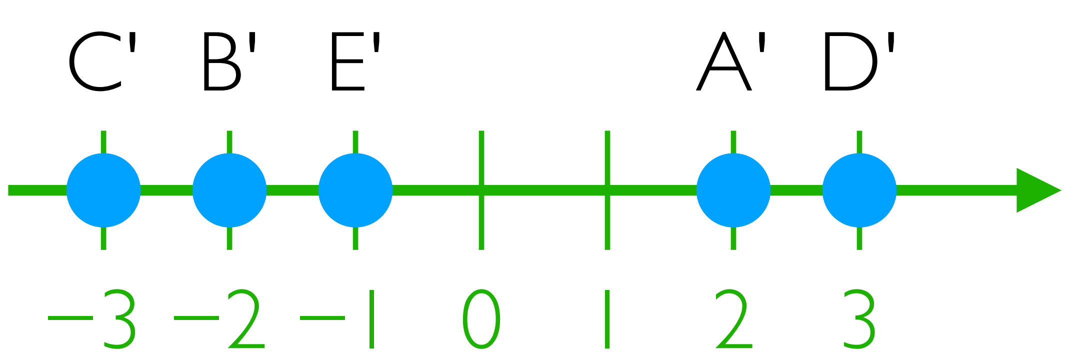
Multidimensional Scaling (MDS)

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'		0	1	5	1
C'			0	6	2
D'				0	4
E'					0

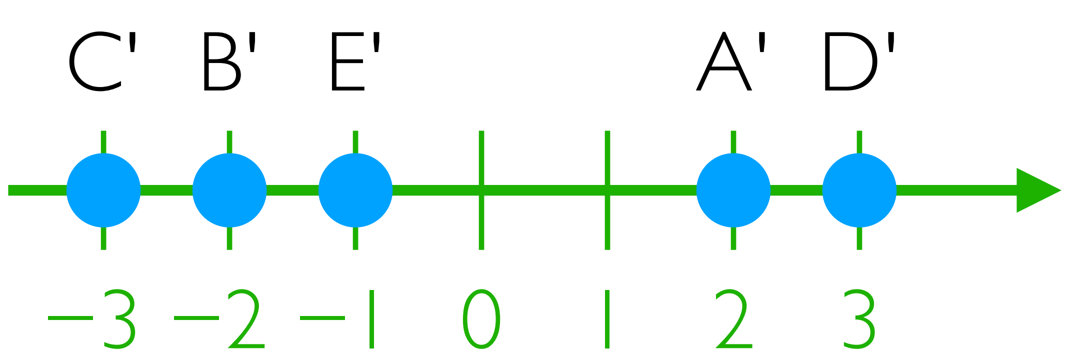
Multidimensional Scaling (MDS)

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

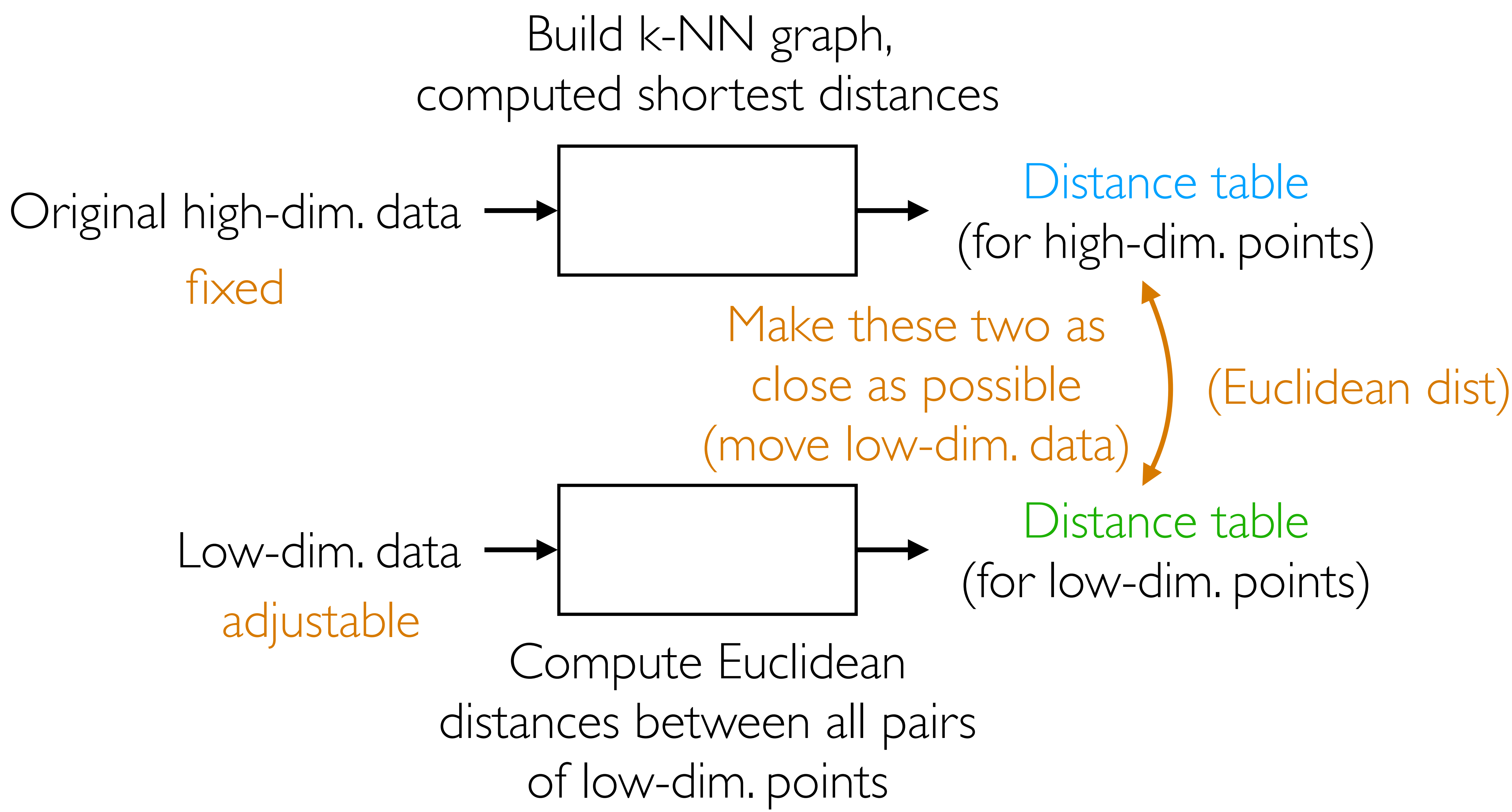
Suppose we have a guess for where the low-dimensional points are



	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

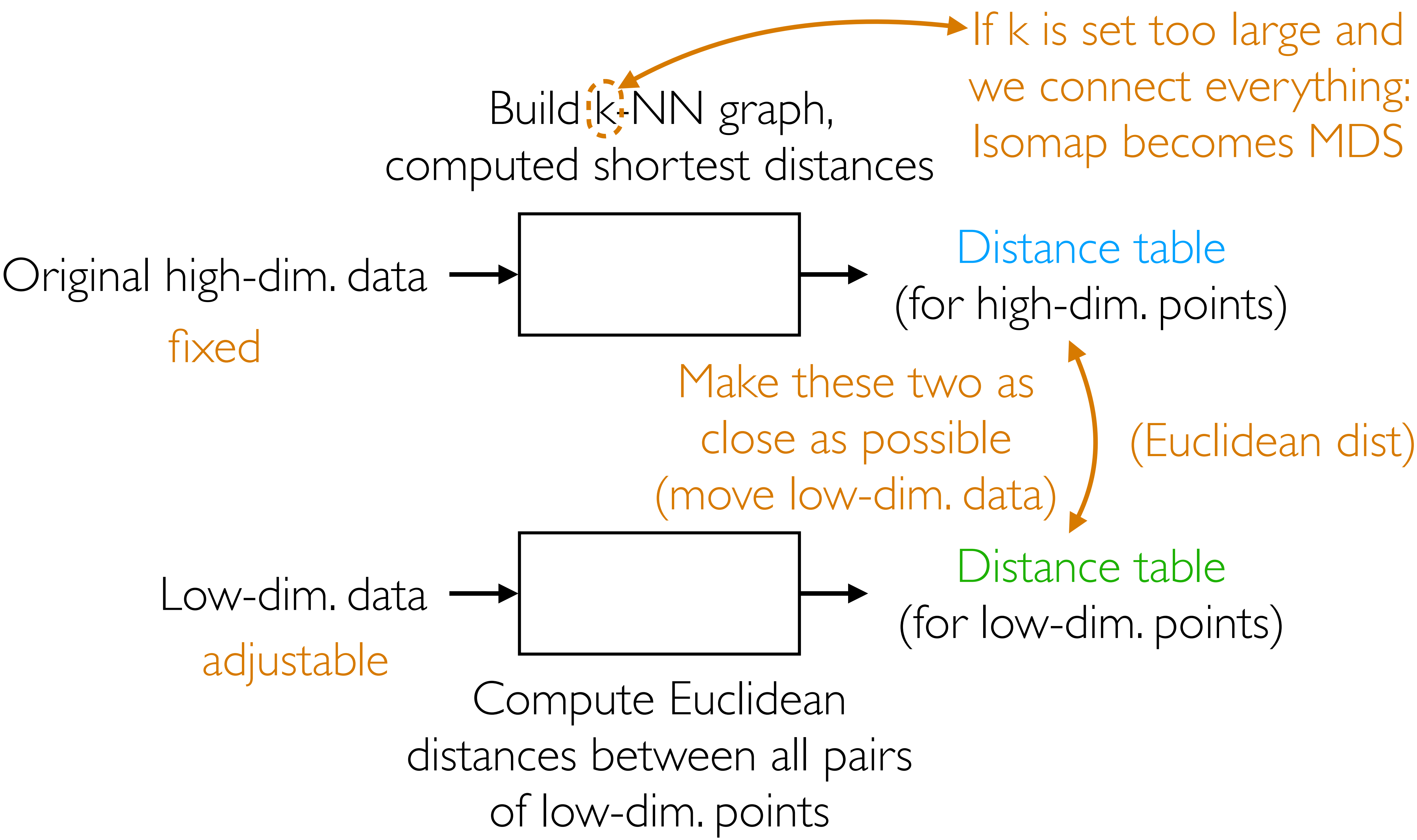


Build k-NN graph,
computed shortest distances
Original high-dim. data
fixed
Distance table
(for high-dim. points)
Make these two as
close as possible
(move low-dim. data)
(Euclidean dist)
Low-dim. data
adjustable
Distance table
(for low-dim. points)
Compute Euclidean
distances between all pairs
of low-dim.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

Isomap Calculation Example

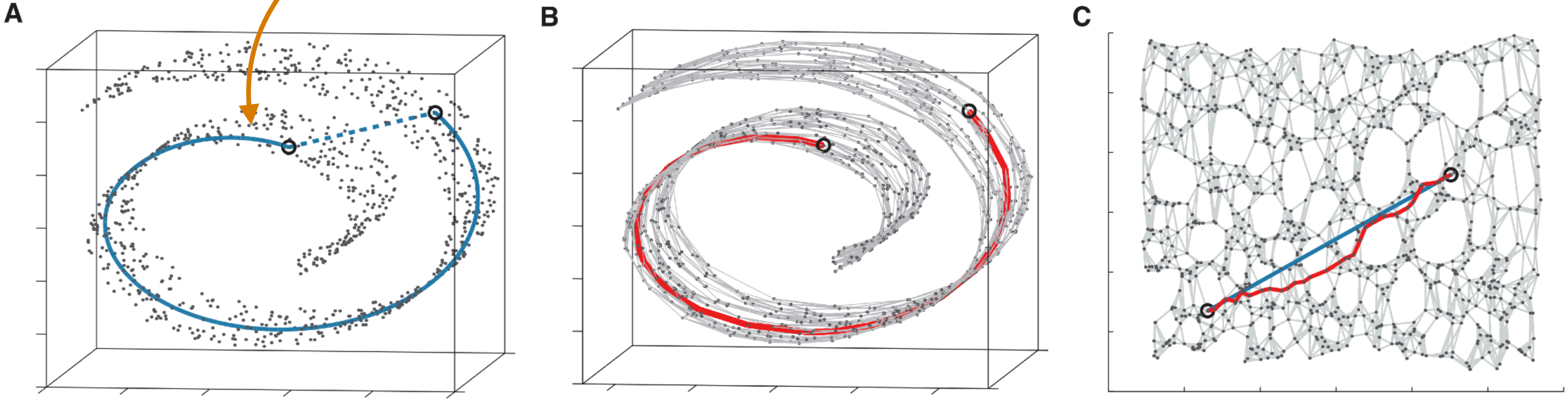
Demo

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

3D Swiss Roll Example

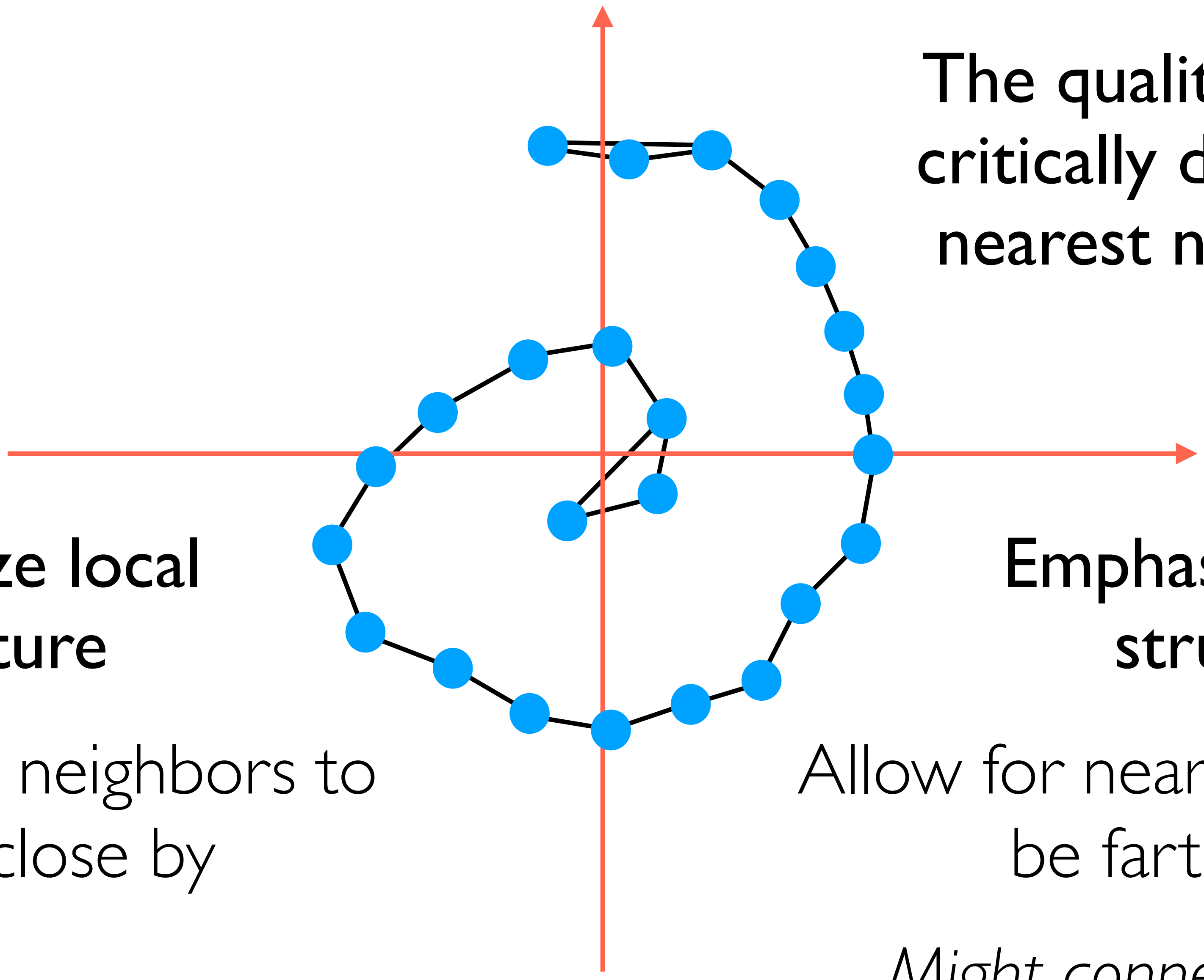
Key idea: true distance on manifold is the blue line



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

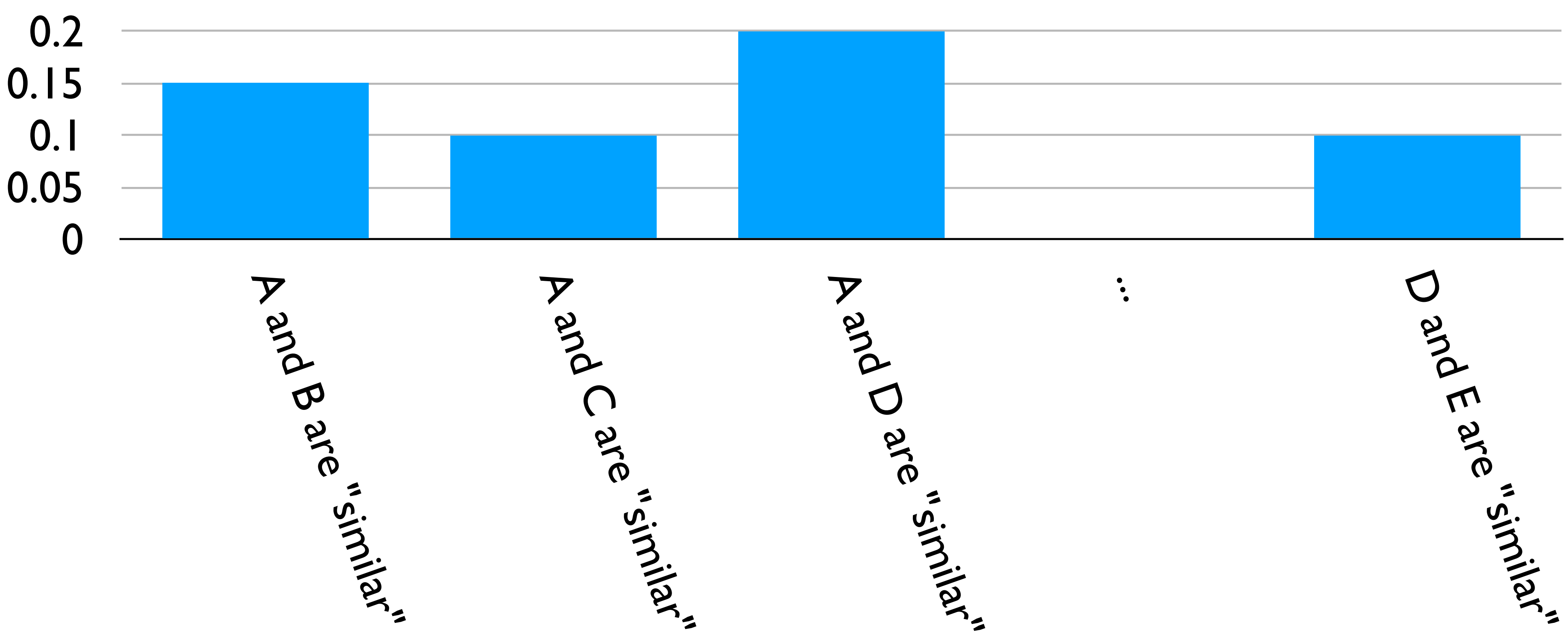
t-SNE
(t-distributed stochastic neighbor embedding)

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 detail: creates probabilities based on Gaussian distribution

Original high-dim. data → → **Probability** table (for high-dim. points)

fixed

Make these two as close as possible (move low-dim. data)

(Technical detail: KL divergence)

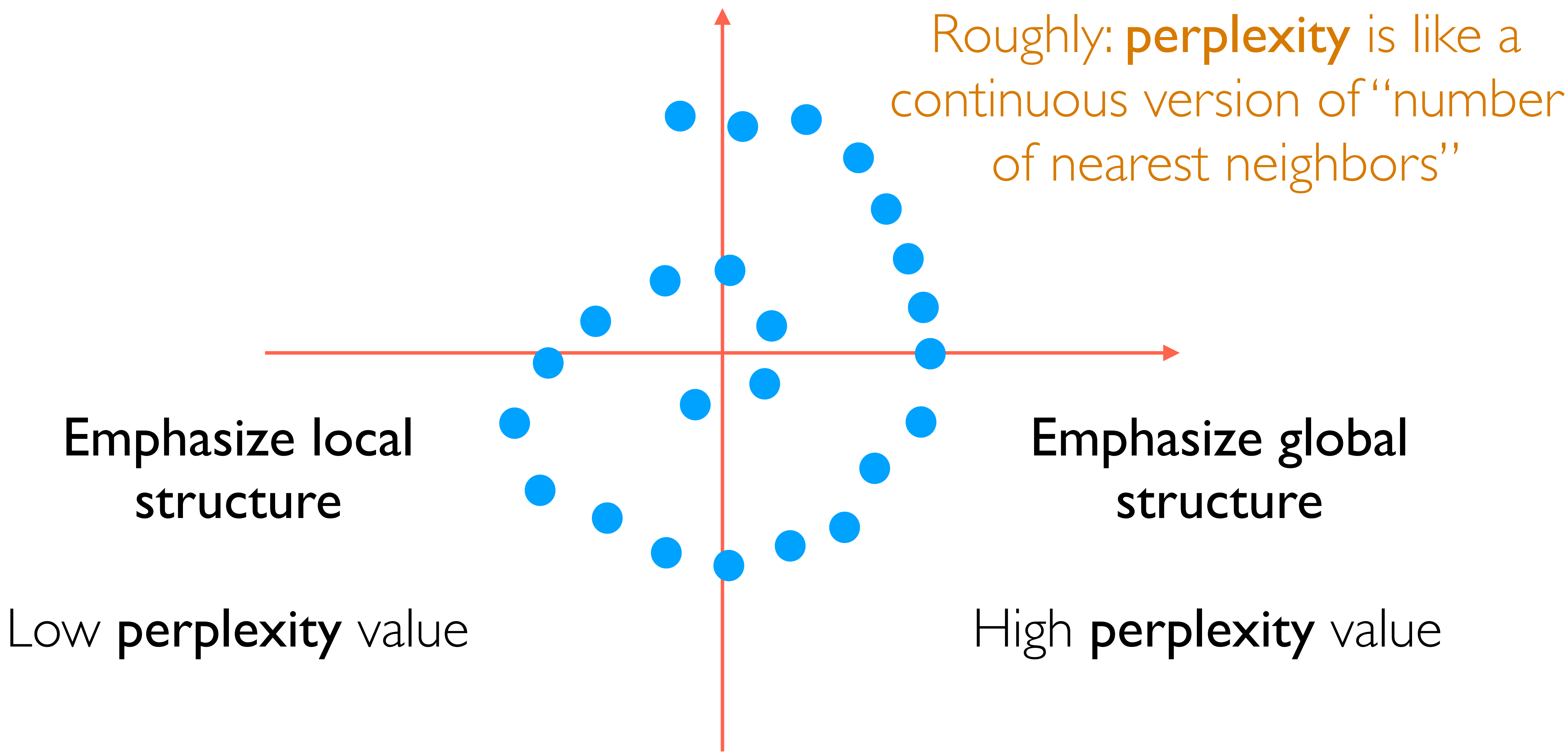
Low-dim. data → → **Probability** table (for low-dim. points)

adjustable

Technical detail: creates probabilities based on Student's *t*-distribution

Technical details are in separate slides (posted on webpage)

t-SNE Parameters…



Also: play with learning rate, # iterations

In practice, often people initialize with PCA

Manifold Learning with t-SNE

Demo

t-SNE Interpretation

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

Dimensionality Reduction for Visualization

- There are *many* methods (I've posted a link on the course webpage to a scikit-learn example using ~10 methods)

- PCA is very well-understood; the new axes can be interpreted

- Nonlinear dimensionality reduction (manifold learning):
  new axes may not really be all that interpretable

- Practice advice for visualization: try PCA first, and if that doesn't work, try t-SNE and then possibly other manifold learning methods

- If you have good reason to believe that only certain features matter, of course you could restrict your analysis to those!