Constructing Maps to Visualize Big Data

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TU Delft

Introduction

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"Have a look at your data!"

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- Good visualizations leverage the human visual system to:
  - Recognize patterns, spot trends, and identify outliers
  - Replace cognitive calculations by perceptual inferences
  - Engage more diverse audiences, *etc.*

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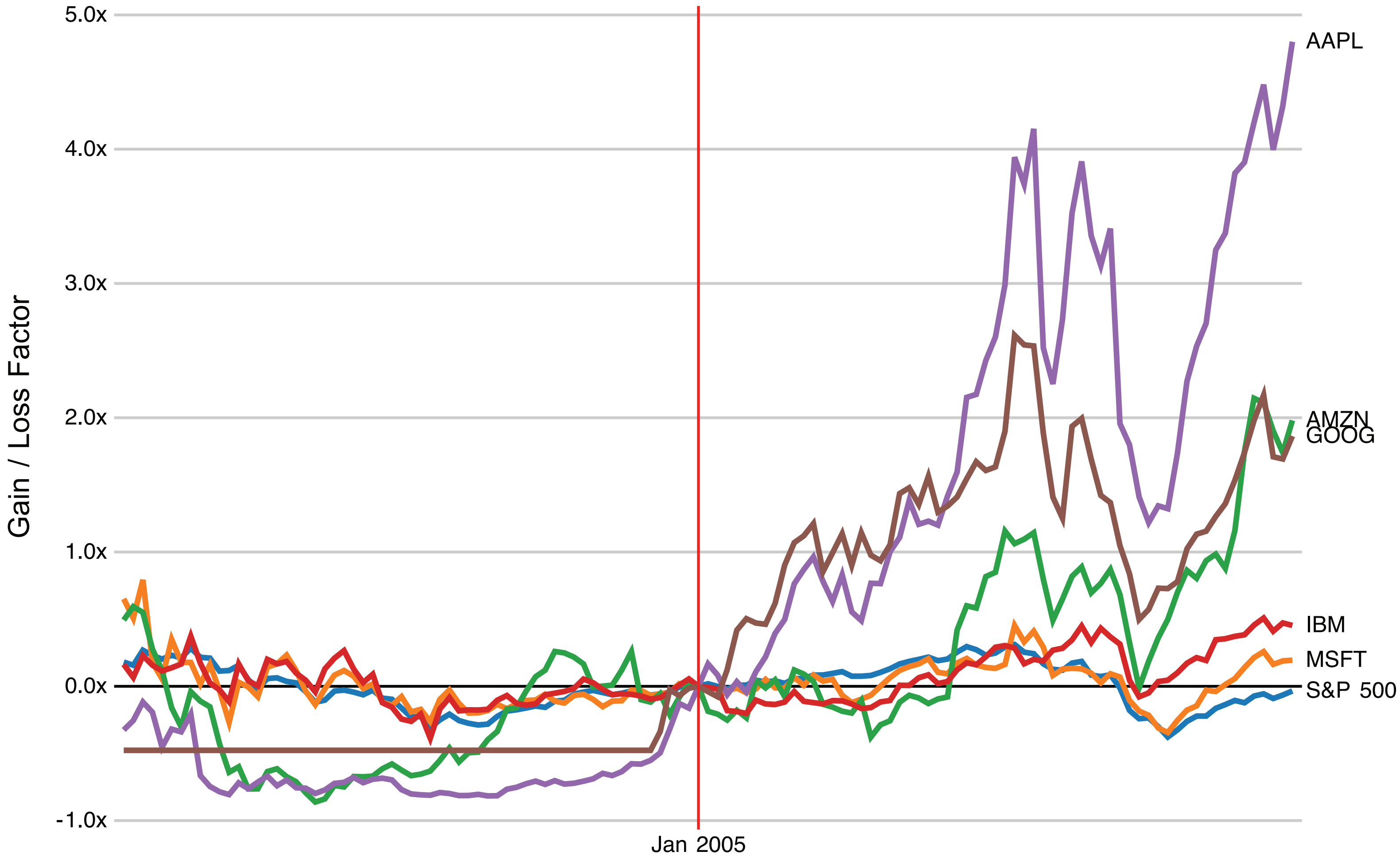
  - For instance, spatial position leads to most accurate coding of numeric data
- Making good visualizations requires a number of iterations

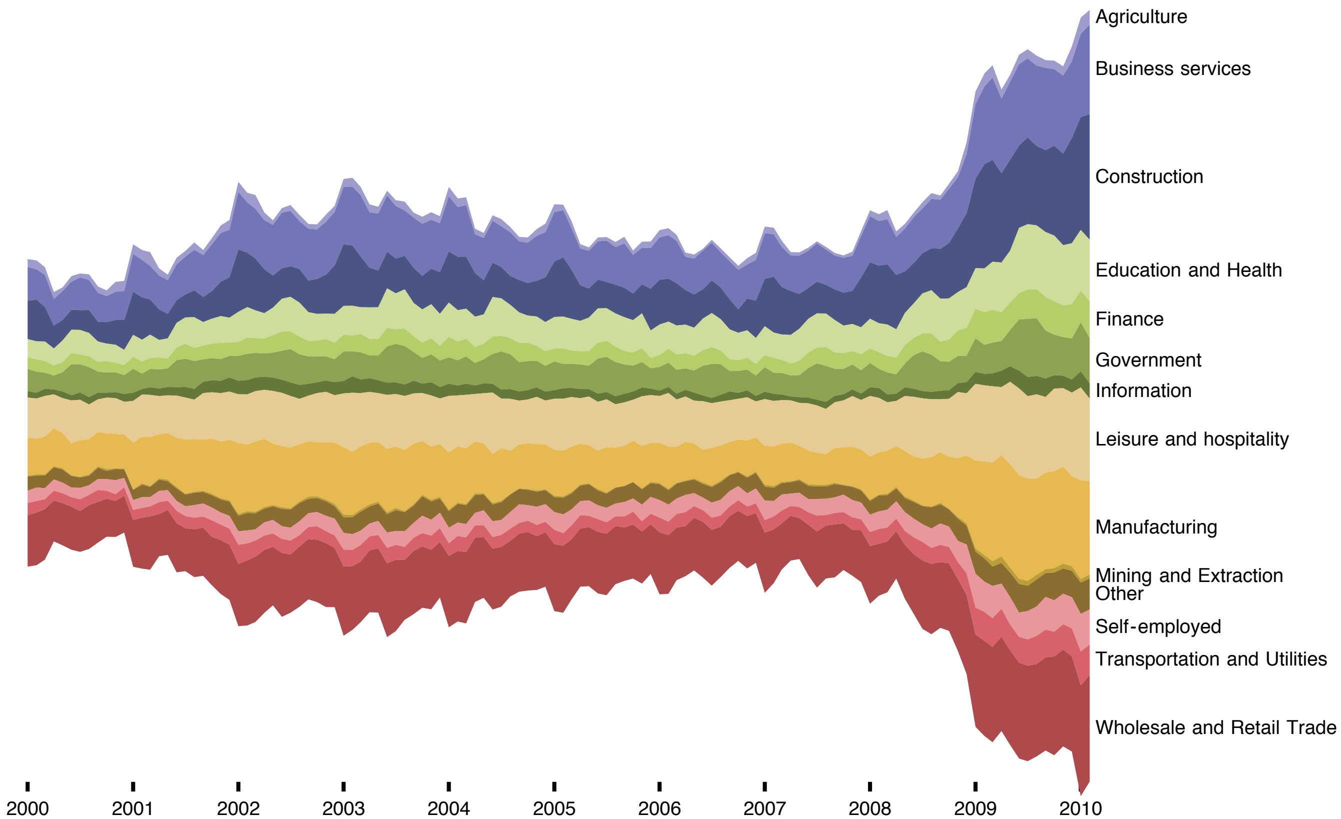
Time series: Index chart

- Displays *relative changes* instead of actual values:



Time series: Stacked graph

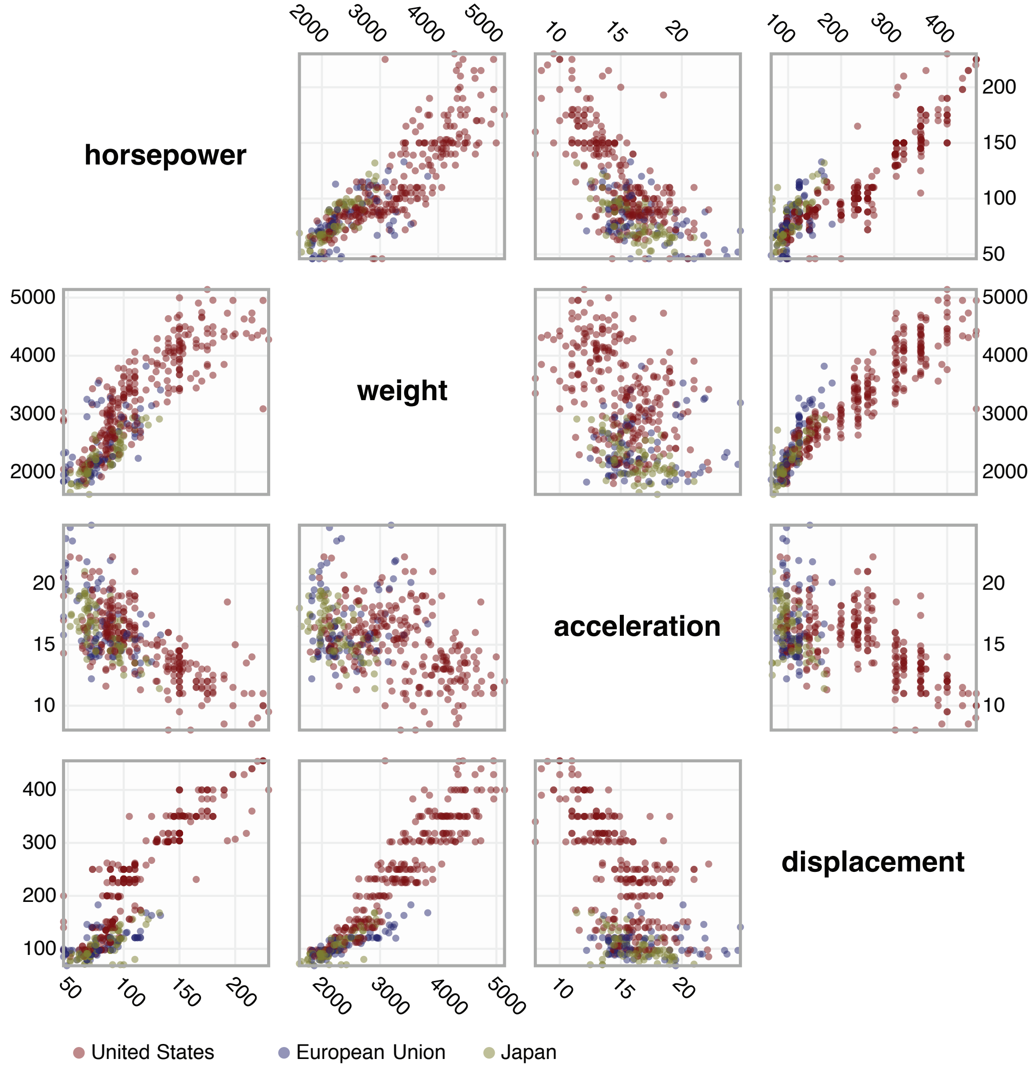
- Shows data in *aggregate*, highlighting *relative changes* in variables:



- Cannot show negative values; hard to interpret trends on top of other curves

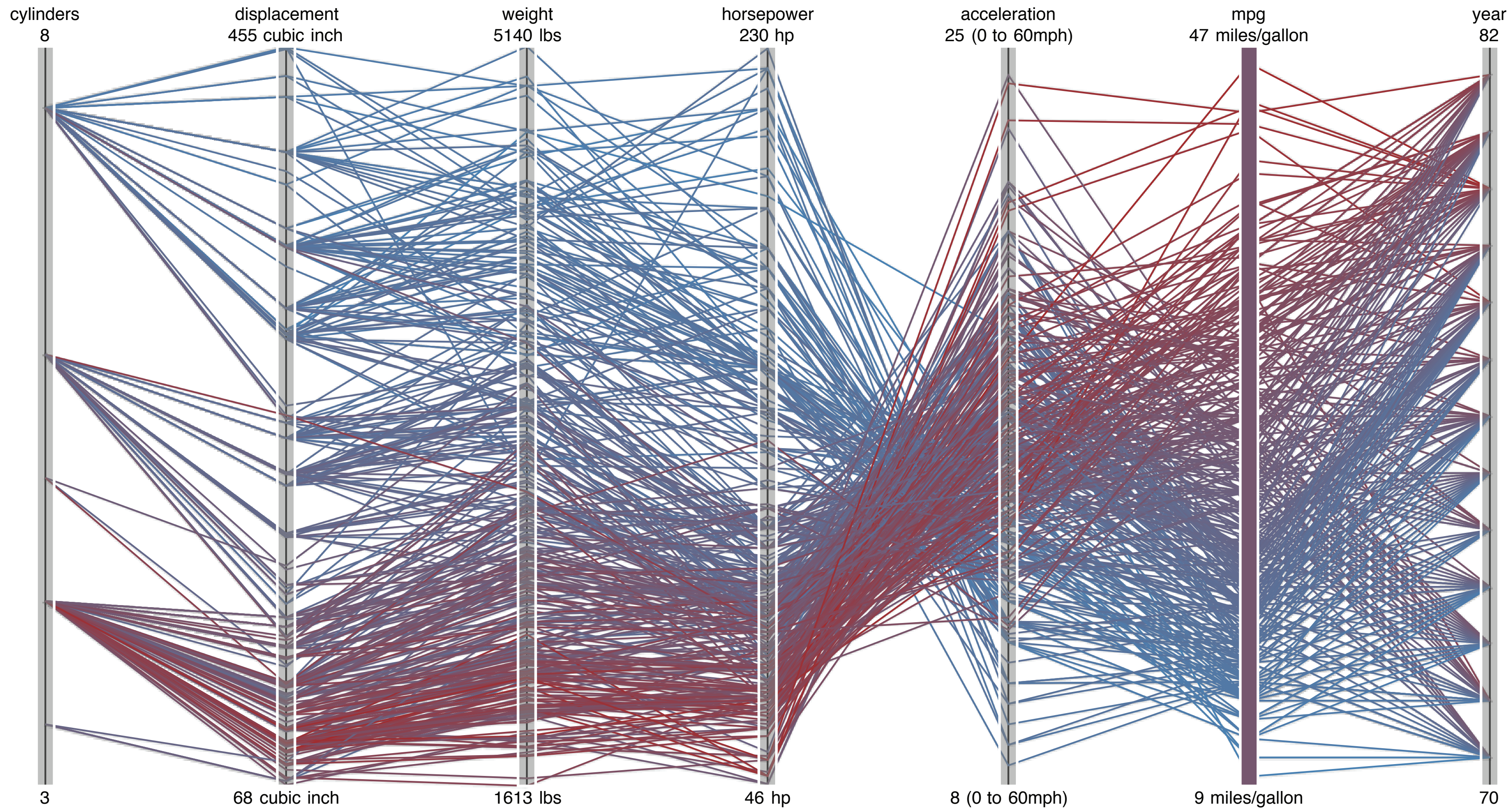
Real-valued data: Scatter plot matrix

- Allows one to quickly spot correlations (if number of variables limited):



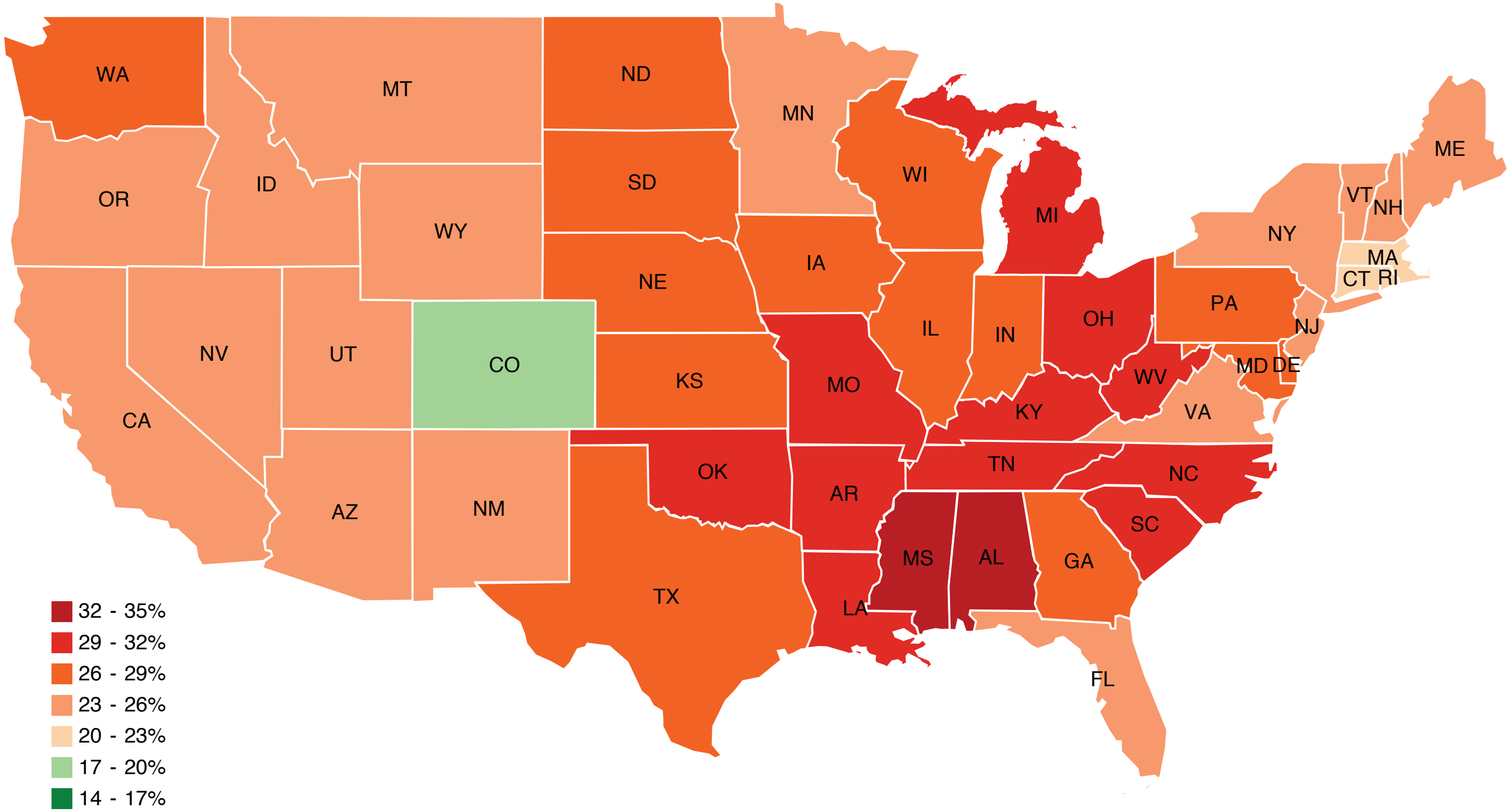
Real-valued data: Parallel coordinates

- Each vertical line corresponds to a variable:



Geographical data: Chloropleth map

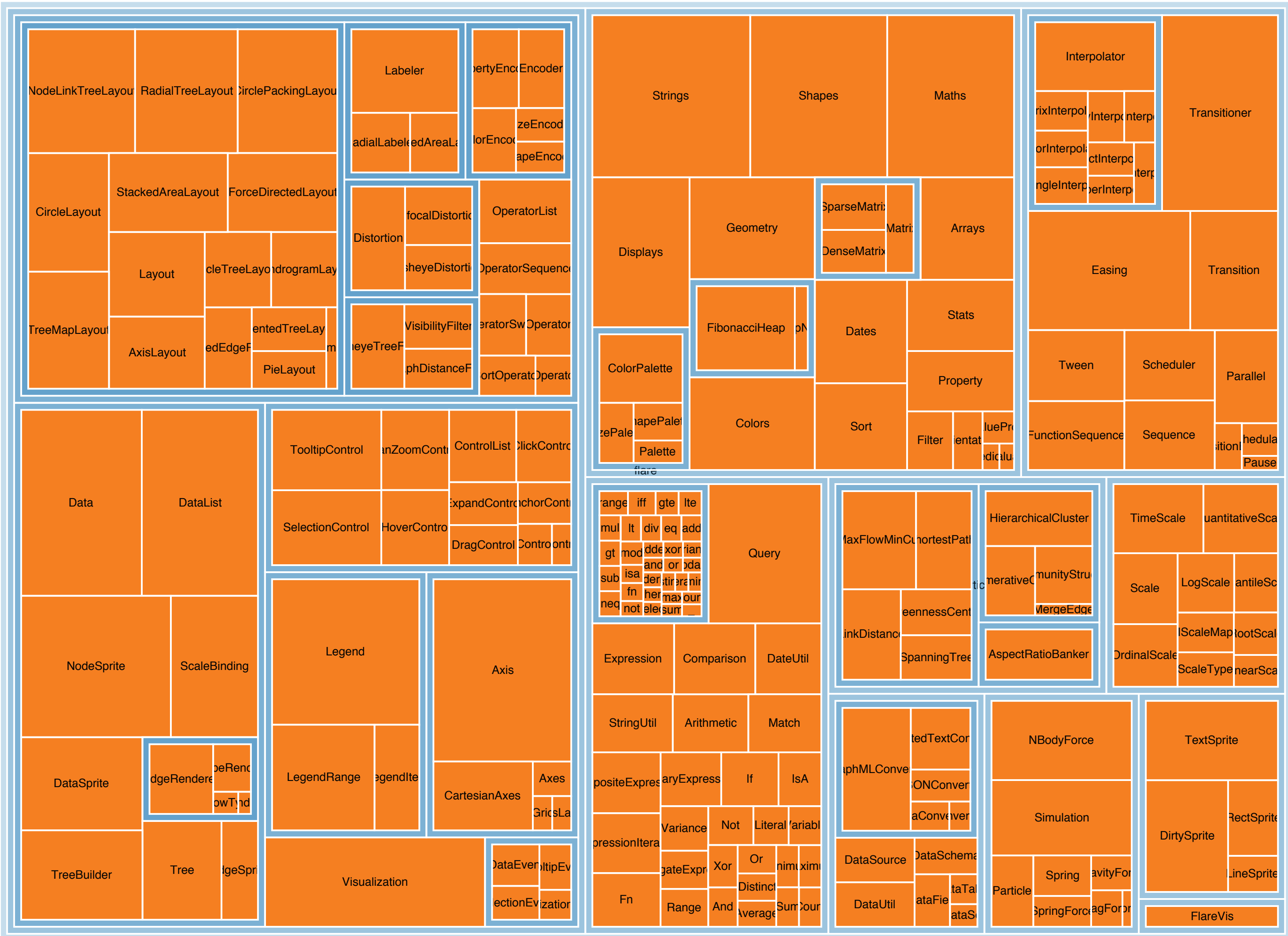
- Visualizes data aggregated by geographic region:



- Disadvantage: perception may be altered by area of geographic region

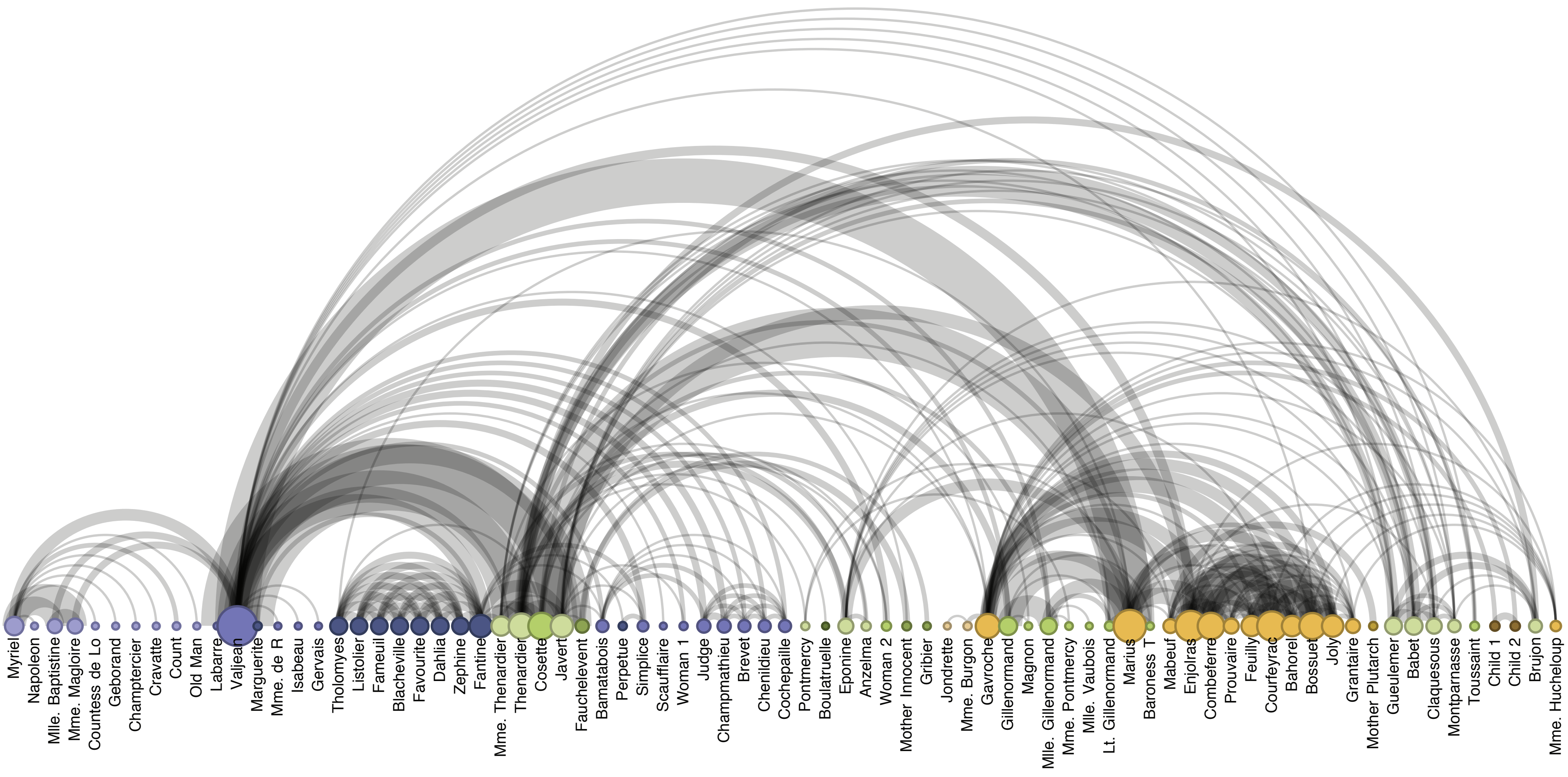
Hierarchies: Treemap / Enclosure diagram

- Effective way to visualize tree with a single variable at each node:



Networks: Arc diagram

- Easy to verify cliques and bridges, but has seriation problem:



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- A plethora of visualization tools / frameworks exist, for instance:
  - d3.js is a popular framework for building web-based visualization
  - VTK is commonly used for 3D and scientific visualization
  - Tools like Matlab, R, Mathematica, and SPSS also provide various visualization tools
  - SynerScope is a Dutch visual-analytics product you will hear more about soon

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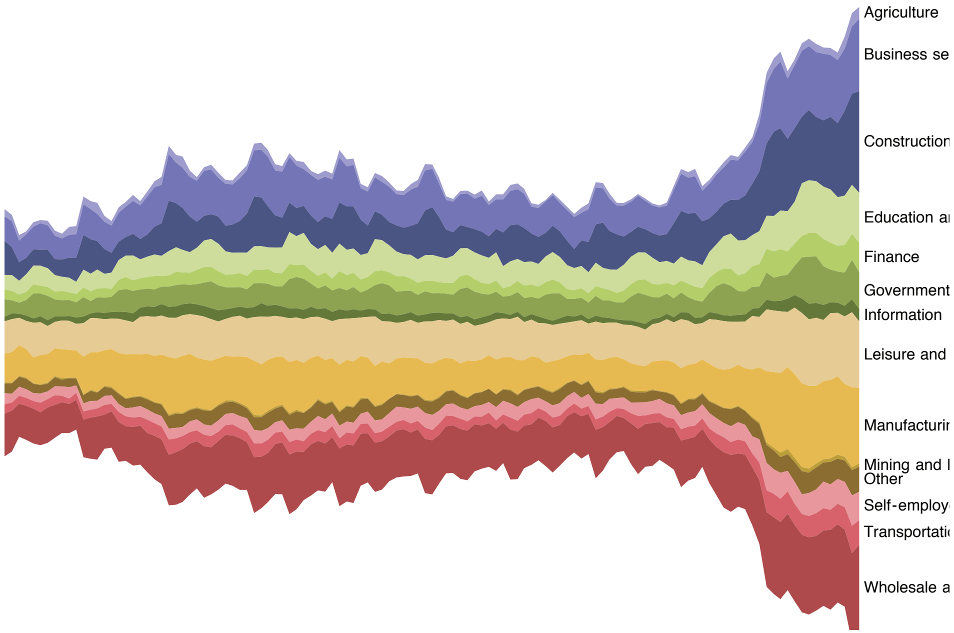

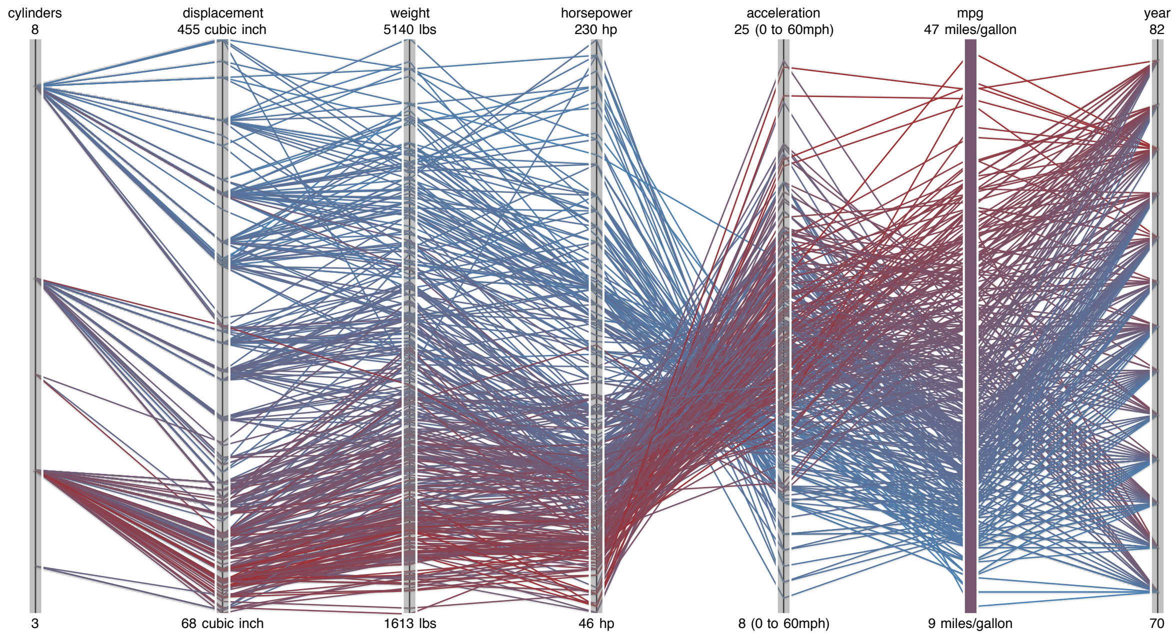

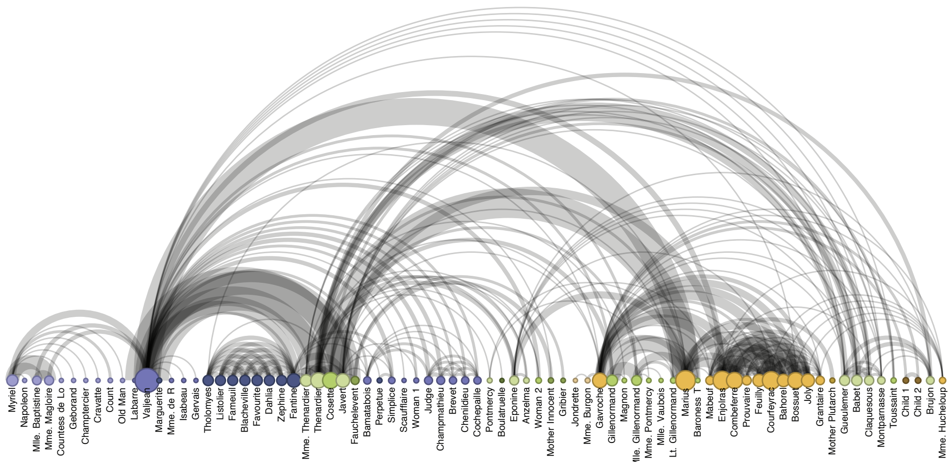

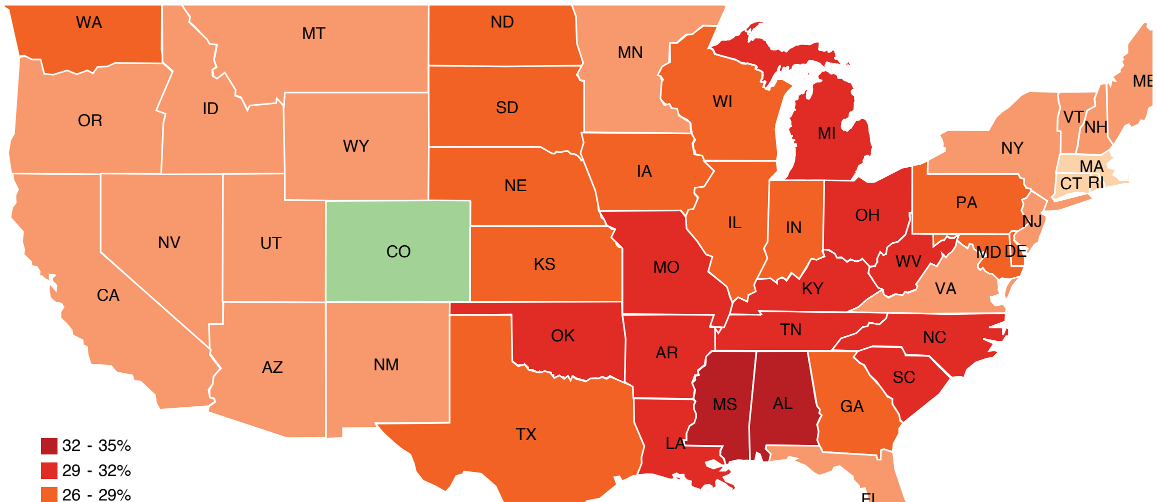

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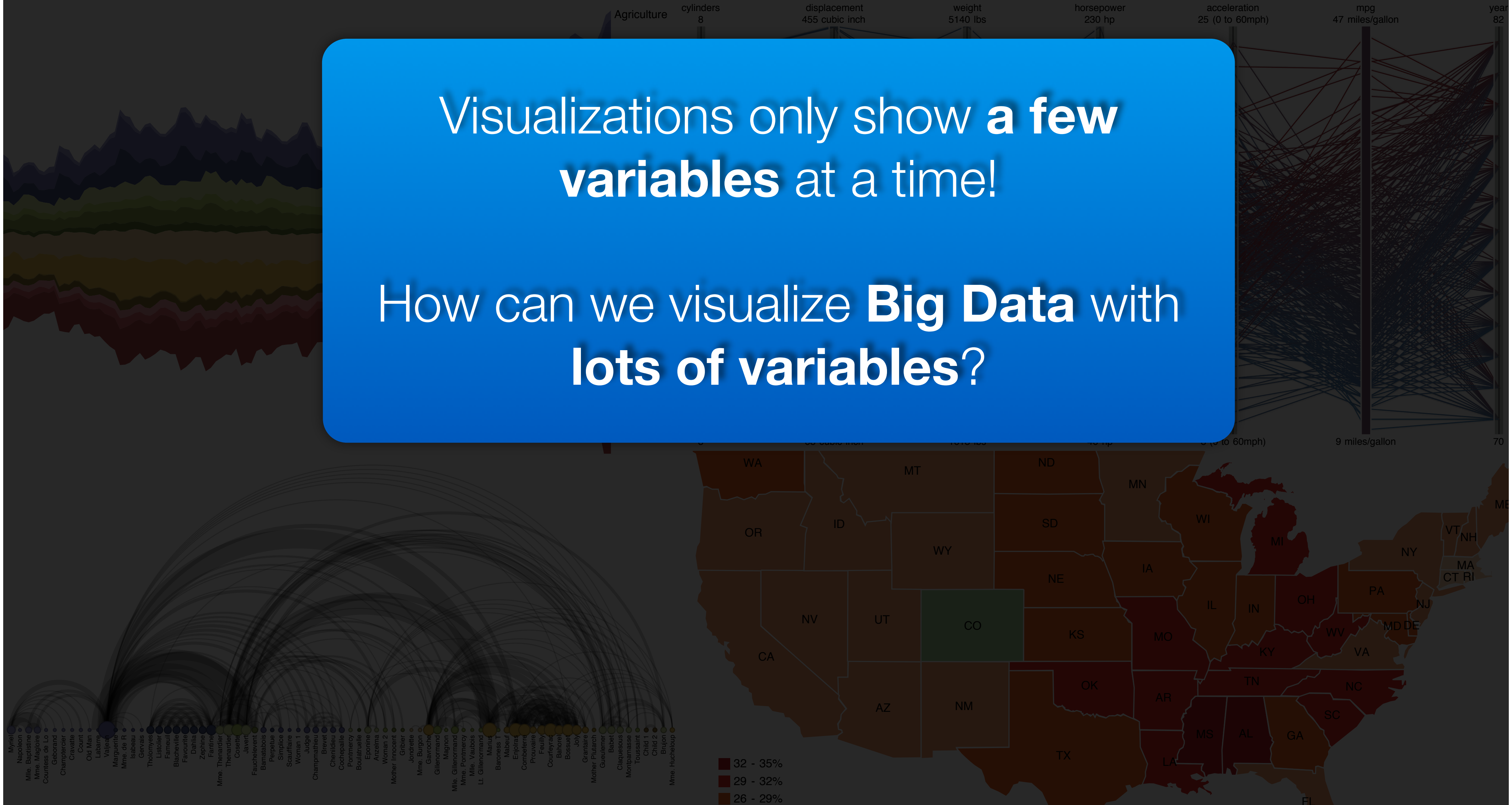

Visualizations only show **a few variables** at a time!

How can we visualize **Big Data** with **lots of variables**?

Visualizing data by constructing maps

Introduction

- Compute *dissimilarity* of all pairs of records in the database:

Ams	800	1	1	0
Rot	700	3	0	1
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- Exact way in which dissimilarities are computed depends on problem at hand

Introduction

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How to build a map from a distance matrix?

Principal components analysis

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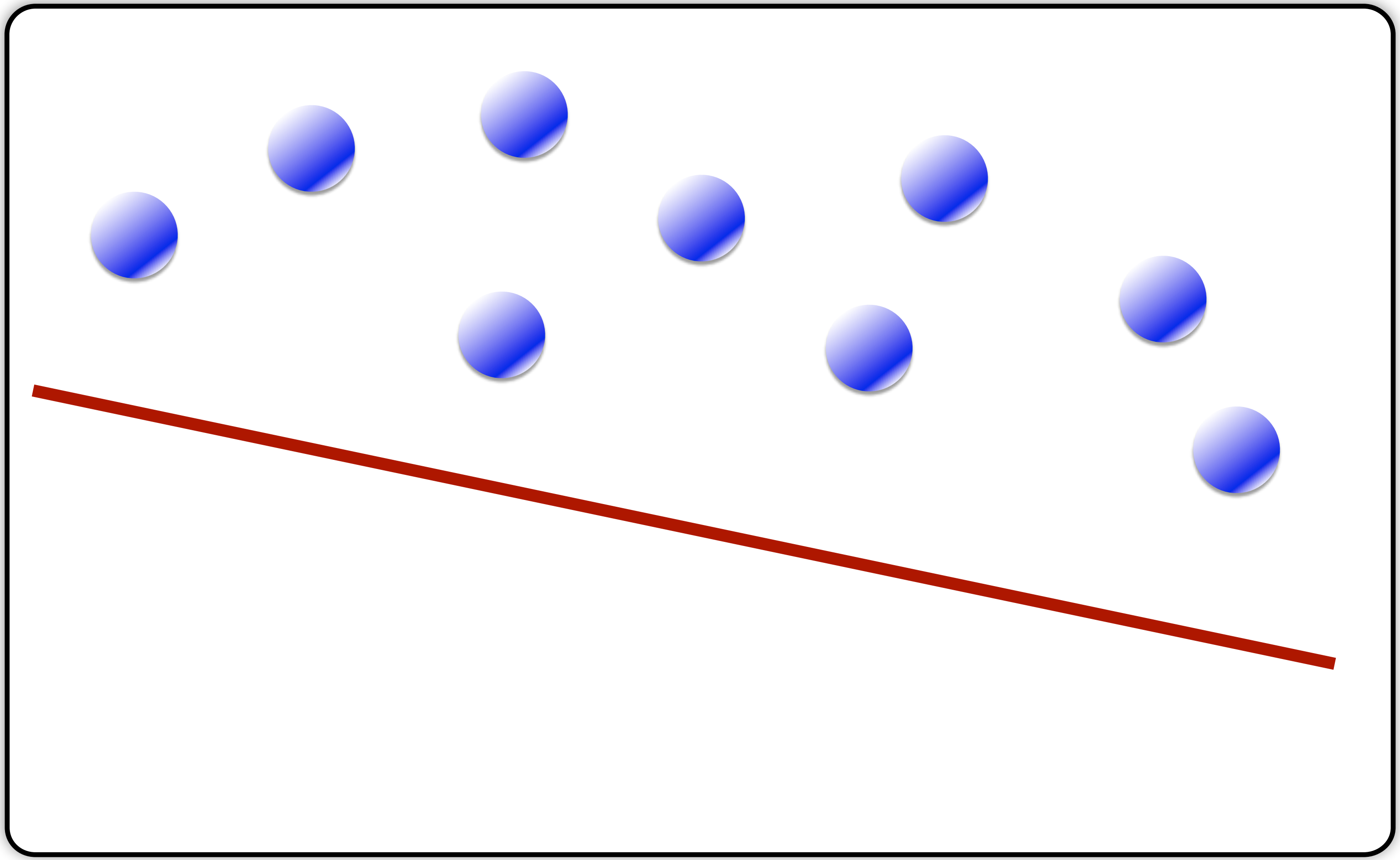

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Principal components analysis

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- Enforce constraint using *Lagrange multiplier*:

$$\max_{\|\mathbf{w}\|^2=1} var(\mathbf{w}^T\mathbf{X}) = \max_{\mathbf{w},\lambda} \mathbf{w}^T\mathbf{C}\mathbf{w} - \lambda(1 - \mathbf{w}^T\mathbf{w})$$

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- Set gradient with respect to $\mathbf{w}$ to zero: $\mathbf{C}\mathbf{w} - \lambda\mathbf{w} = 0$

$$\mathbf{C}\mathbf{w} = \lambda\mathbf{w}$$

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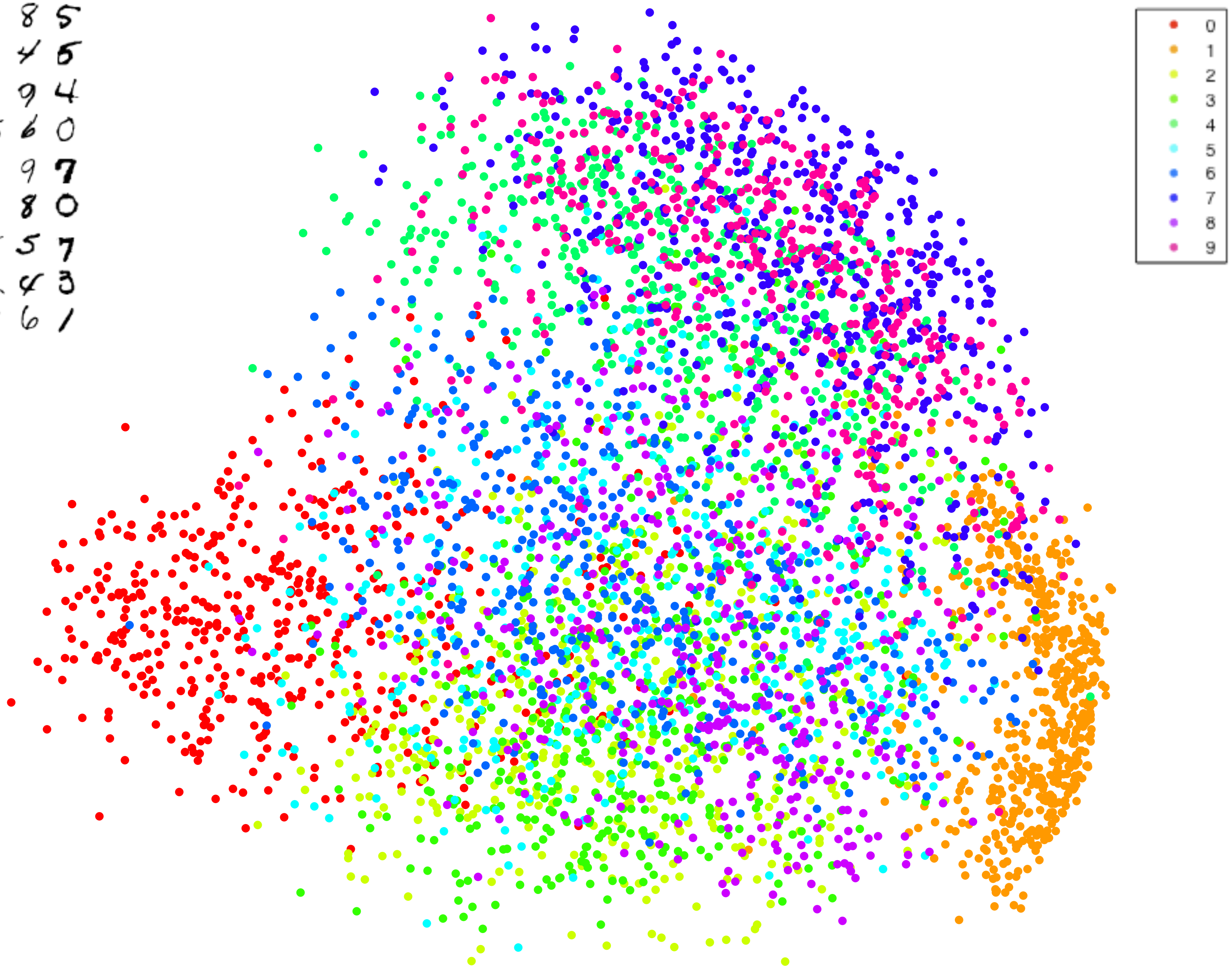
  - Compute the principal eigenvectors of the resulting matrix
- These eigenvectors are identical to the projected data computed by PCA:
  - Identity is due to a relation between eigenvectors of inner and outer products

Principal components analysis



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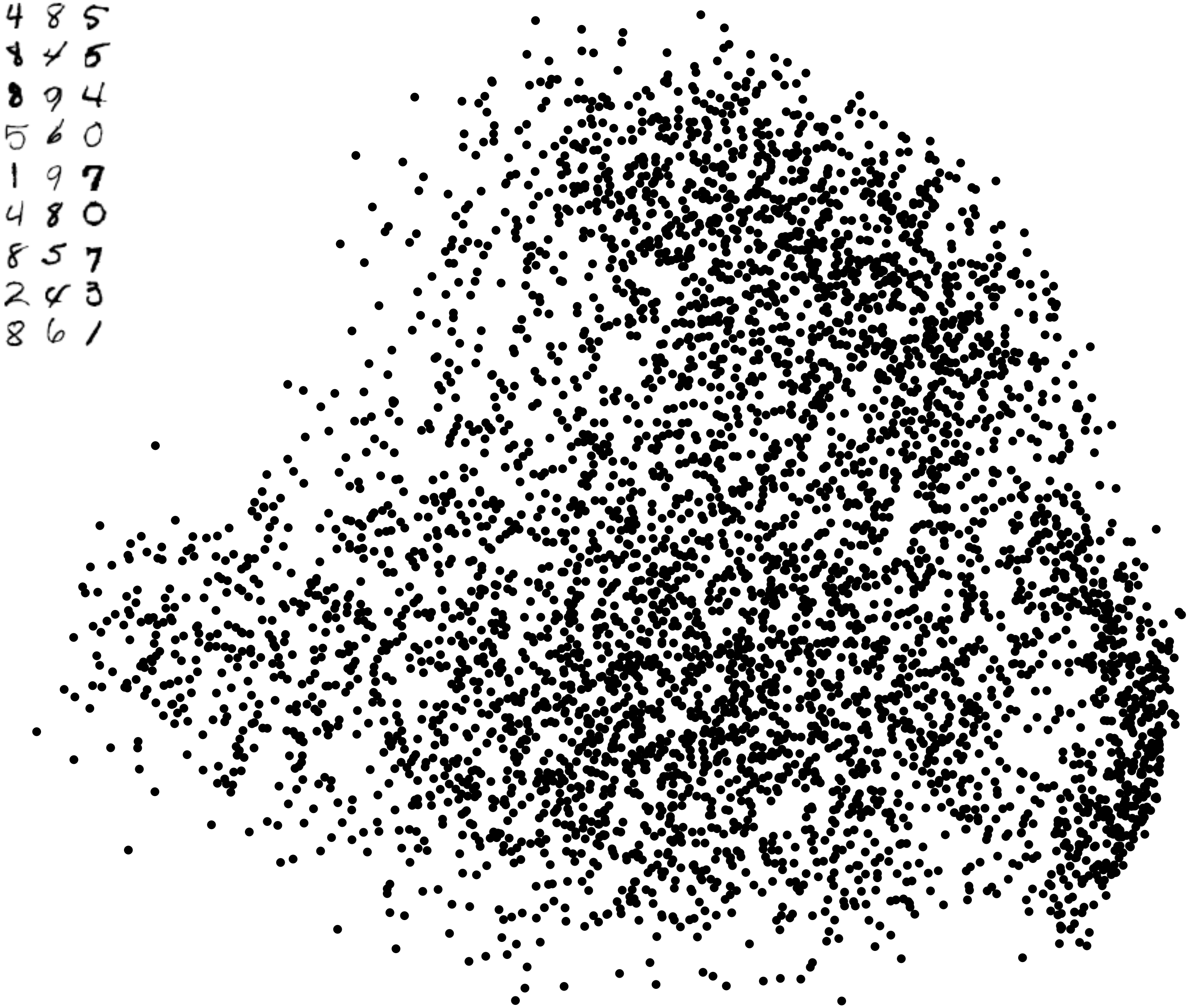

What distances to preserve?

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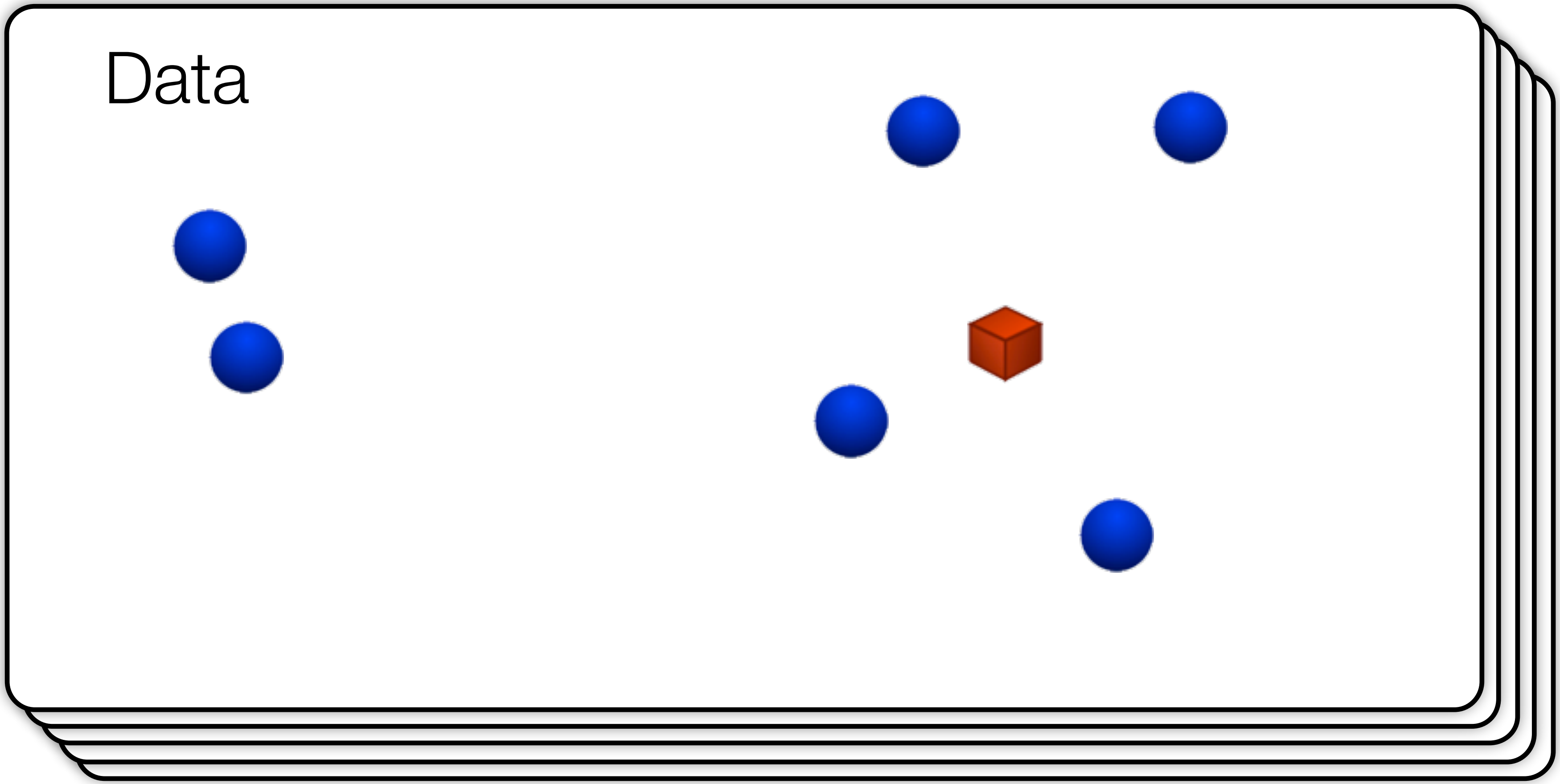
- Large pairwise distances, however, are relatively unimportant in visualizations
    - Do we really care exactly how dissimilar zeros and ones are?

t-Distributed Stochastic Neighbor Embedding

- Compute "local" pairwise similarities based on pairwise distances:



$$p_{ij} = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma^2)}{\sum_k \sum_{l \neq k} \exp(-\|\mathbf{x}_k - \mathbf{x}_l\|^2/2\sigma^2)}$$

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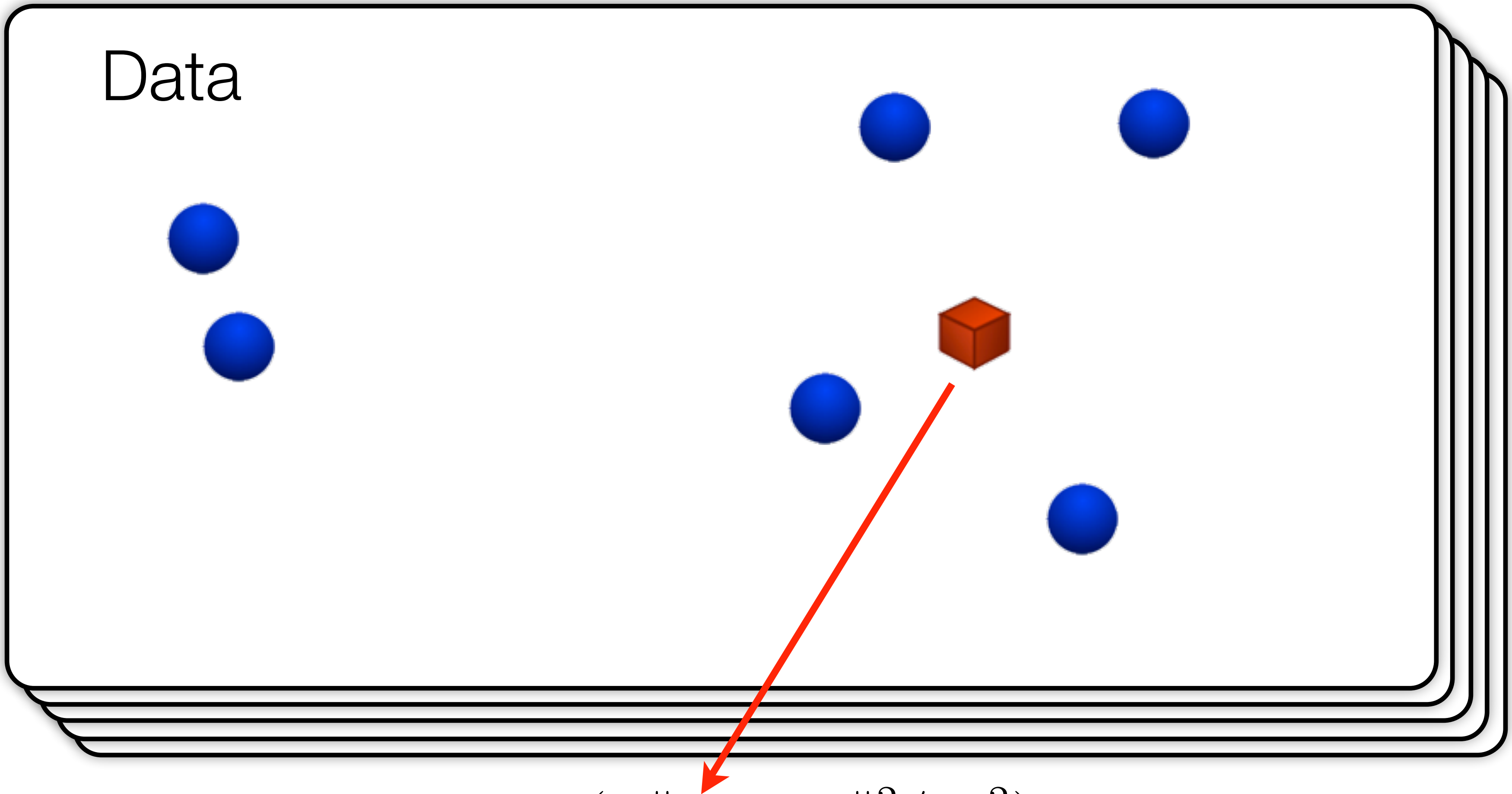

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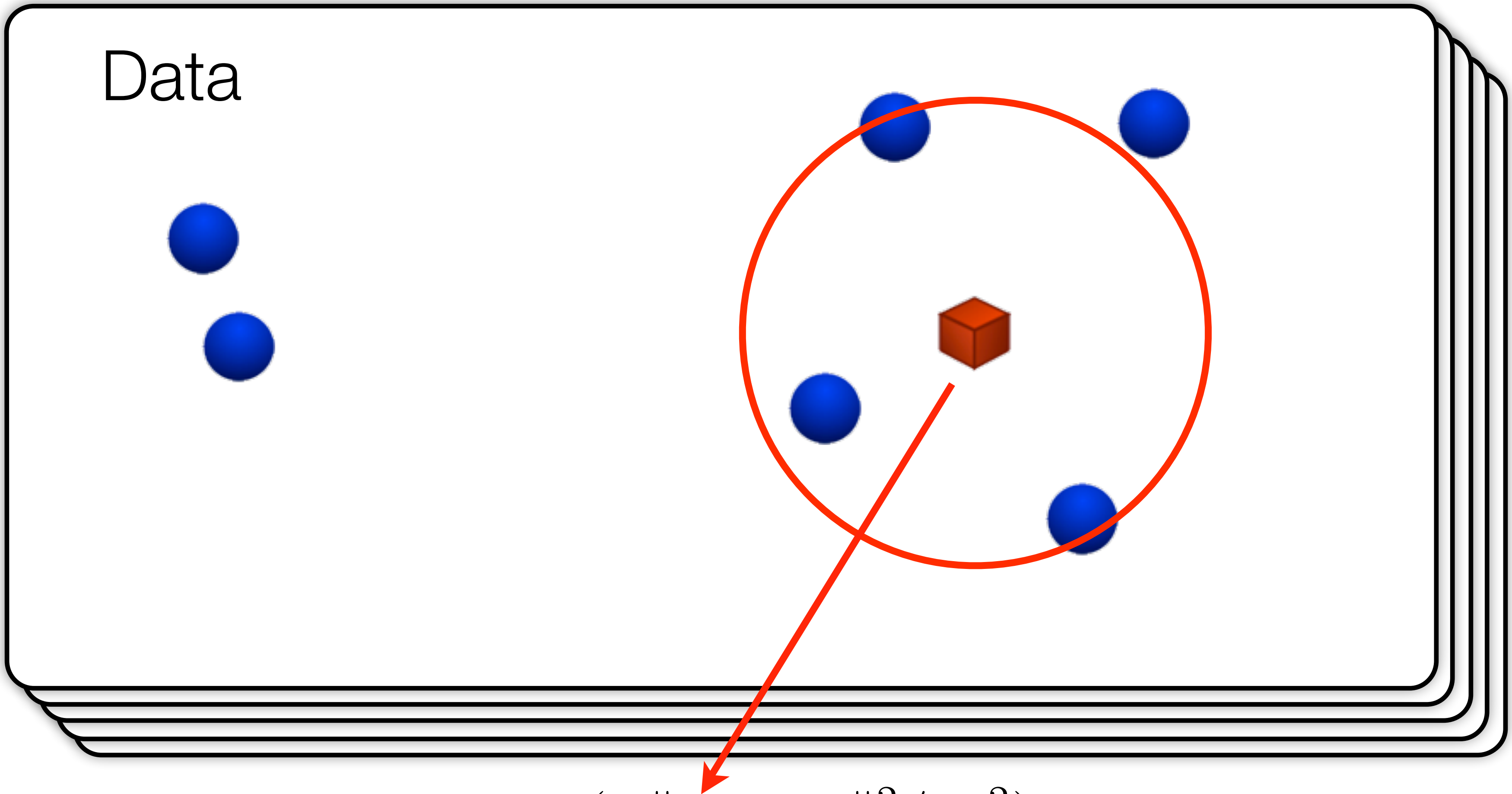

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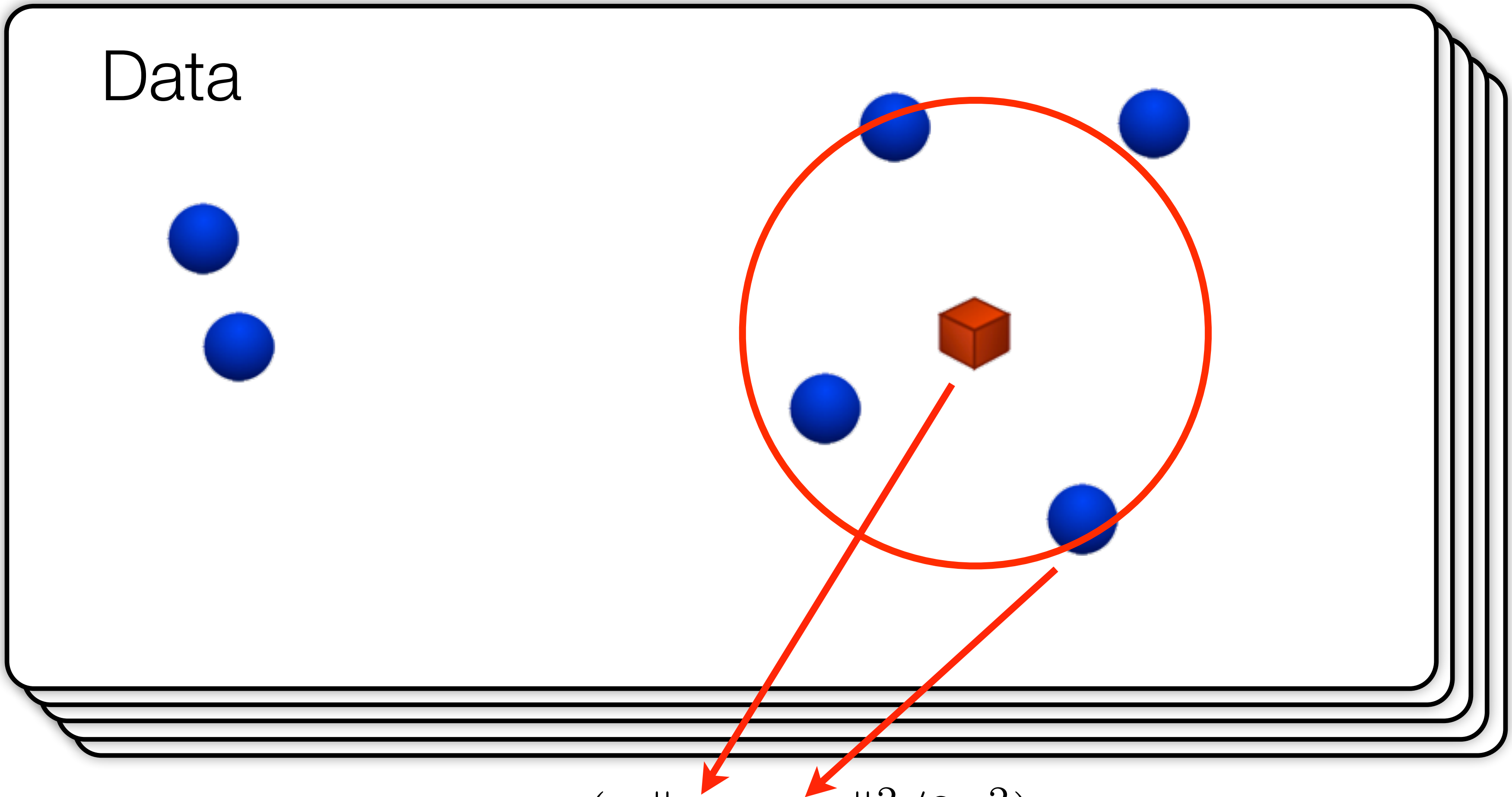

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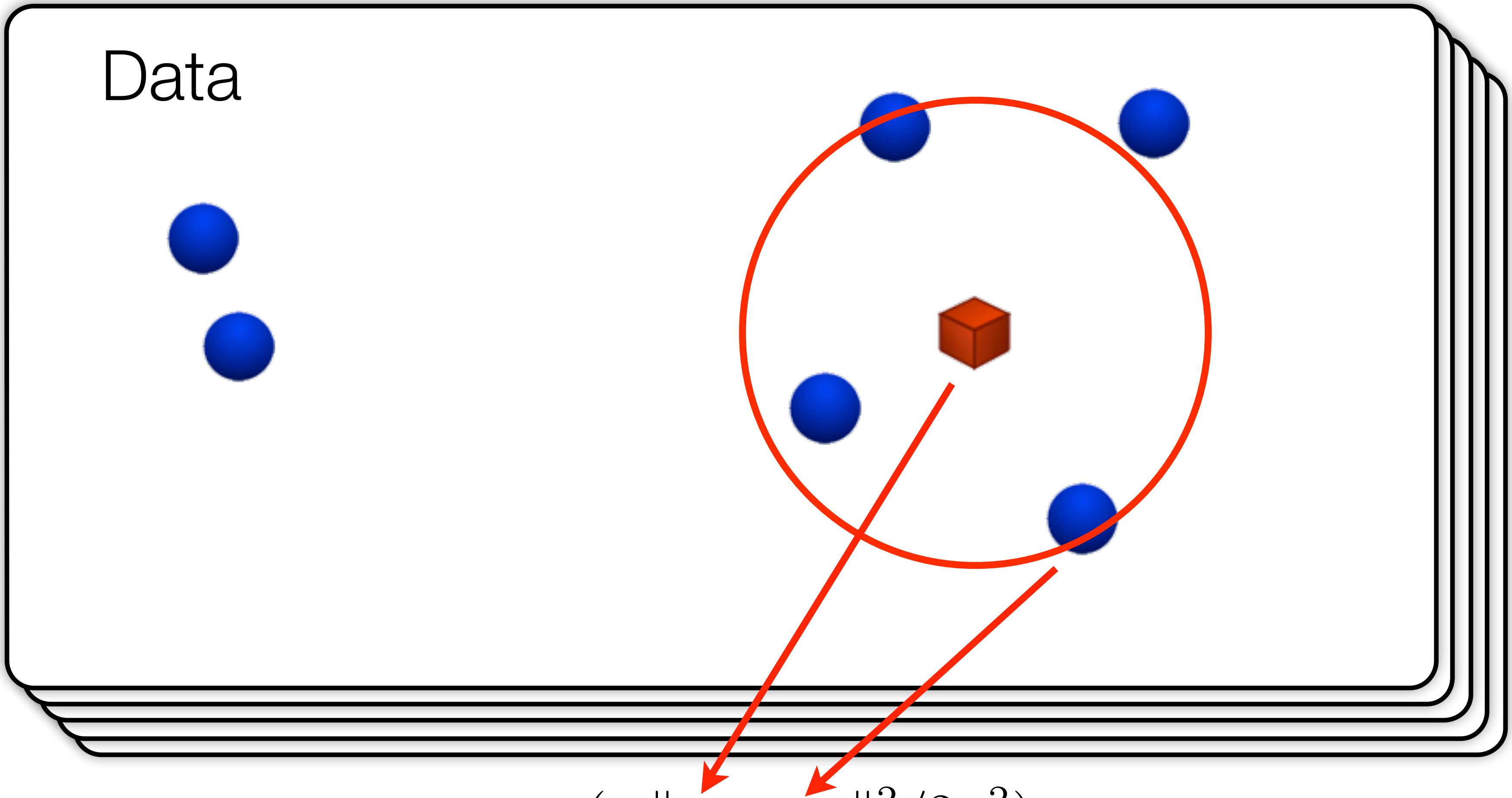

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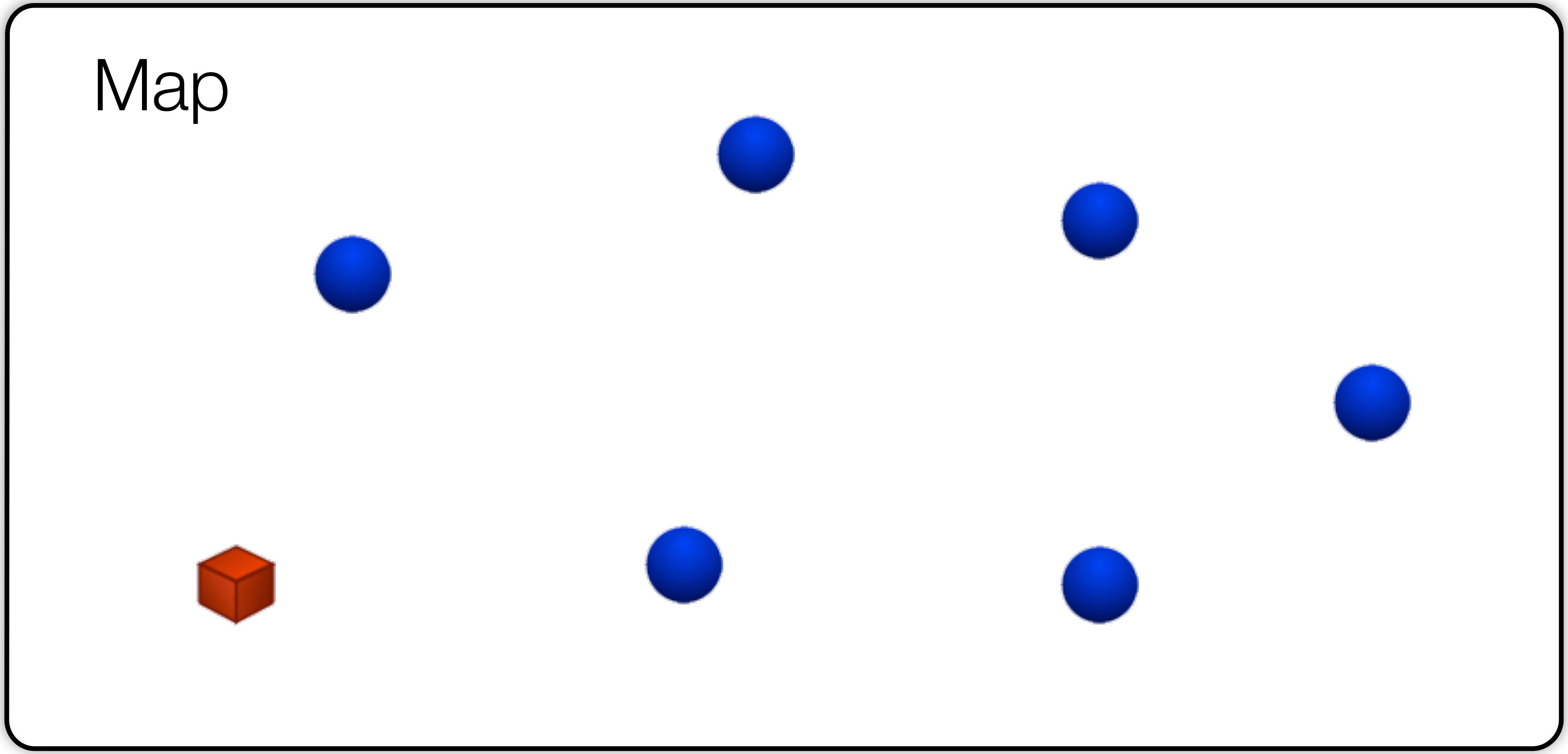
- Measure pairwise similarities between corresponding points in the map:



$$q_{ij} = \frac{(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}}{\sum_k \sum_{l \neq k} (1 + \|\mathbf{y}_k - \mathbf{y}_l\|^2)^{-1}}$$

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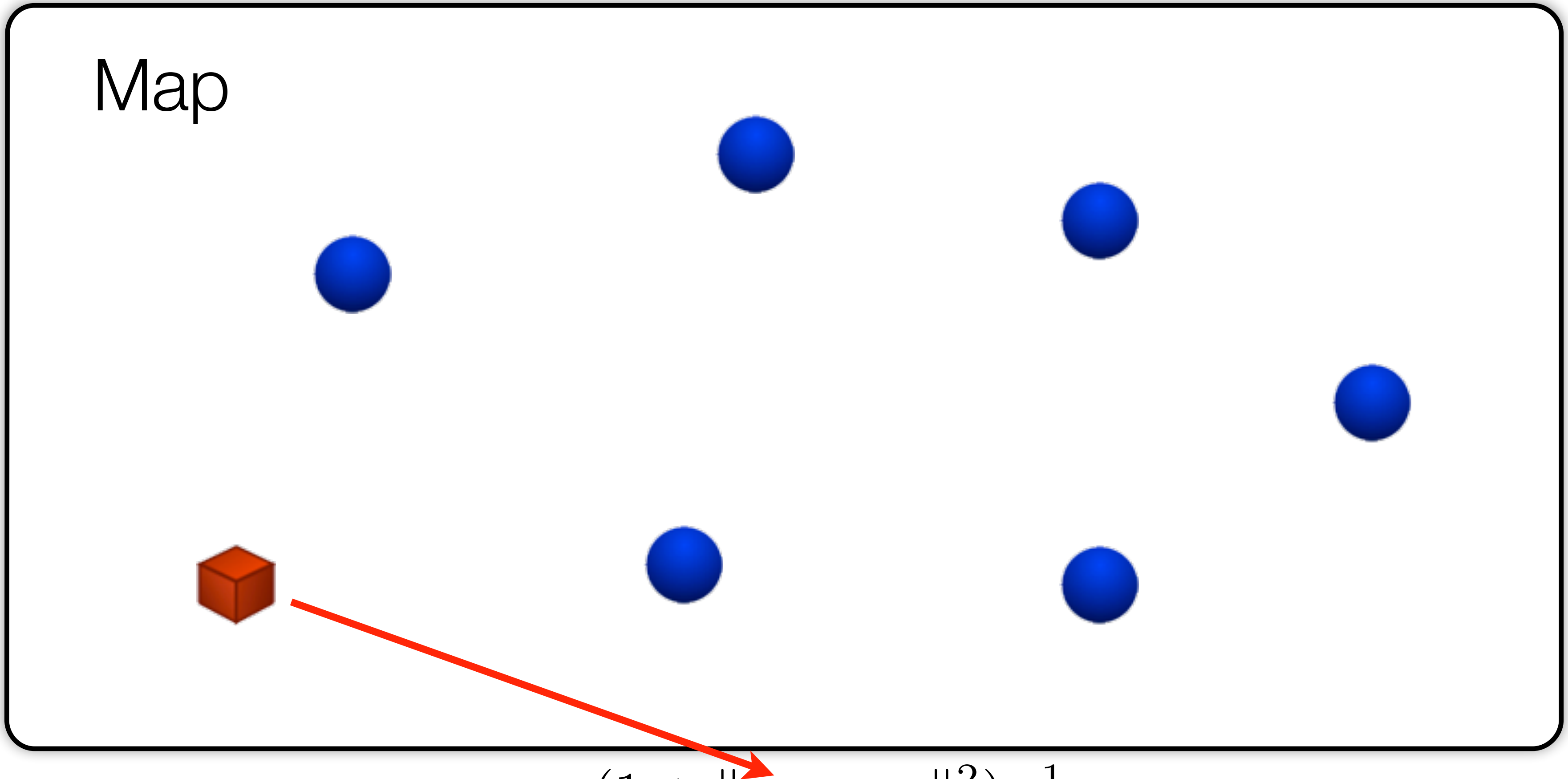

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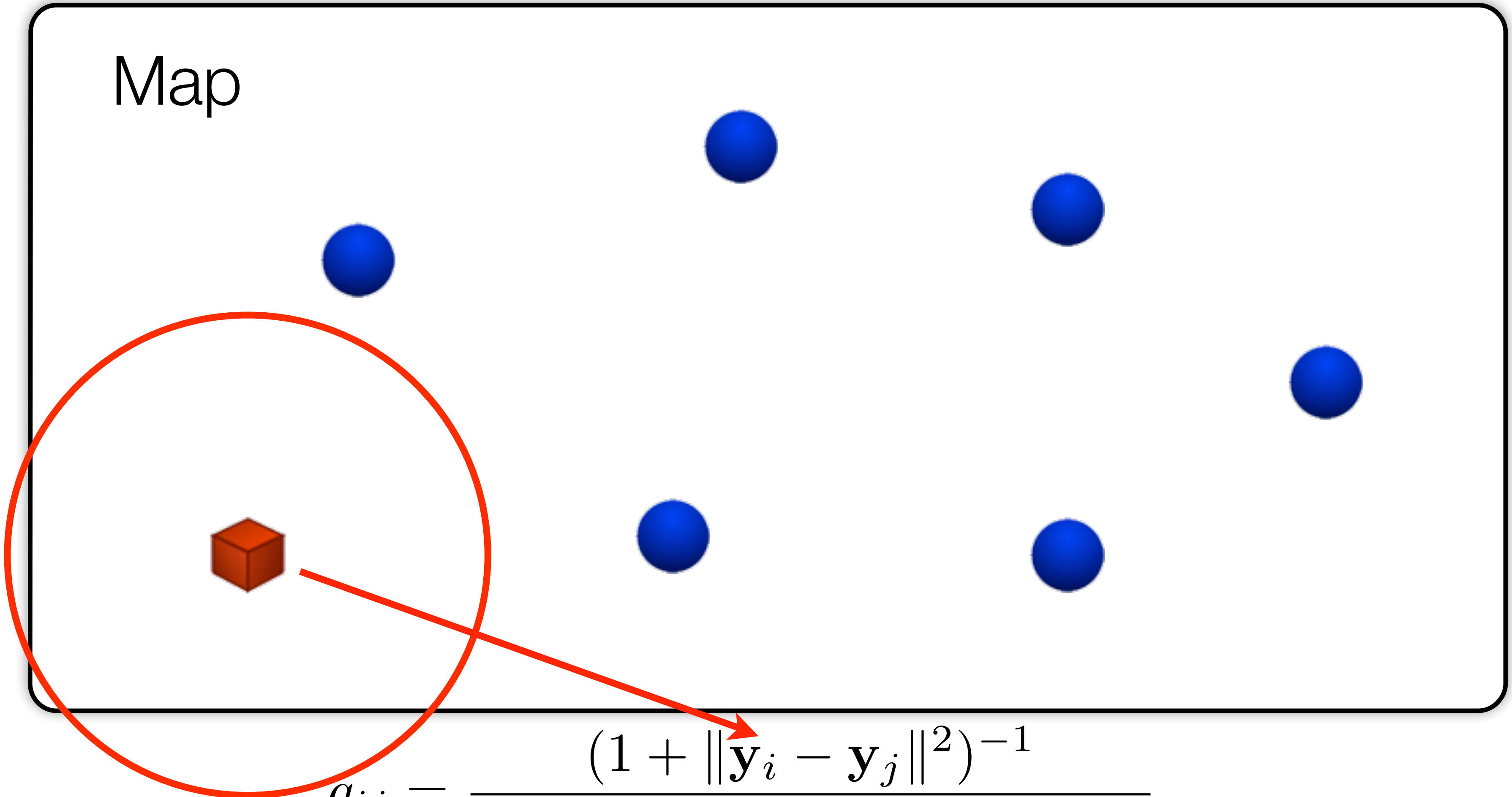

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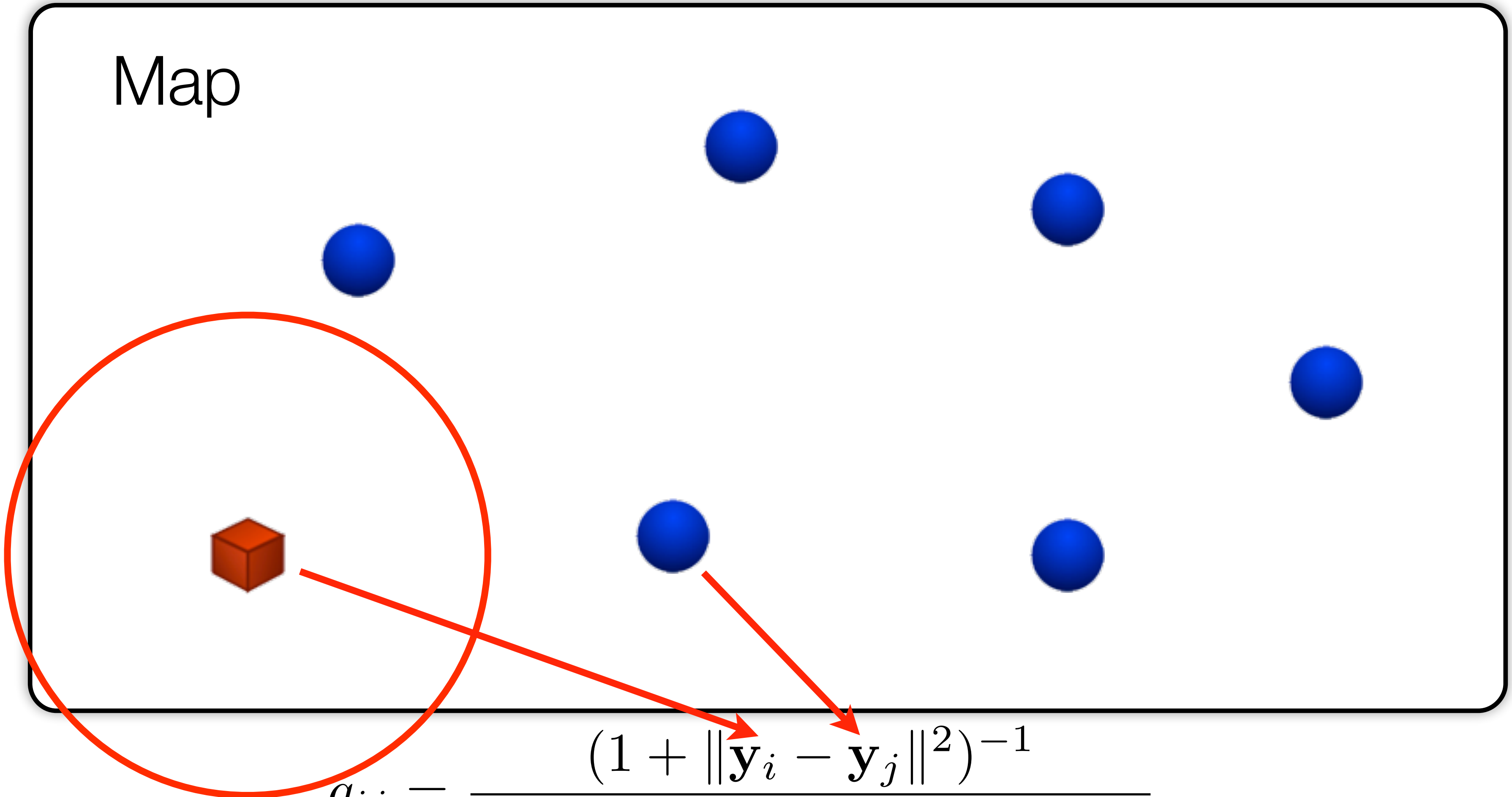

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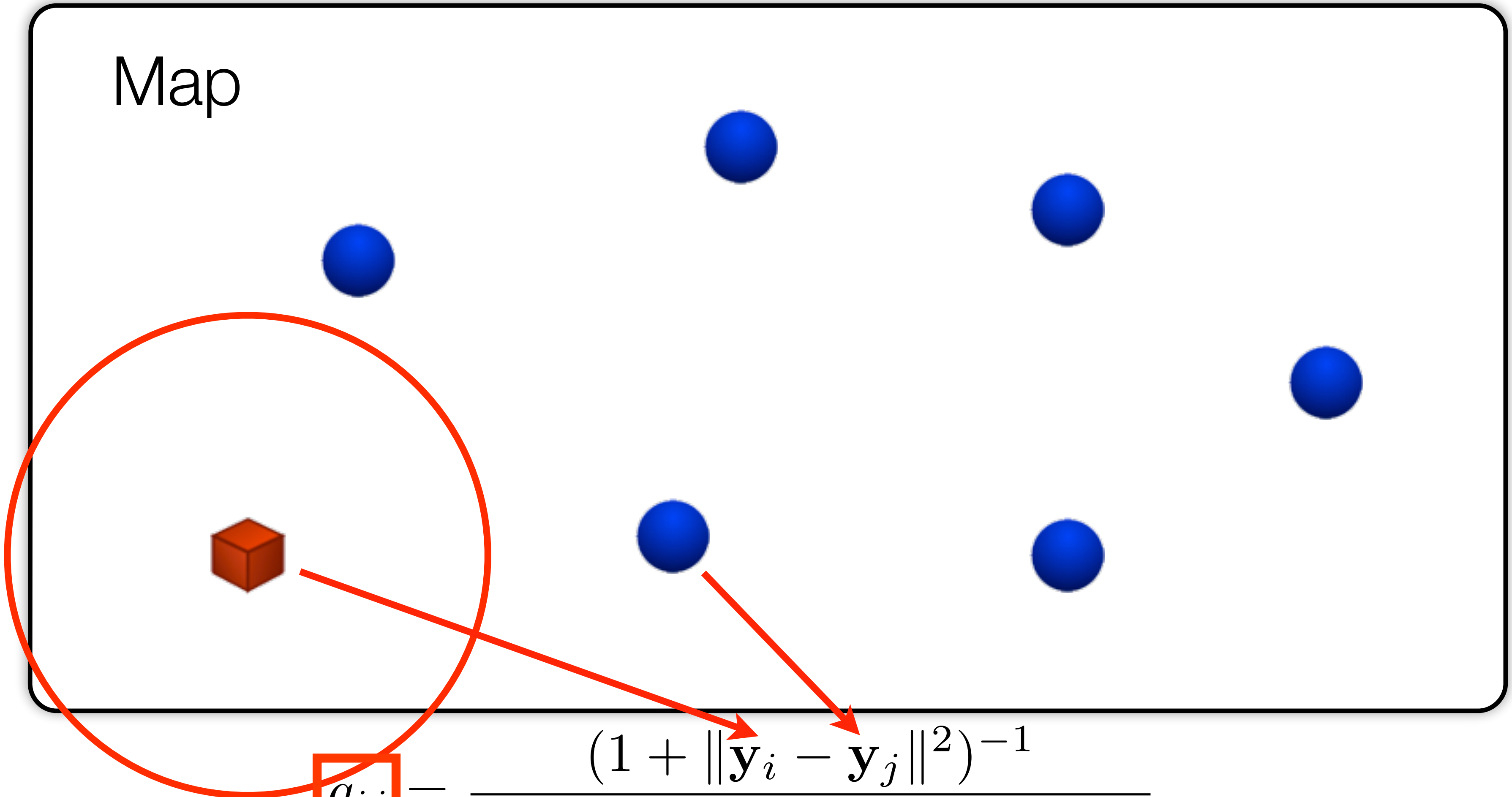

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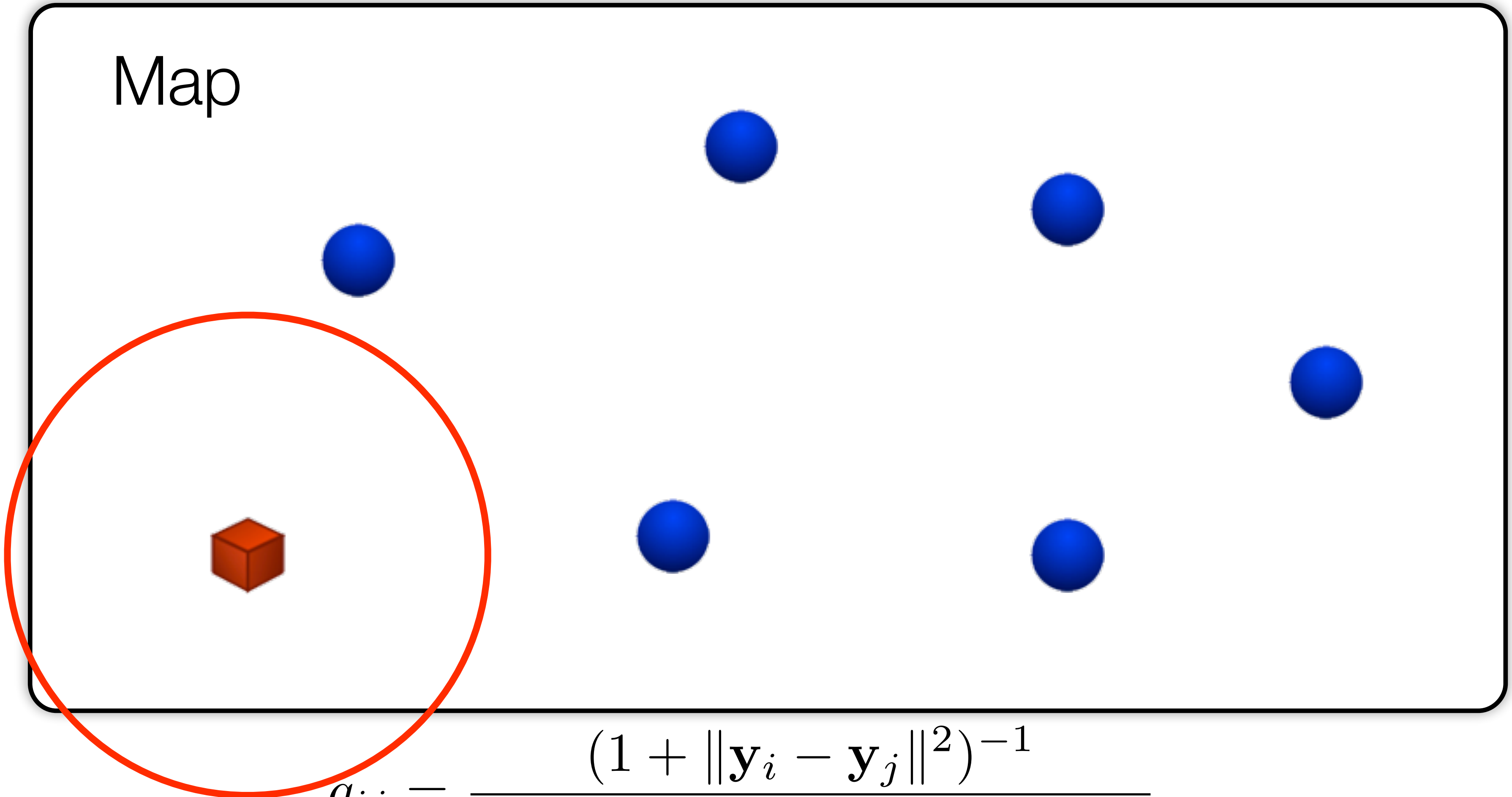
t-Distributed Stochastic Neighbor Embedding

- Move points around to minimize: $KL(P||Q) = \sum_i \sum_{j \neq i} p_{ij} \log \frac{p_{ij}}{q_{ij}}$



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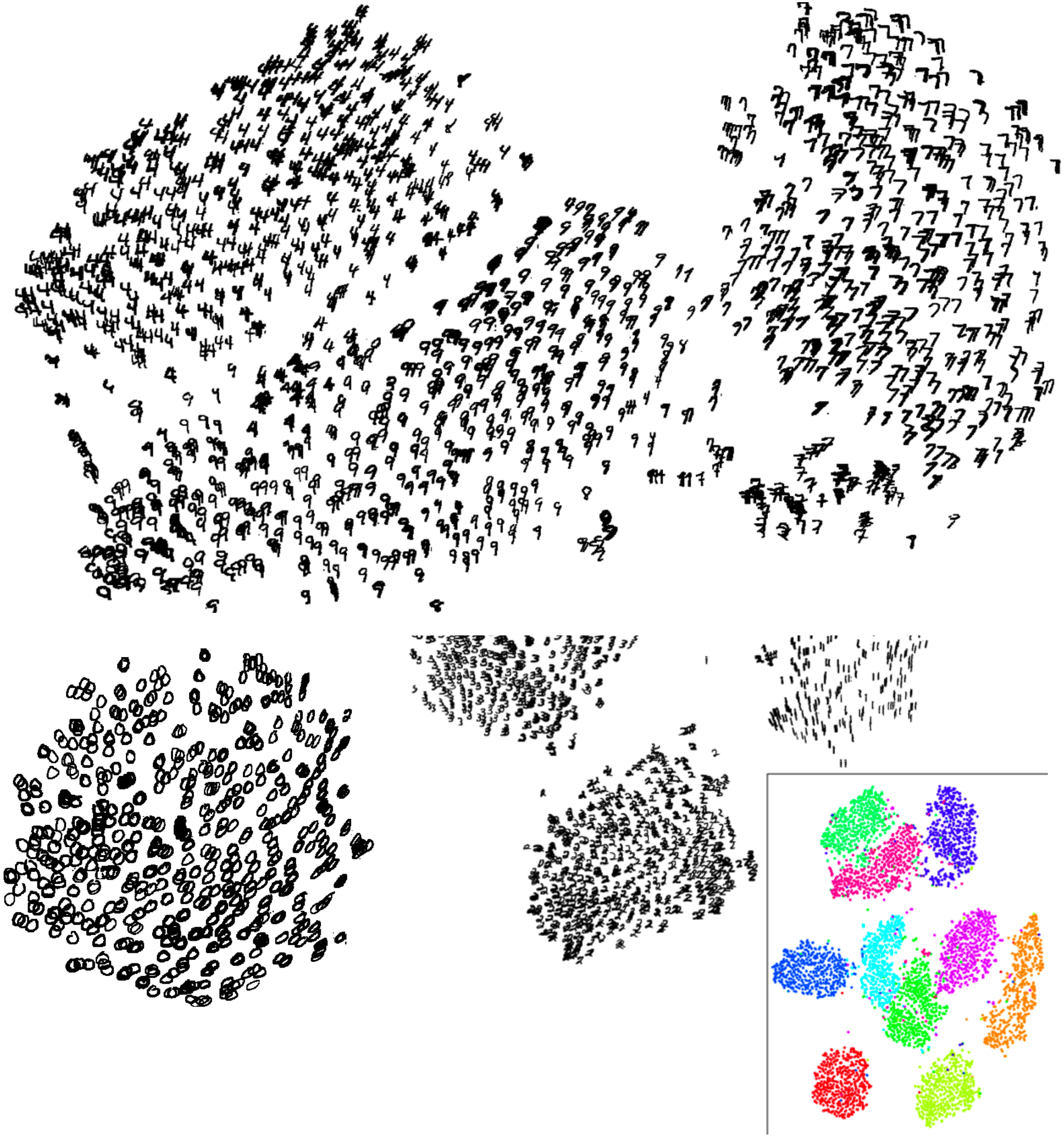
- Hence, t-SNE mainly preserves *local similarity structure* of the data


0
1
2
3
4
5
6
7
8
9



Why a Student-t distribution?

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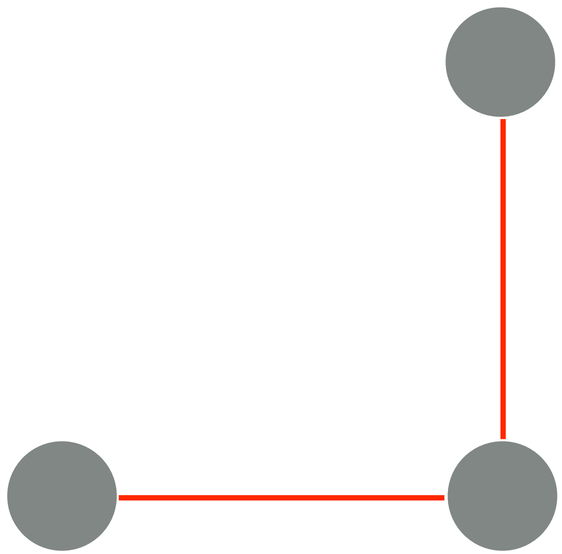
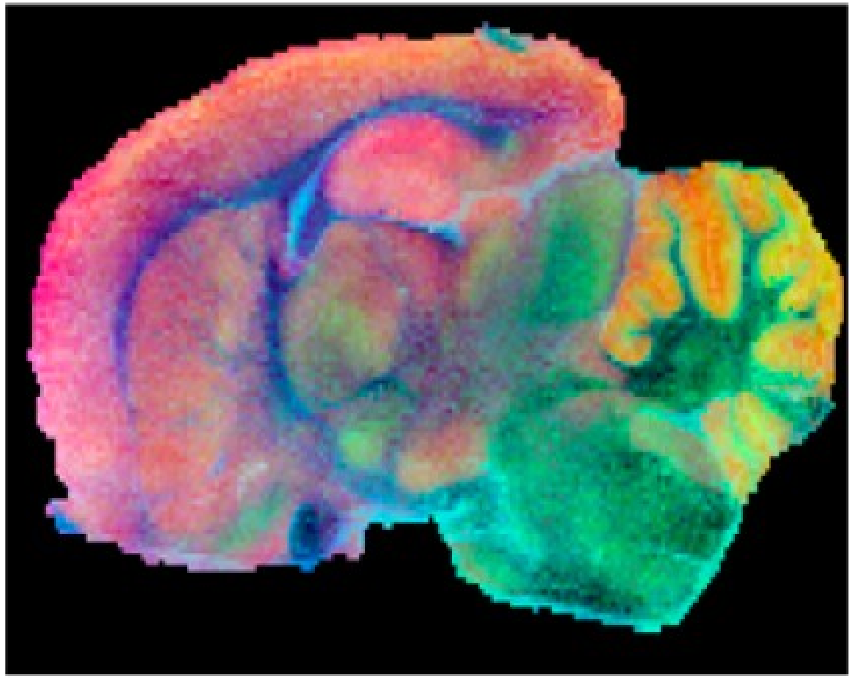
- Suppose data is *intrinsically* high-dimensional
- We try to model the *local structure* of this data in the map
- Result: dissimilar points have to be modeled as too far apart in the map!



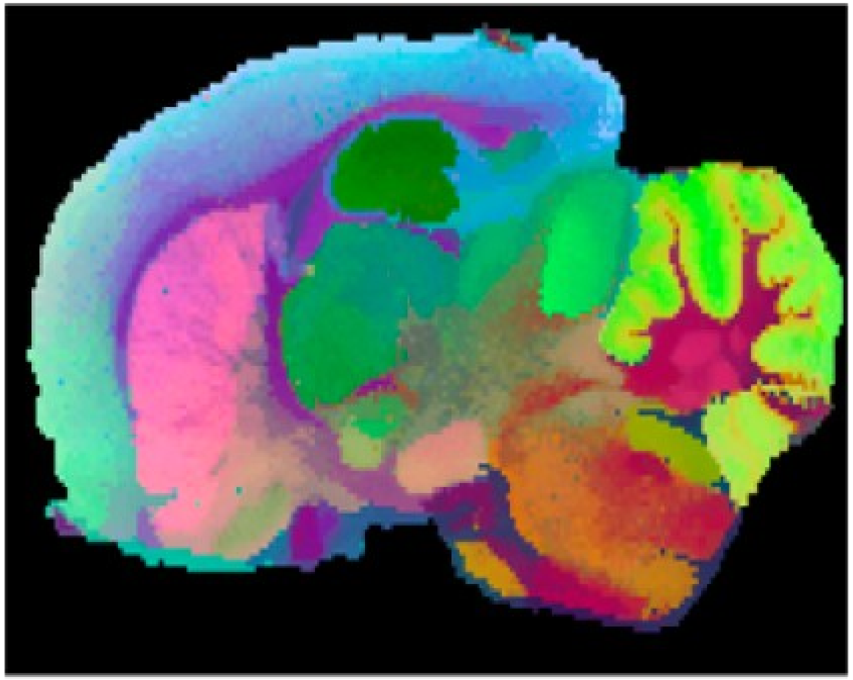
Visualizing mass spectrometry data

A mass spectrum is a plot of the ion signal as a function of the mass-to-charge ratio. It helps identify the amount and type of chemicals present in a sample.

PCA

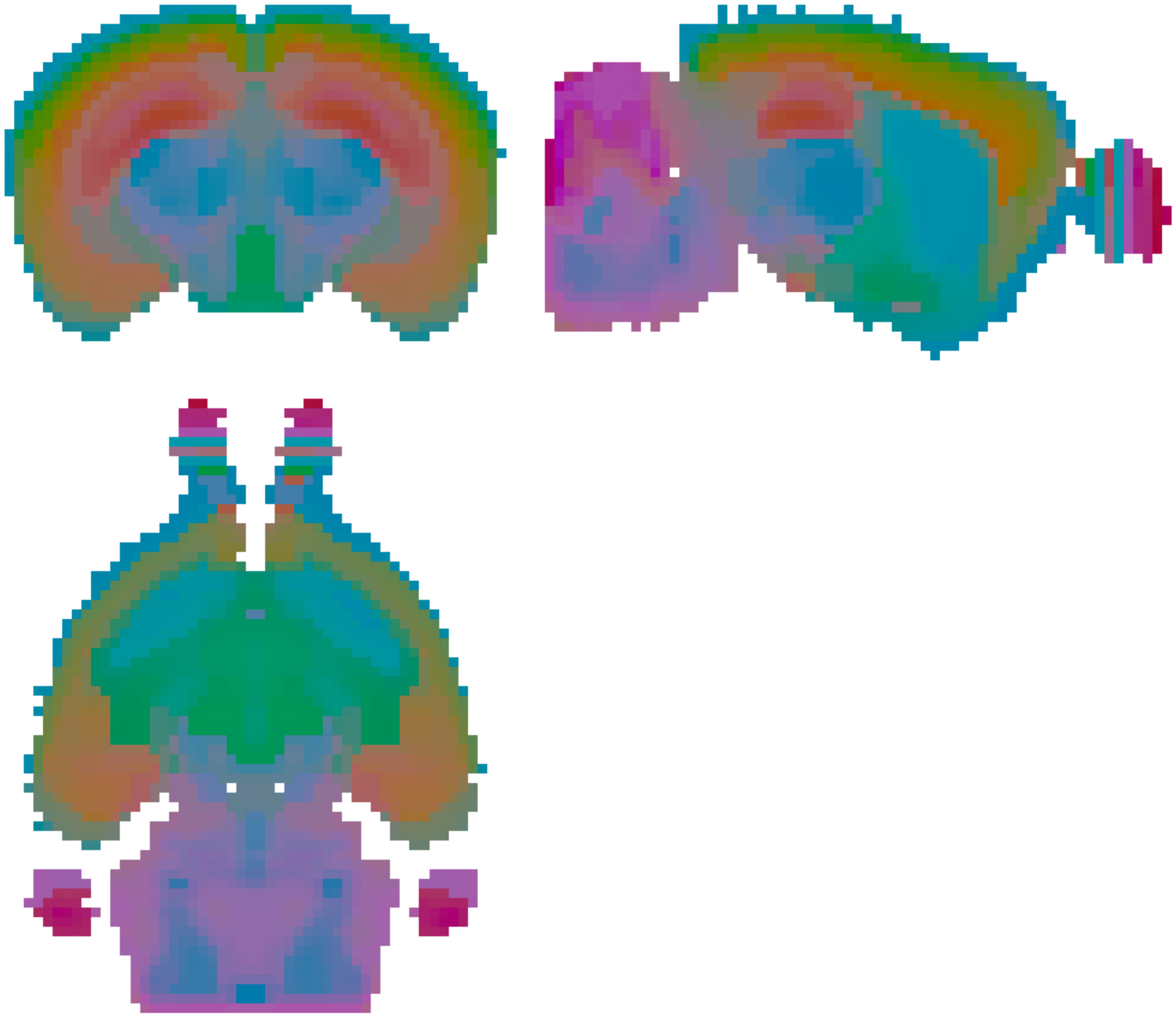


t-SNE



* Figure adopted from: J. Fonville *et al.*, *Anal. Chem.* 85(3), 2013.

Visualizing gene expression data



* Joint work with the LUMC and the Allen Brain Institute.

Human embryo data

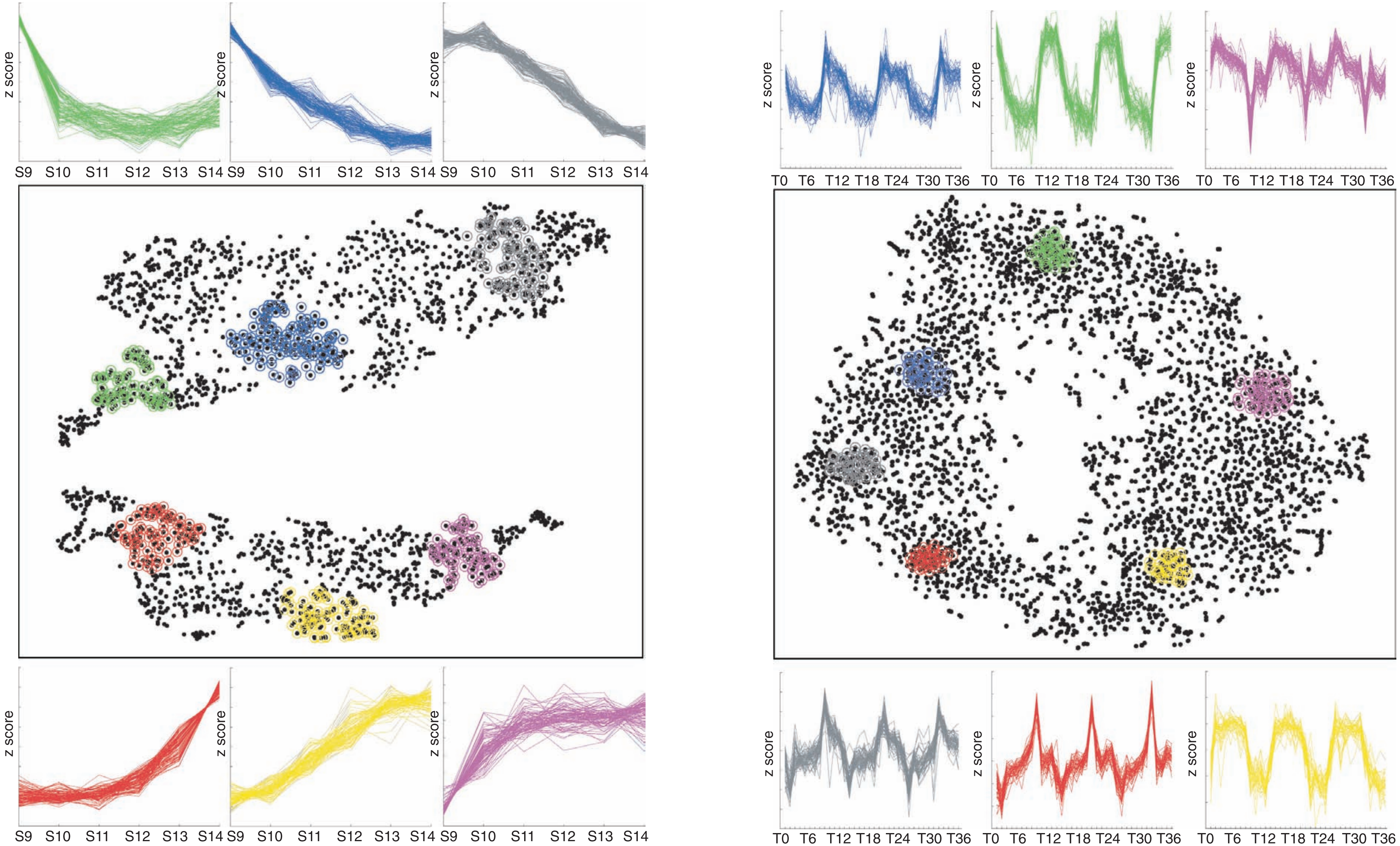
Two groups: one set of genes gets up-regulated and one set of genes gets down-regulated. (6D)

g gene expression data

Yeast metabolic cycle data

Cyclic behavior causes ring-like structure. (36D)

- Visualizing human embryo data and yeast metabolic cycle data:

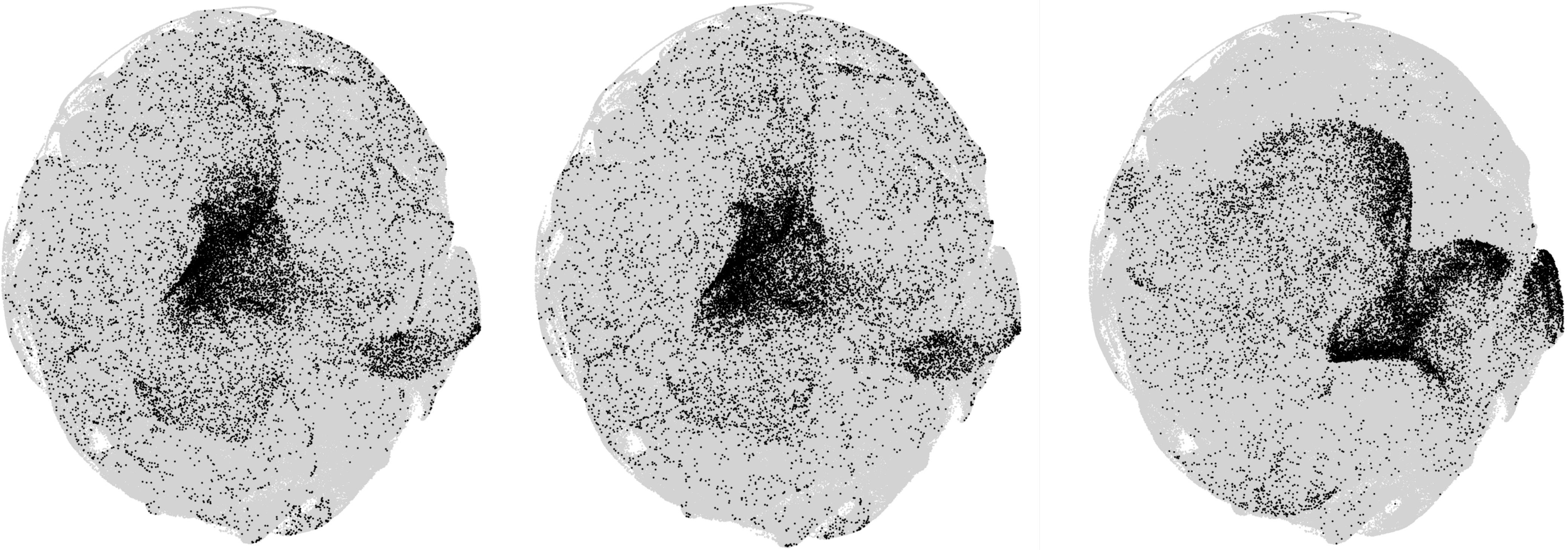


* Figure adopted from: N. Bushati *et al.*, *Nucleic Acids Res.* 39(17), 2011.

Visualizing flowcytometry data

- Flowcytometry data (= blood cell measurements) of leukemic and healthy kids:

Healthy | Healthy | Leukemia

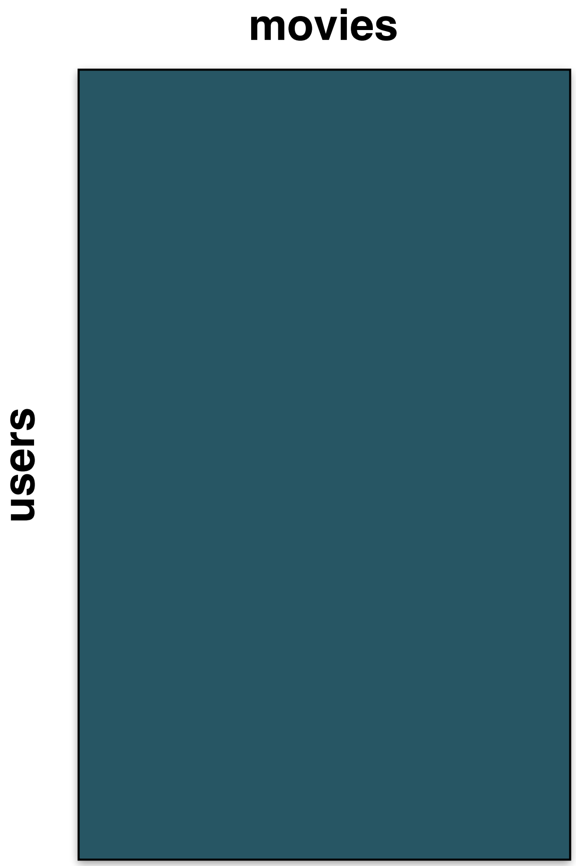


* Joint work with SickKids Hospital Toronto.


COFFEE!

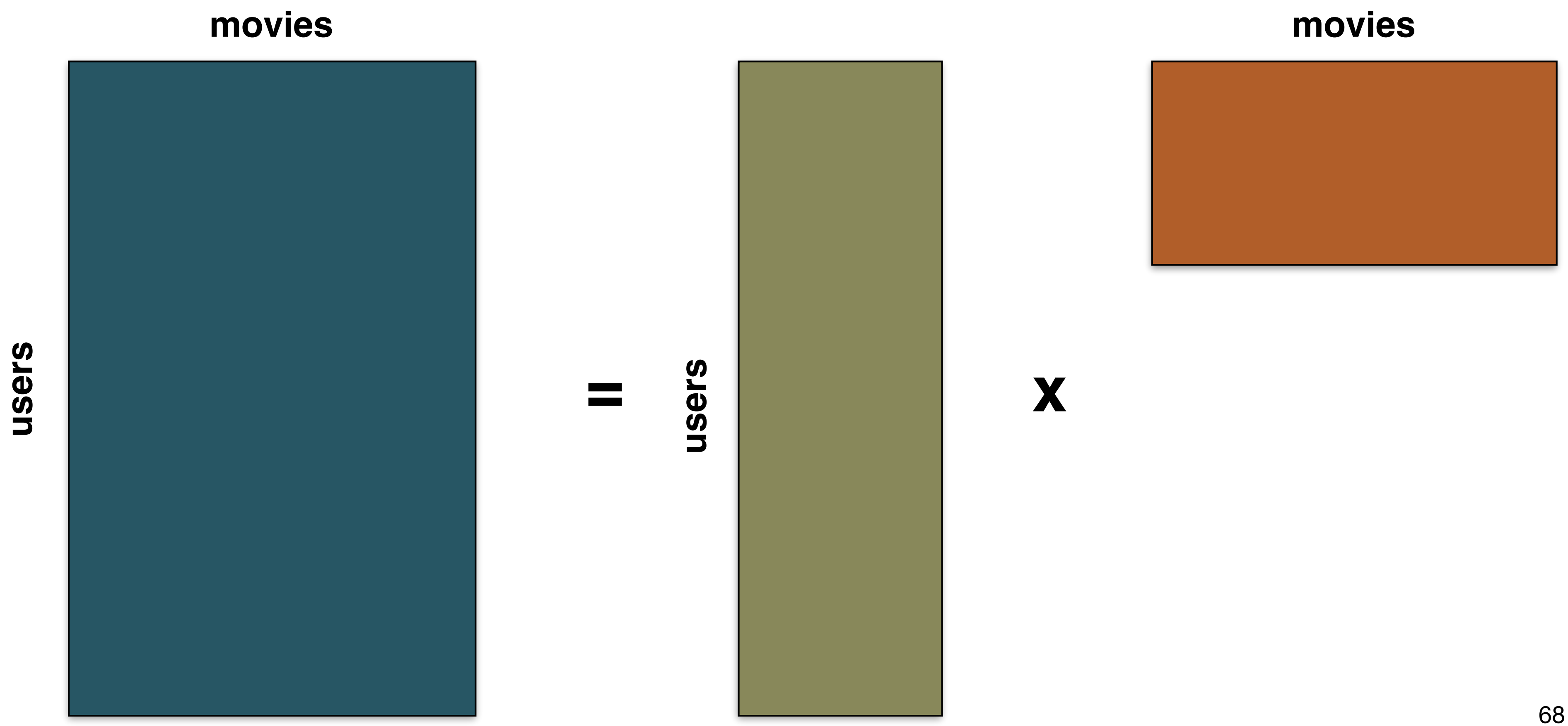
Visualizing movies

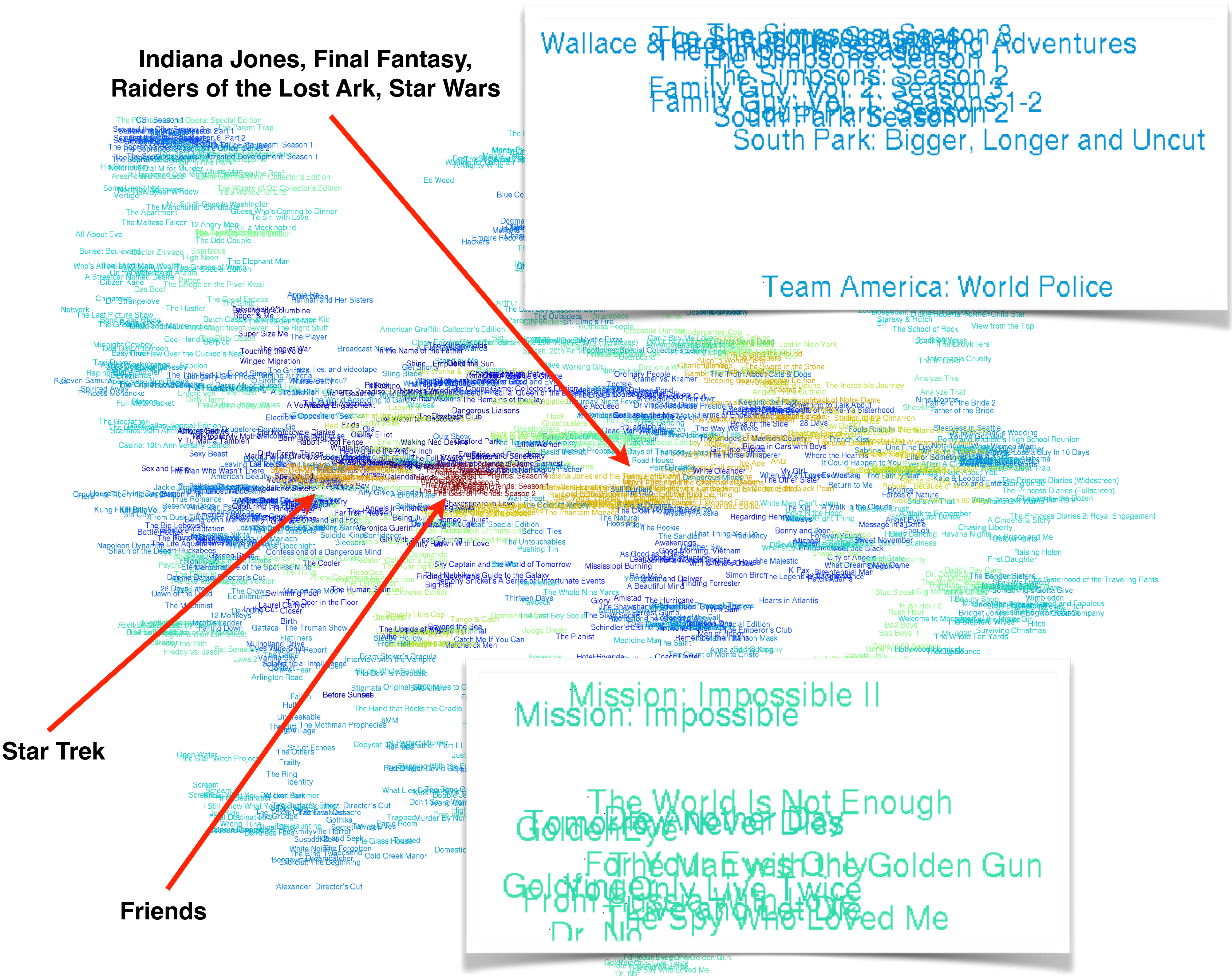
- Netflix has a large collection of user-movie ratings stored in a *rating matrix*



Visualizing movies

- Netflix has a large collection of user-movie ratings stored in a *rating matrix*
- *Decompose* the rating matrix to obtain *user features* and *movie features*:




Indiana Jones, Final Fantasy, Raiders of the Lost Ark, Star Wars
Star Trek
Friends
South Park: Bigger, Longer and Uncut
Team America: World Police
Mission: Impossible II
Mission: Impossible
The World Is Not Enough
The Spy Who Loved Me

What about Big Data?

- All the approaches I presented so far scale quadratically (or worse):
  - How do you make maps of data with lots of instances / records?

- Trick 1: Construct sparse matrix (approximate) input similarities

- Trick 2: Approximate interactions between points in map during learning

Computing high-dimensional similarities efficiently

Finding nearest neighbors

- What is the most common value in the input similarity matrix *P*?

Finding nearest neighbors

- What is the most common value in the input similarity matrix *P*? Infinitesimal!

Finding nearest neighbors

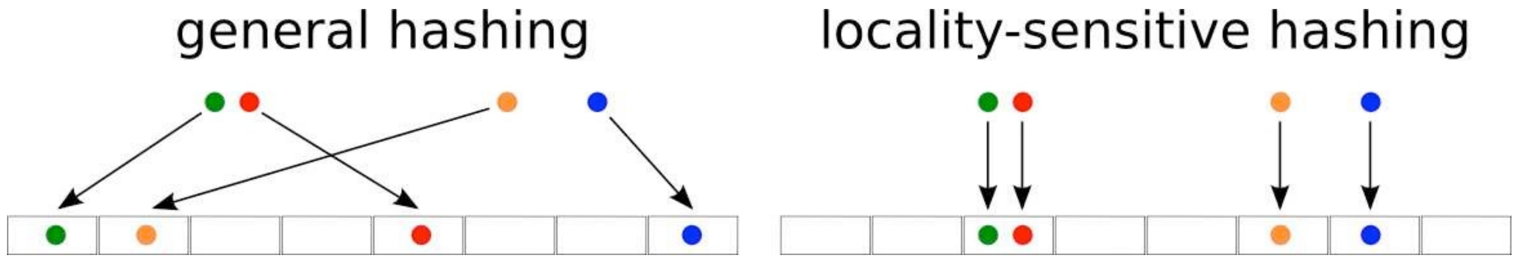
- What is the most common value in the input similarity matrix *P*? Infinitesimal!

- Good approximation: only compute p_{ij} for pairs of near neighbors

- Finding near neighbors (approximately) can be performed very efficiently:
    - Using a trick called *locality-sensitive hashing*
    - Using clever data structures such as *vantage-point trees*

Locality-sensitive hashing

- LSH uses hashing functions that take “location” of object in consideration:



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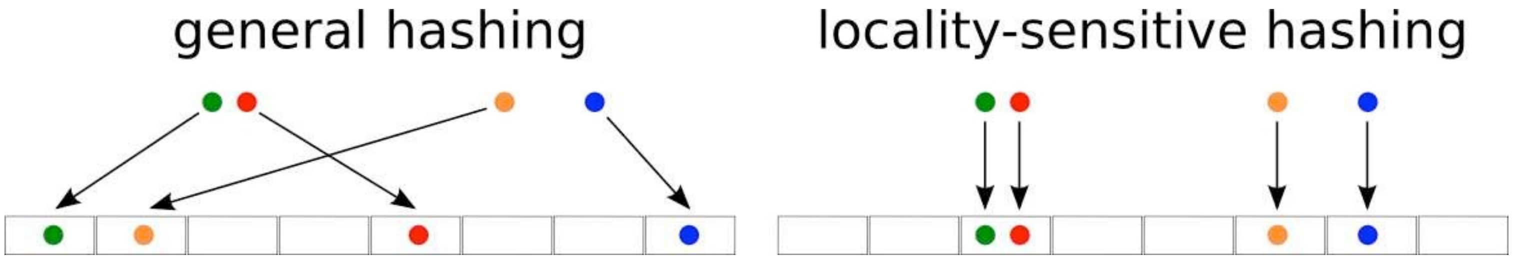
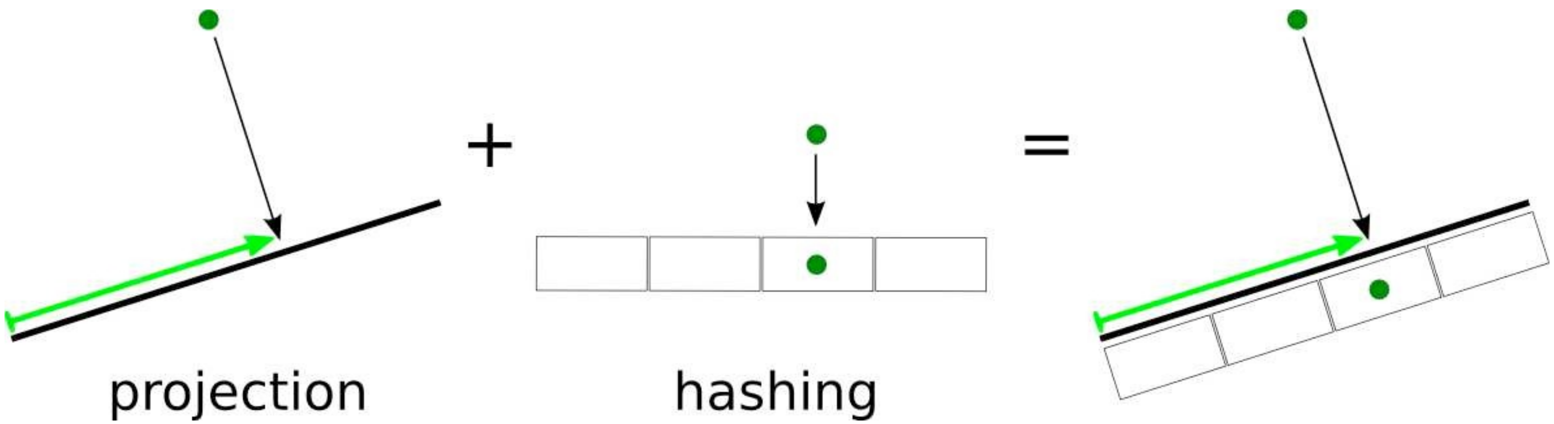


- Example of a locality-sensitive hashing function for points in a space:
  - Project the point onto a random subspace; divide result into 4 buckets (2 bits)



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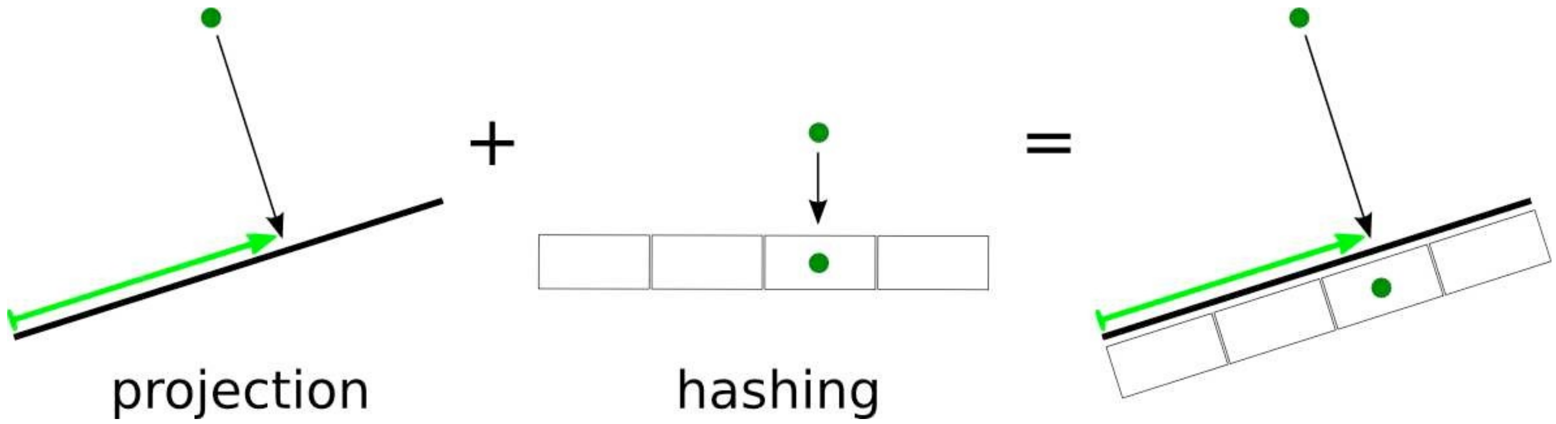
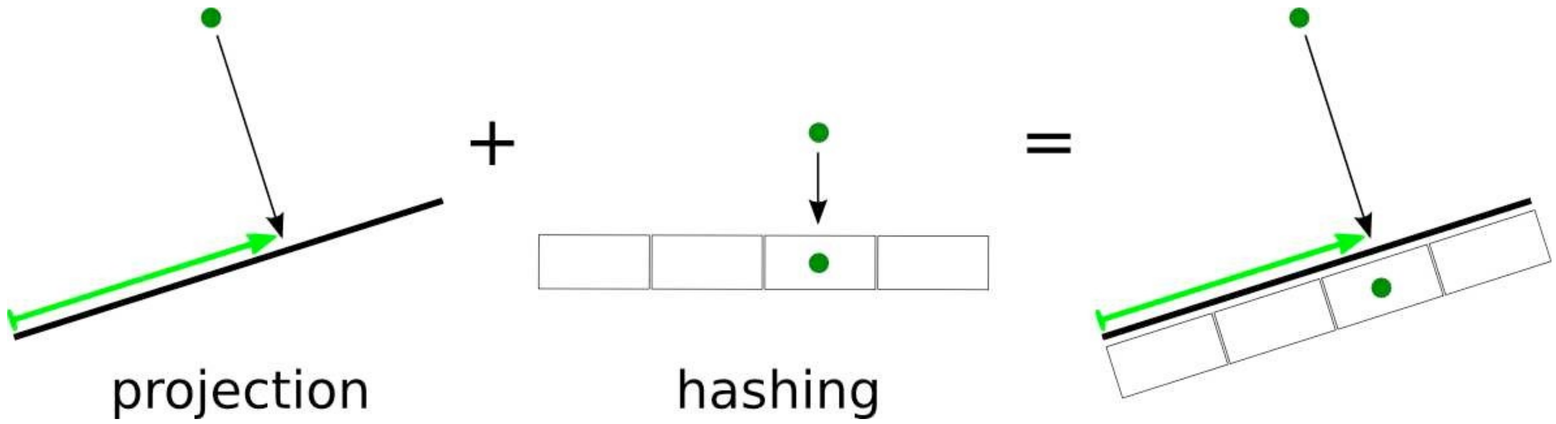


- Mathematically, we could express this locality sensitive hash function as:

$$h(\mathbf{x}) = \begin{cases} 0 & \text{if} \quad \mathbf{w}^\top \mathbf{x} \leq -\tau \\ 1 & \text{if} \quad -\tau < \mathbf{w}^\top \mathbf{x} \leq 0 \\ 2 & \text{if} \quad 0 < \mathbf{w}^\top \mathbf{x} \leq \tau \\ 3 & \text{if} \quad \mathbf{w}^\top \mathbf{x} > \tau \end{cases}$$

Locality-sensitive hashing



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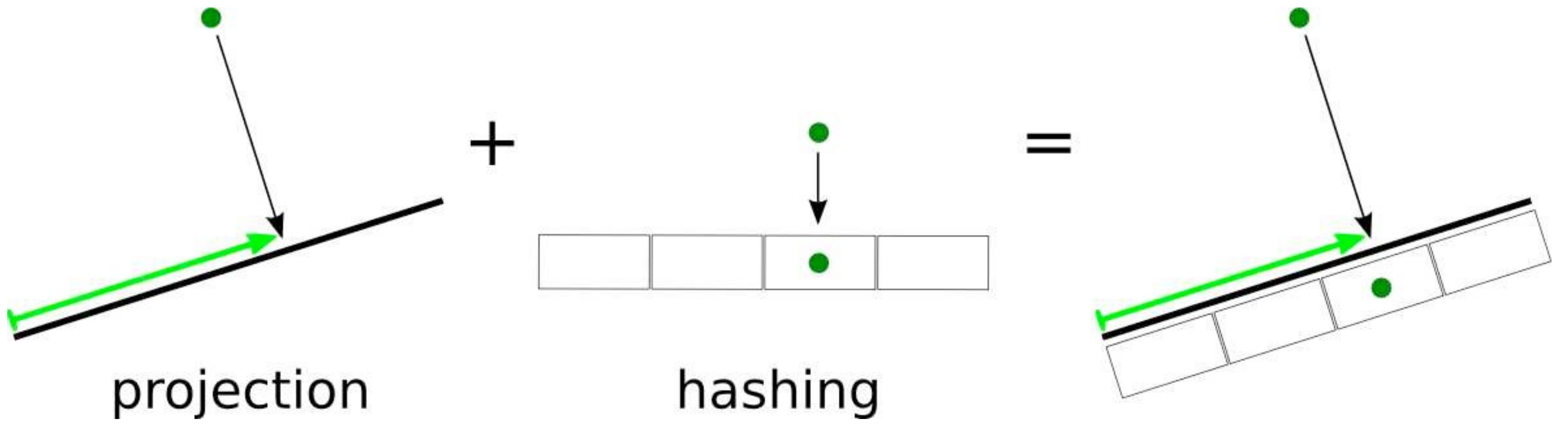
random projection

Locality-sensitive hashing



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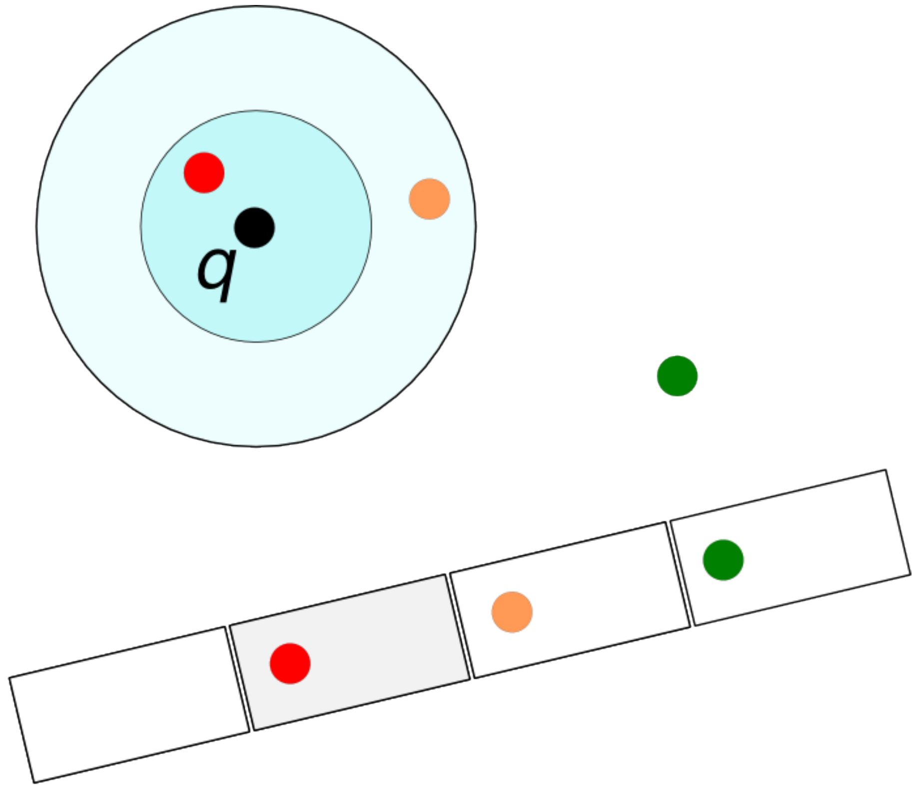
random projection

threshold parameter

Locality-sensitive hashing

- Retrieval of nearest neighbors of a query point *q* using LSH works as follows:



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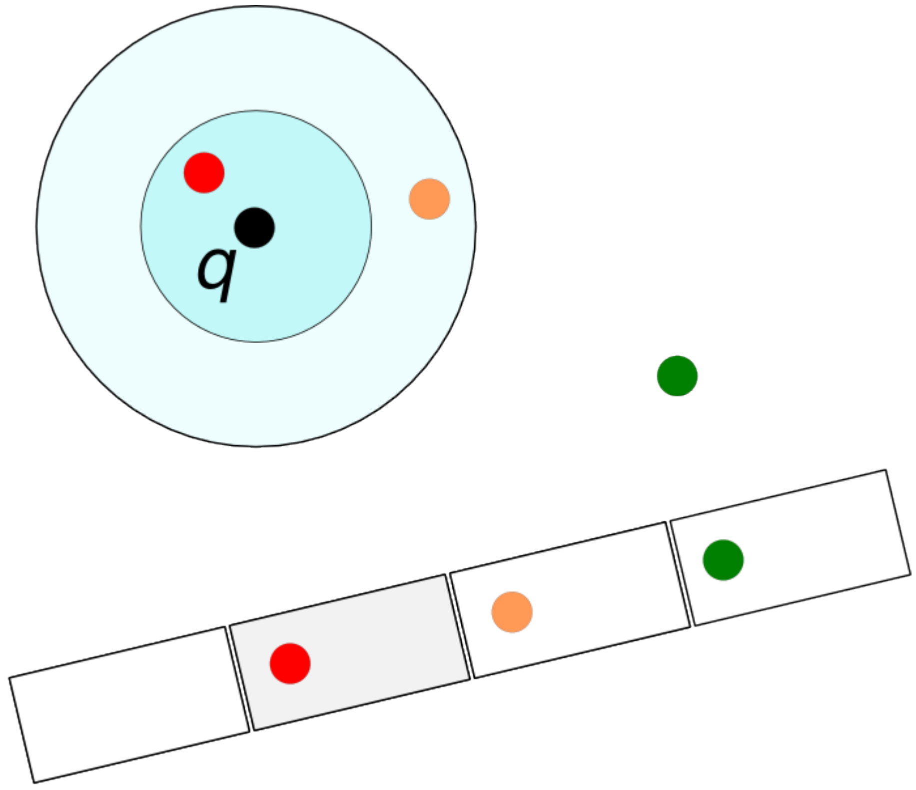

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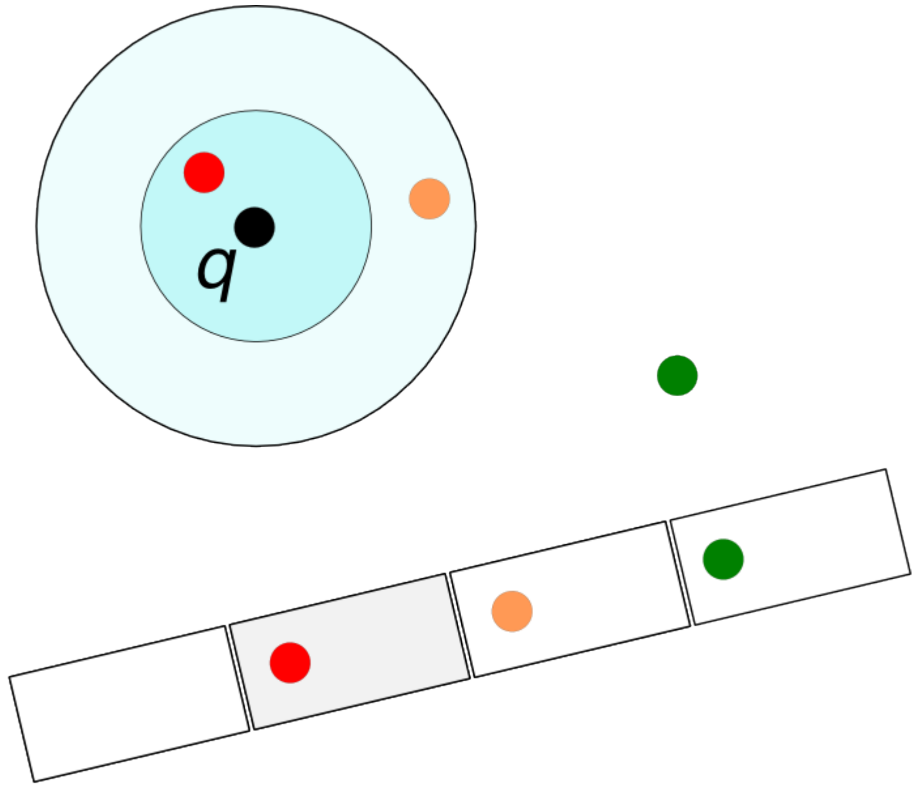

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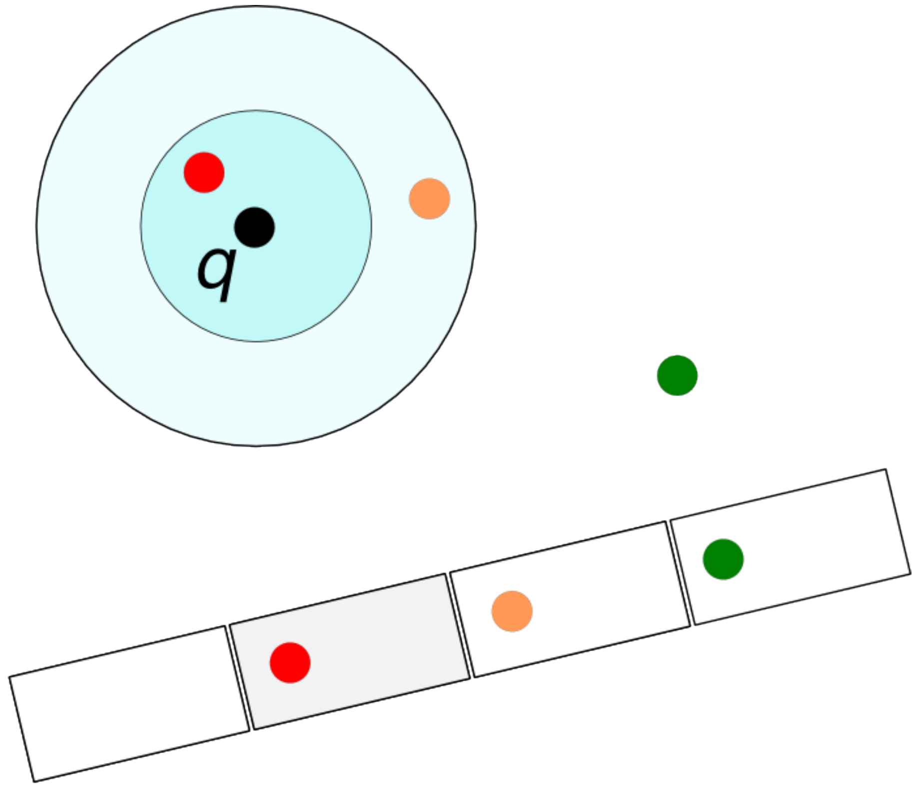

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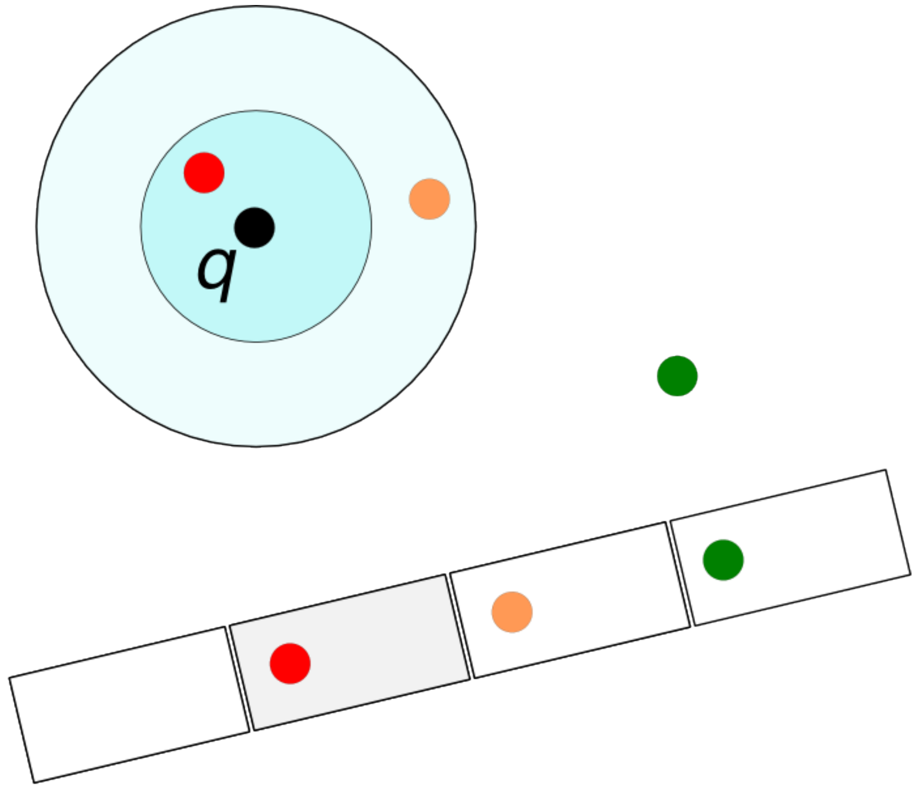
  - Compute locality-sensitive hash of query point
  - All data points in the bucket are candidate near neighbors
  - Compute distances to candidate points to find true nearest neighbors



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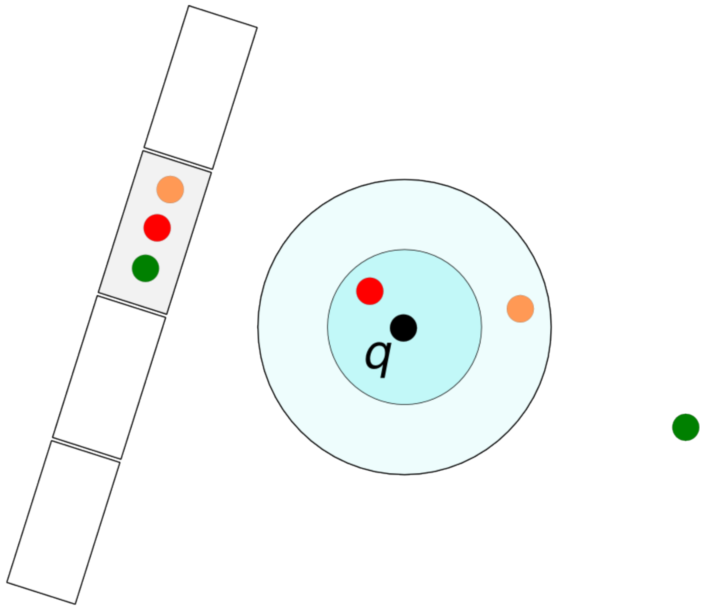

“Collision”: Distant points
hashed in the same bucket

Locality-sensitive hashing

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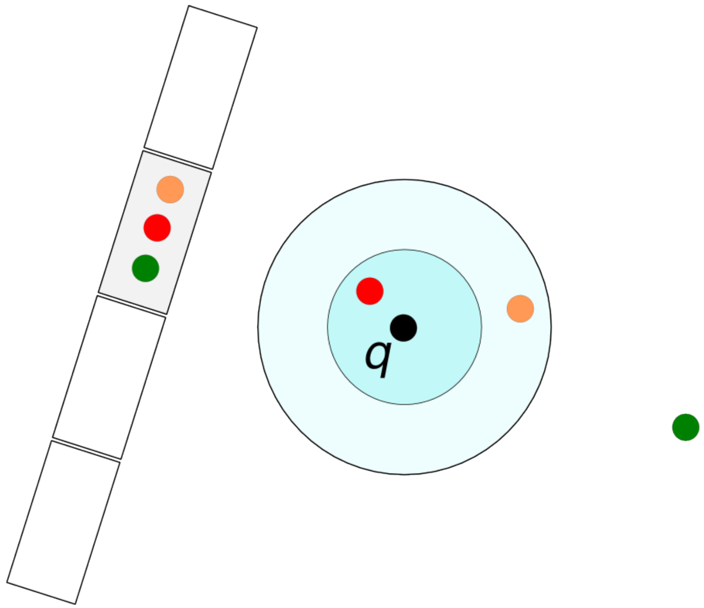

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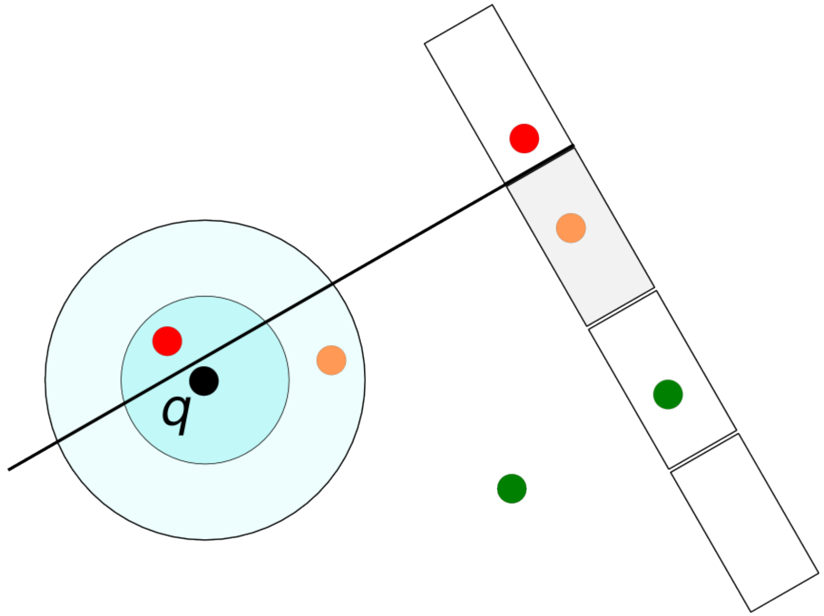
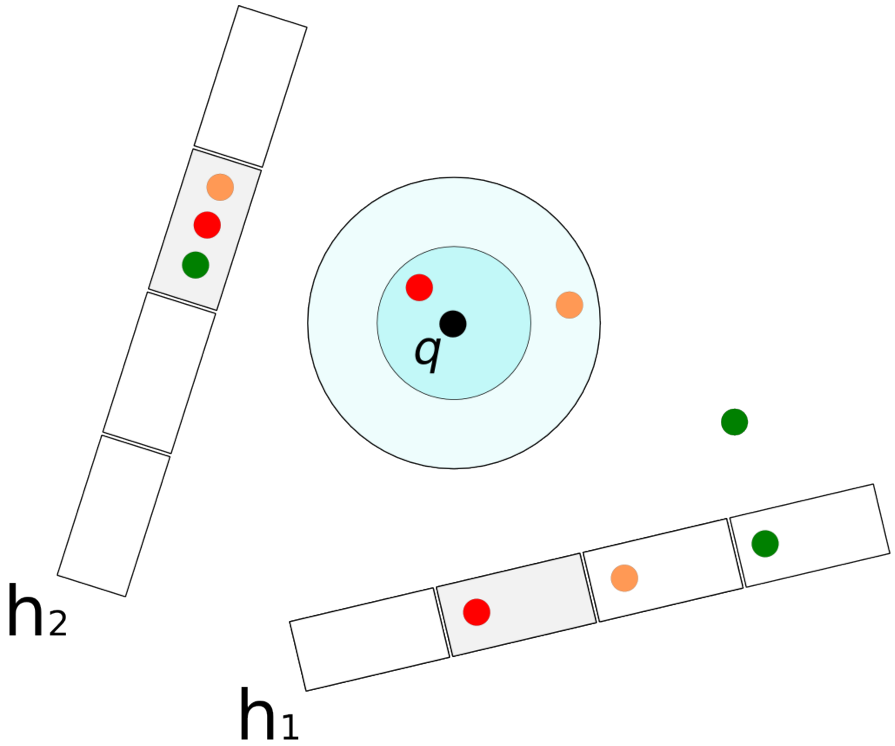


“Split”: Nearby points
hashed in different buckets

Locality-sensitive hashing

- Using multiple projections in an LSH resolves “collisions”:



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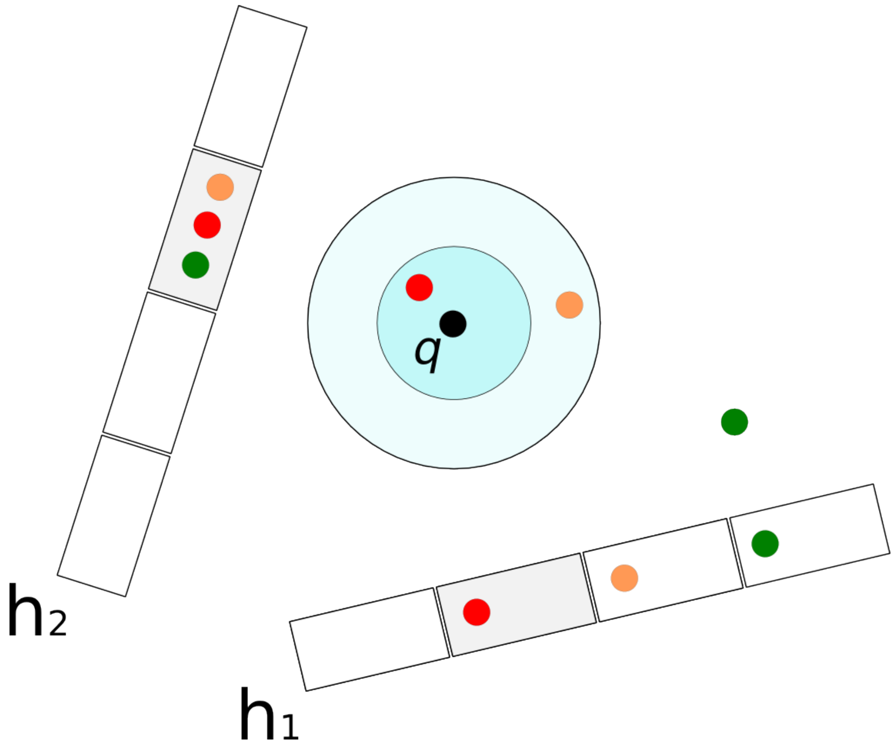
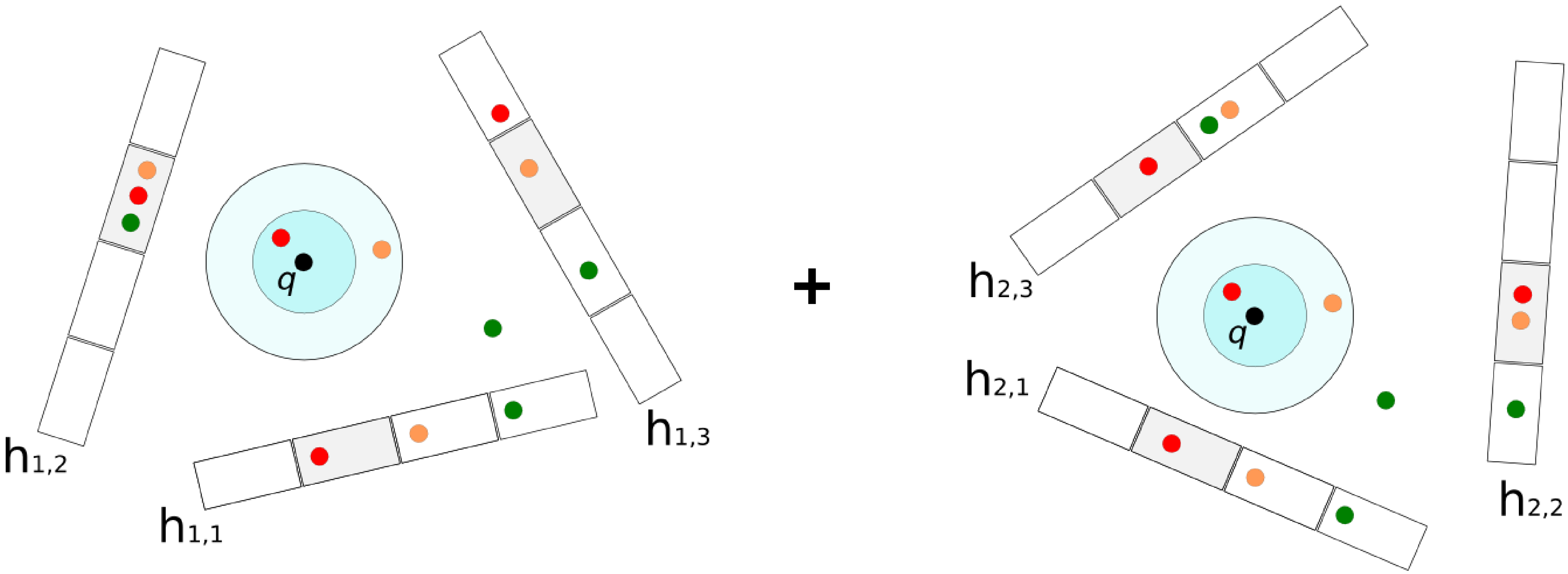


- The LSH is given by a concatenation of all individual buckets

Locality-sensitive hashing

- Using multiple separate hash tables when doing LSH resolves “splits”:



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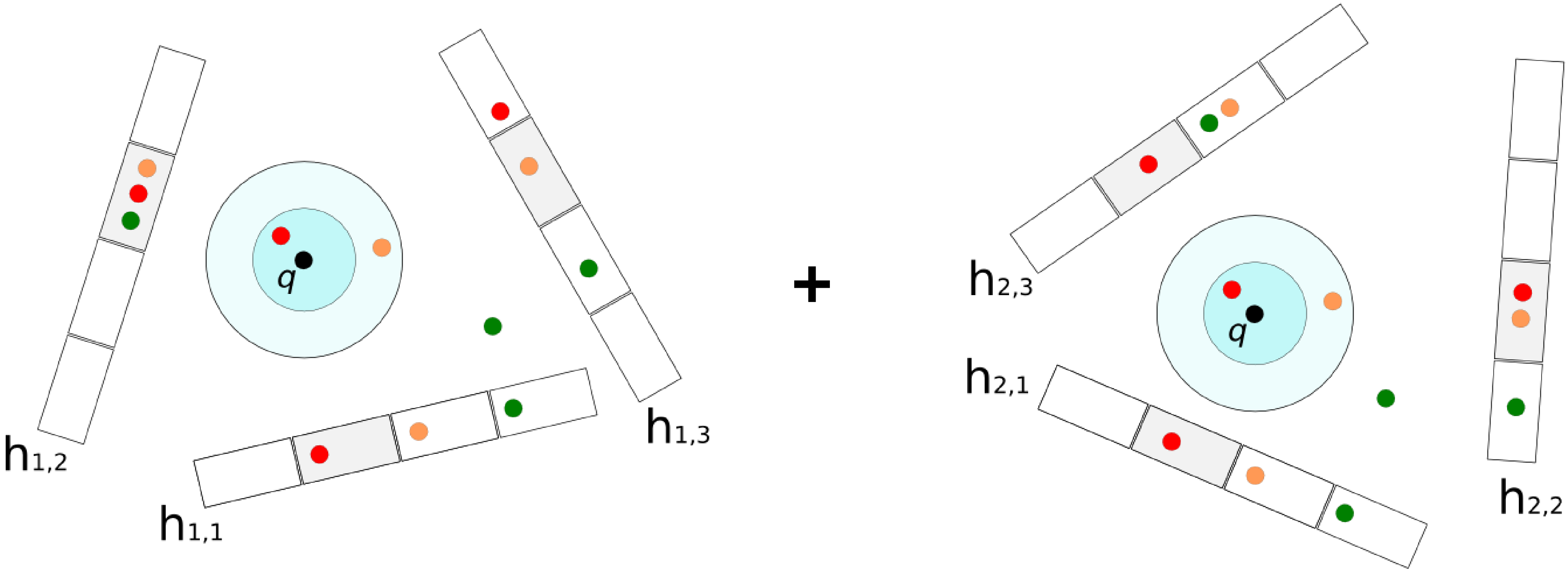


- Points are candidate neighbors if candidate in *any* of the hash tables

Locality-sensitive hashing

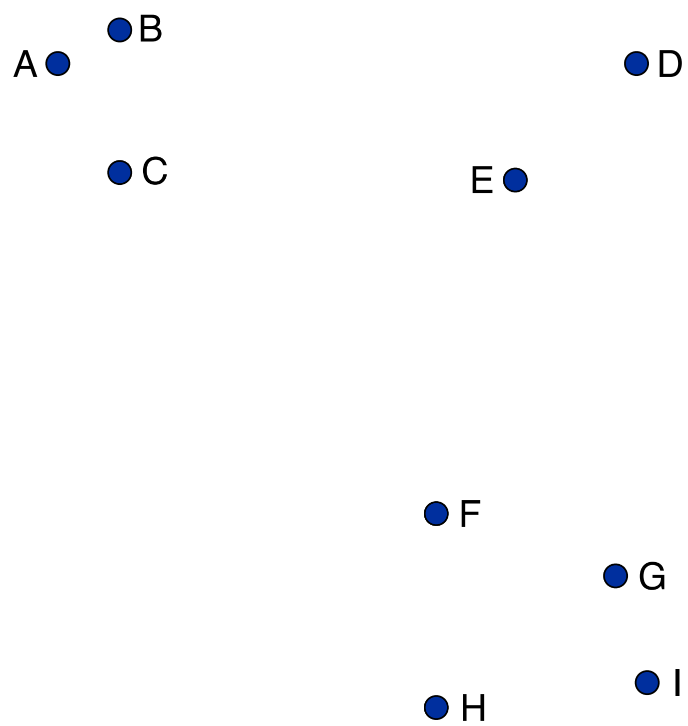
- Efficient algorithm to compute a sparse *P*-matrix:
    - Load all data in a locality-sensitive hash
    - For each data point, retrieve the *candidate near neighbors* from the LSH
    - For these candidates, compute the *P*-value using a Gaussian kernel

Constructing maps efficiently

Gradient interpretation

- We can interpret building a t-SNE map as a simulation of an *N-body system*:

$$\frac{\partial C}{\partial \mathbf{y}_i} = 4 \sum_{j \neq i} (p_{ij} - q_{ij})(1 + \|\mathbf{y}_i - \mathbf{y}_j\|^2)^{-1}(\mathbf{y}_i - \mathbf{y}_j)$$



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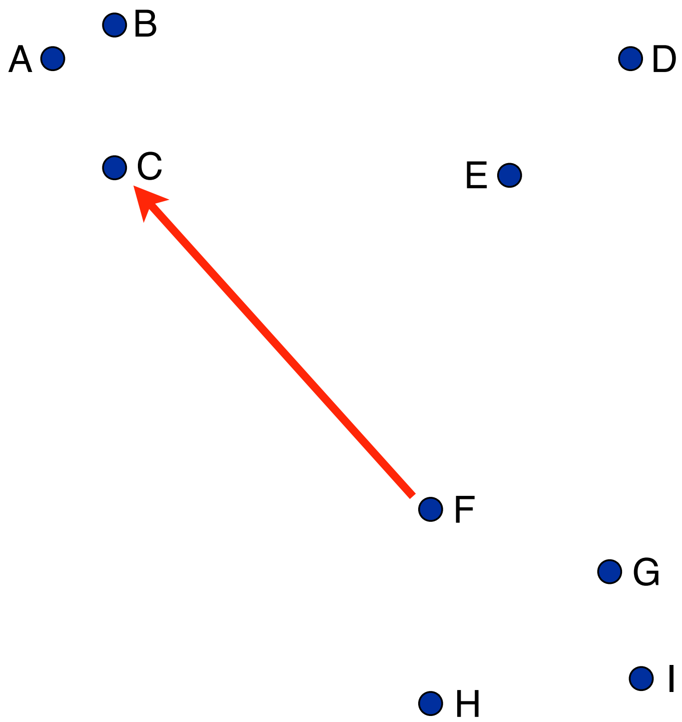
spring



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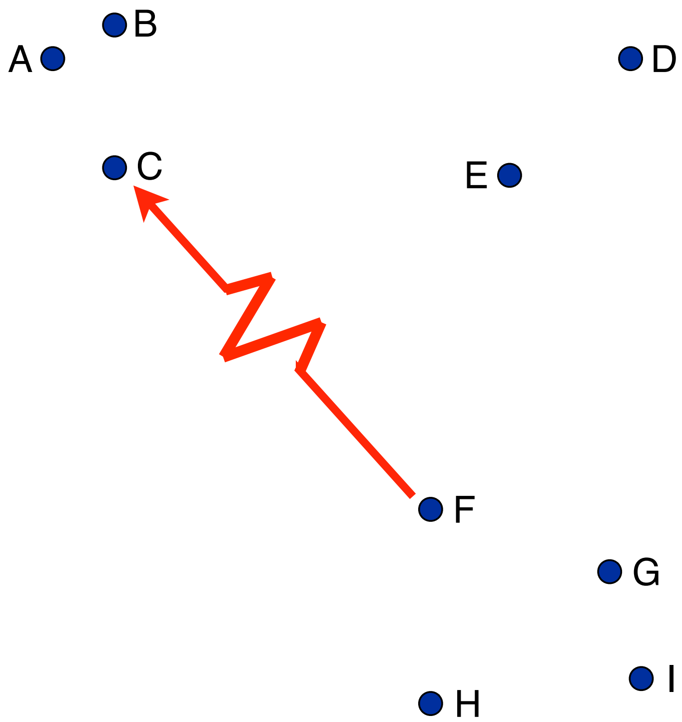
exertion / compression



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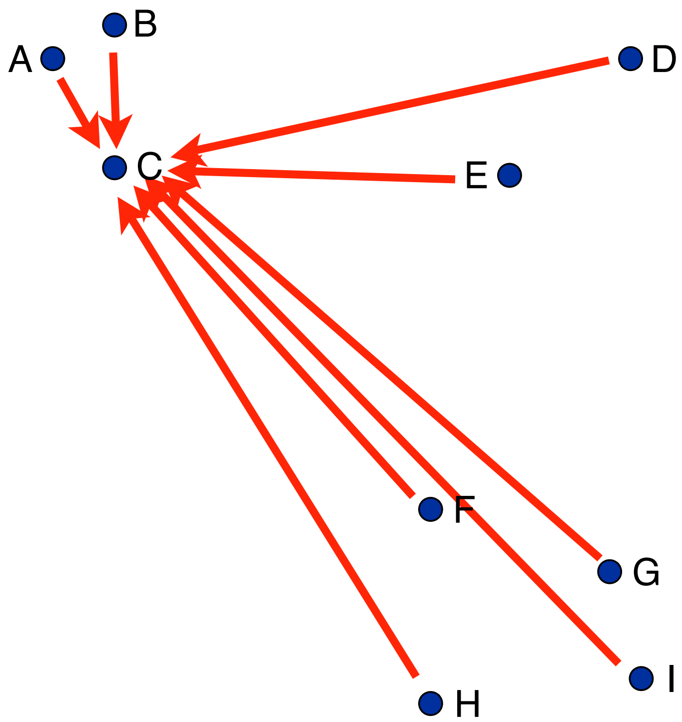
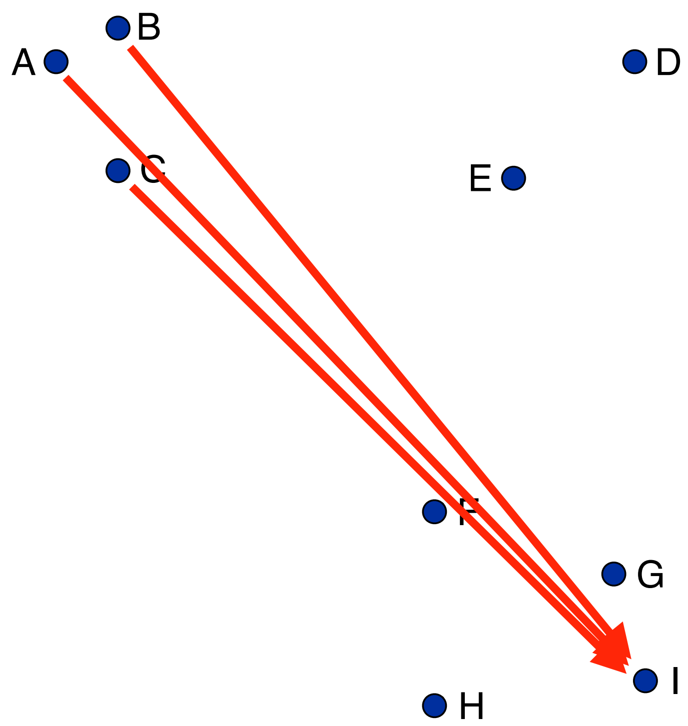


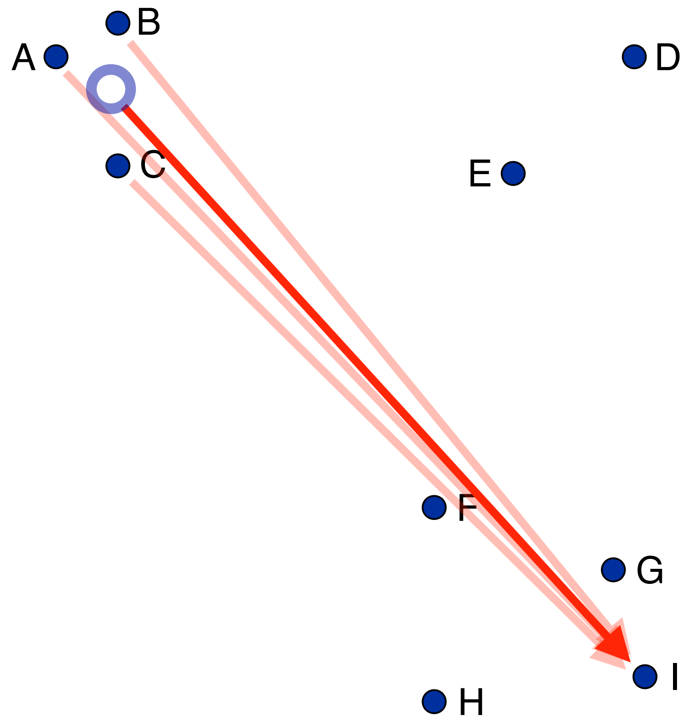
Barnes-Hut approximation

- Many of the pairwise interactions between points are very similar:



Barnes-Hut approximation

- Approximate such similar interactions by a *single* interaction:



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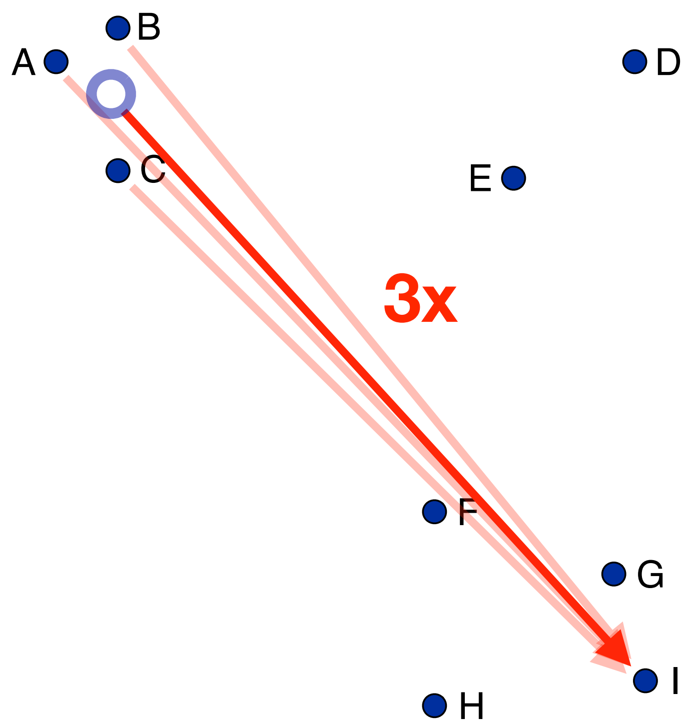


Barnes-Hut-SNE

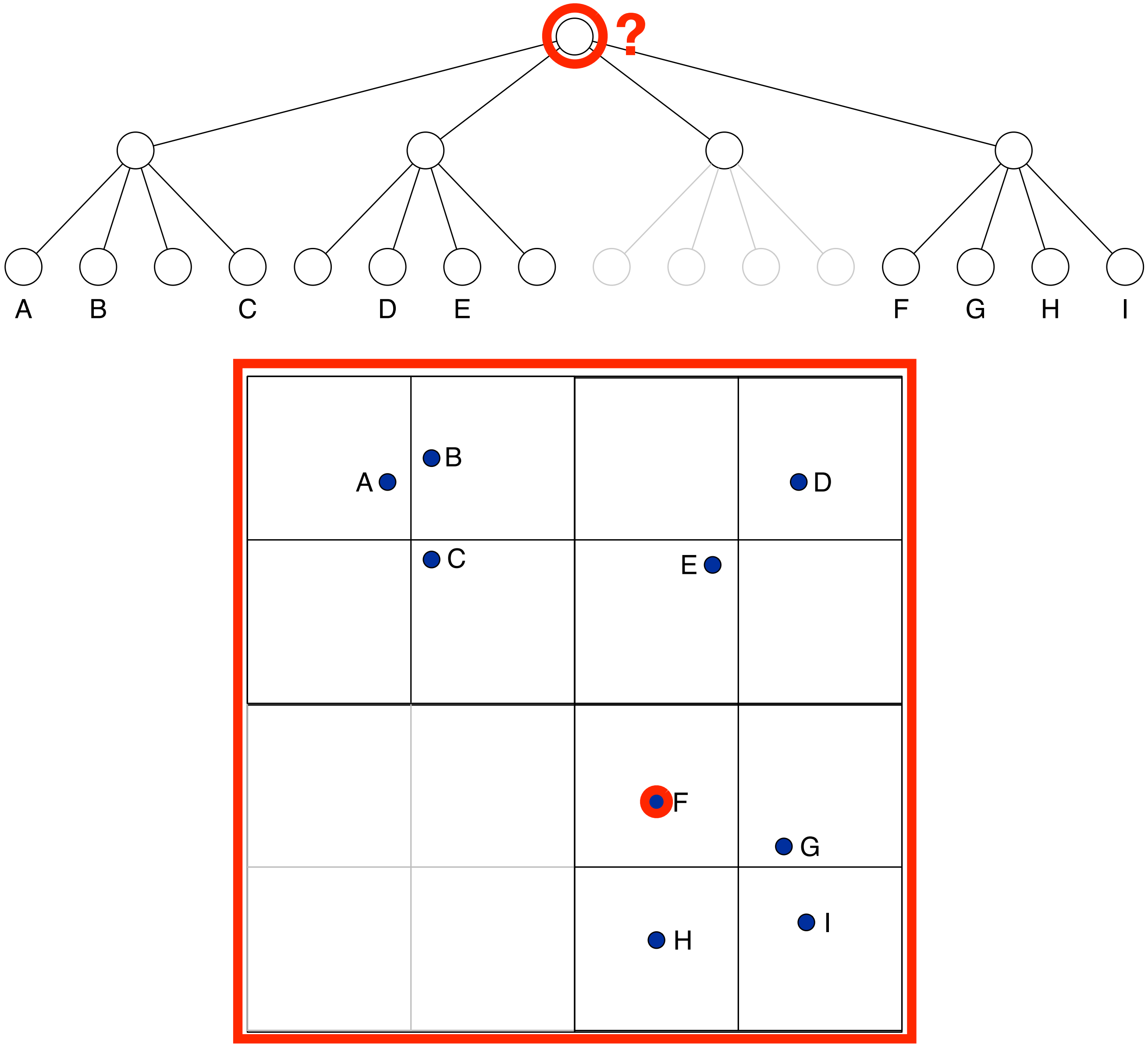
- Split up the t-SNE gradient into two main parts:

$$\frac{\partial C}{\partial \mathbf{y}_i} = 4(F_{attr} - F_{rep}) = 4\left(\sum_{j \neq i} p_{ij} q_{ij} Z(\mathbf{y}_i - \mathbf{y}_j) - \sum_{j \neq i} q_{ij}^2 Z(\mathbf{y}_i - \mathbf{y}_j)\right)$$

- Compute $\sum_{j \neq i} p_{ij} q_{ij} Z(\mathbf{y}_i - \mathbf{y}_j)$ exactly (possible because *P*-values are sparse)

- Approximate $\sum_{j \neq i} q_{ij}^2 Z^2(\mathbf{y}_i - \mathbf{y}_j)$ and Z with two Barnes-Hut algorithms

Barnes-Hut-SNE



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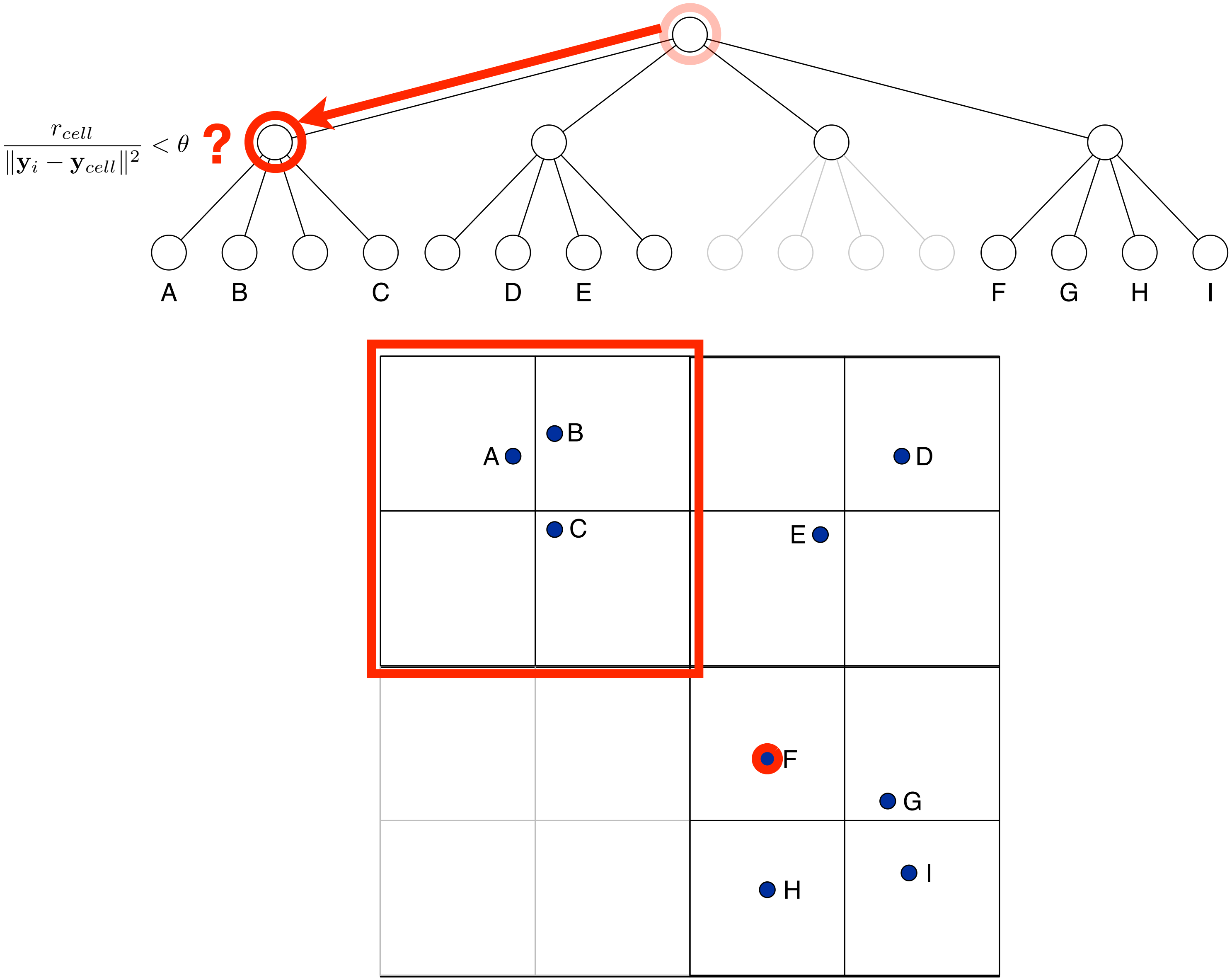

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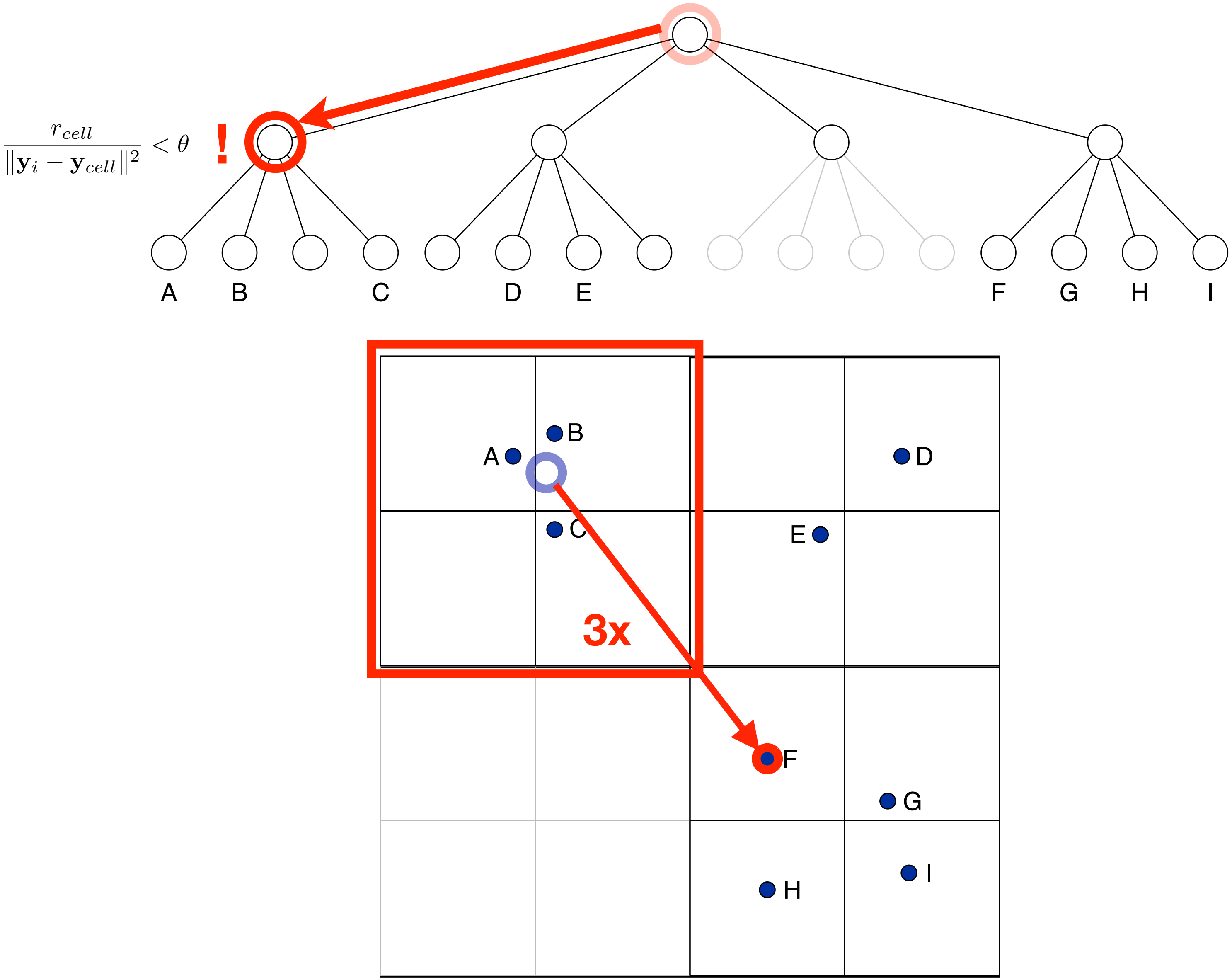

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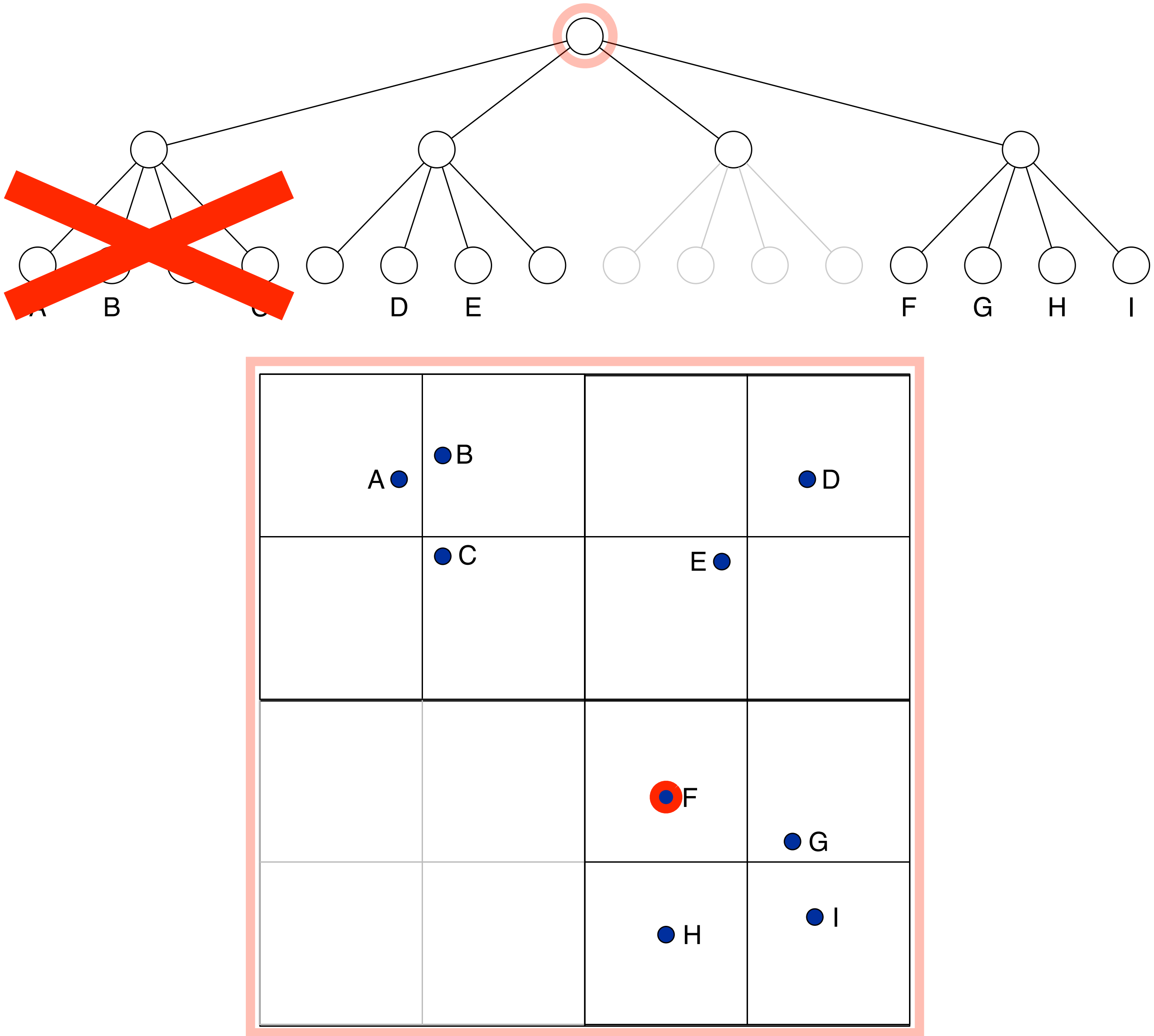

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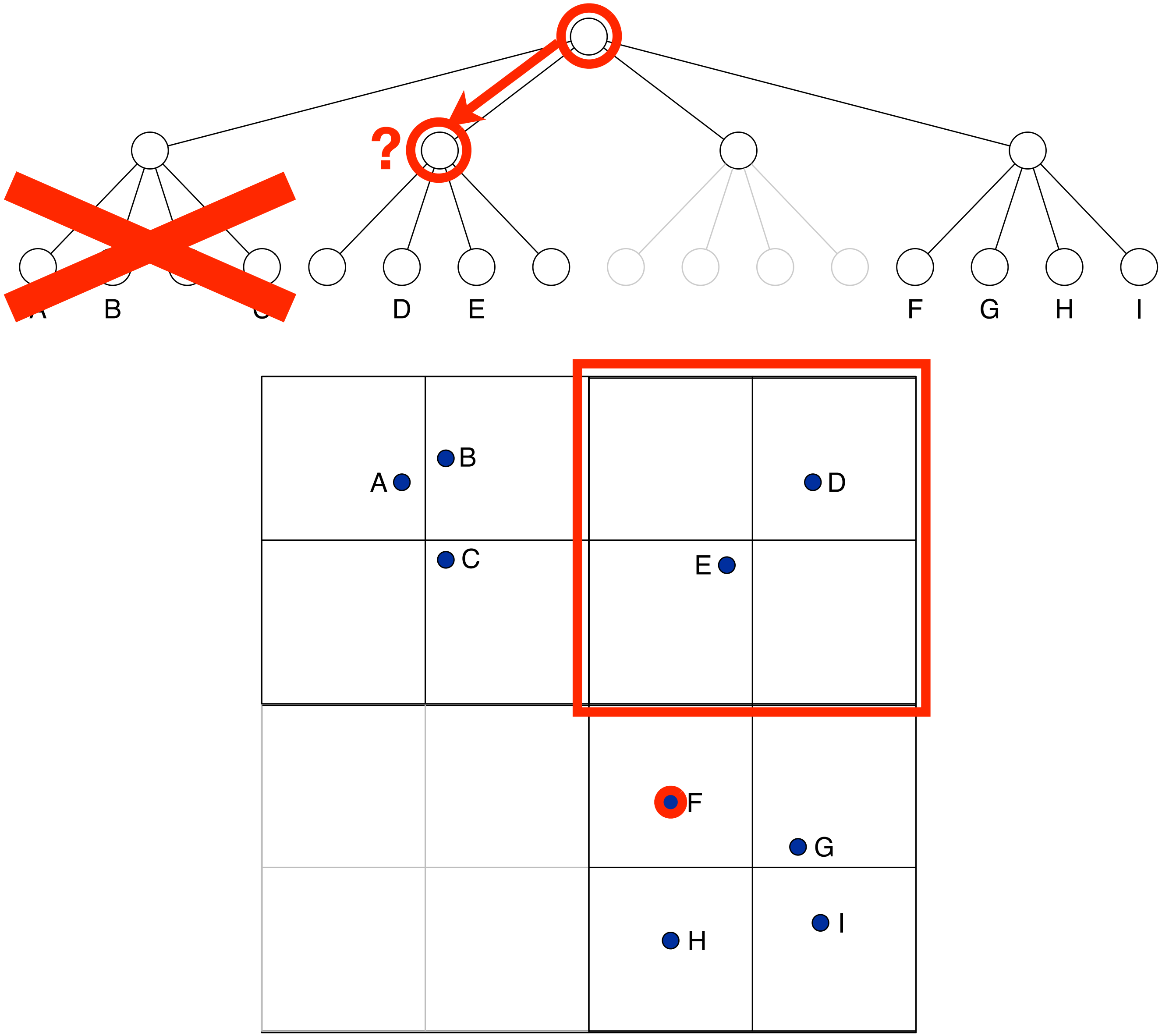

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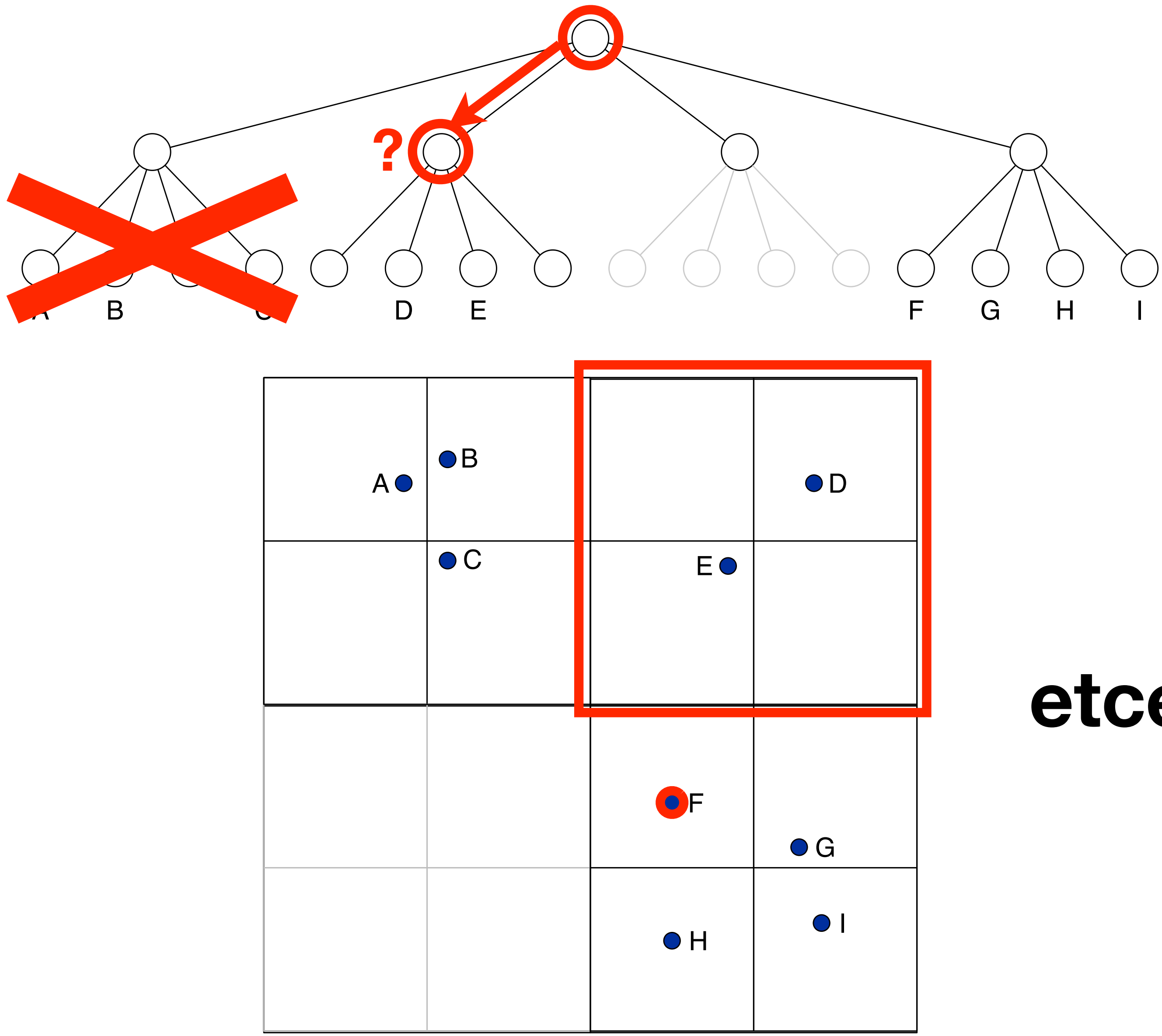
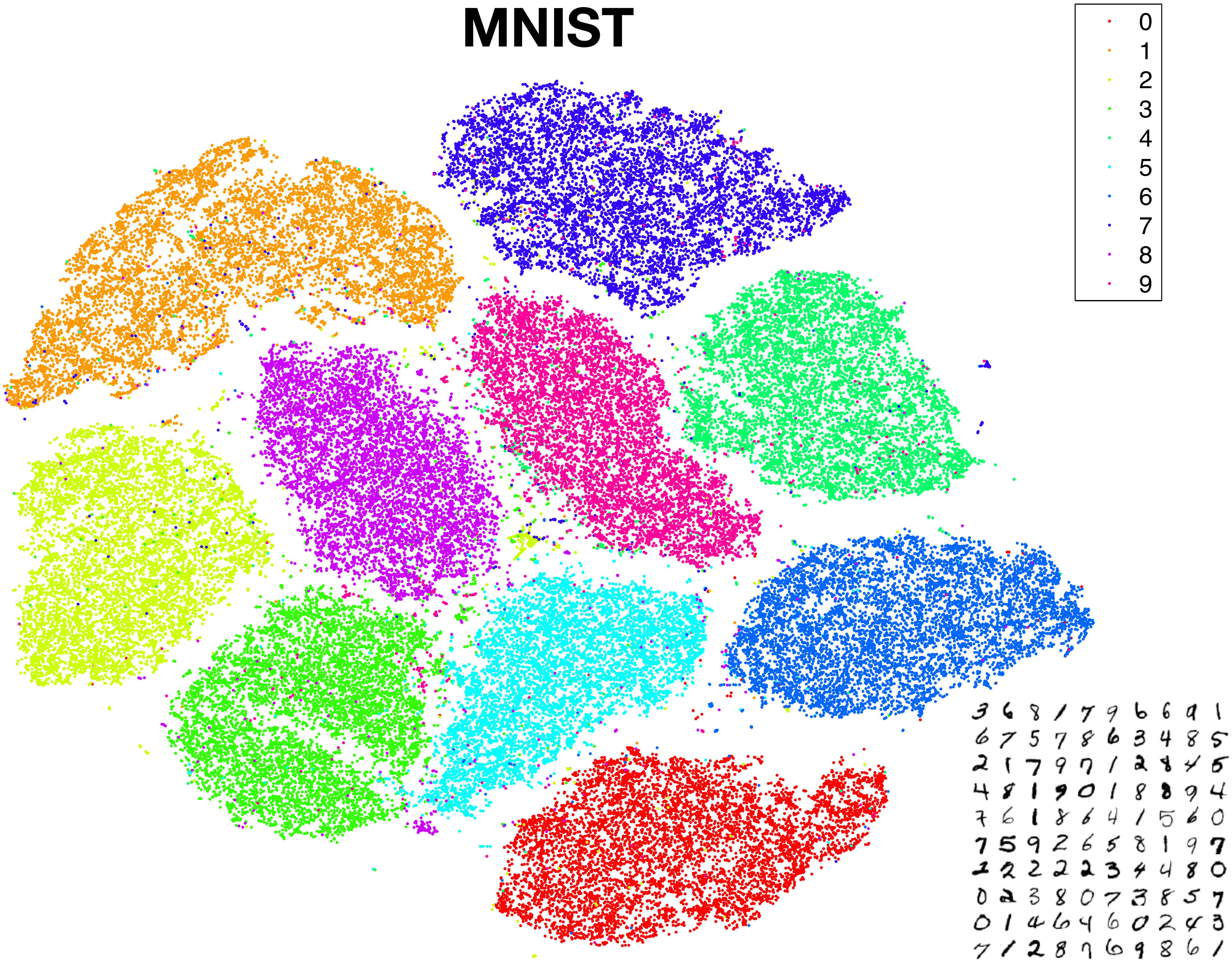


etcetera...


MNIST
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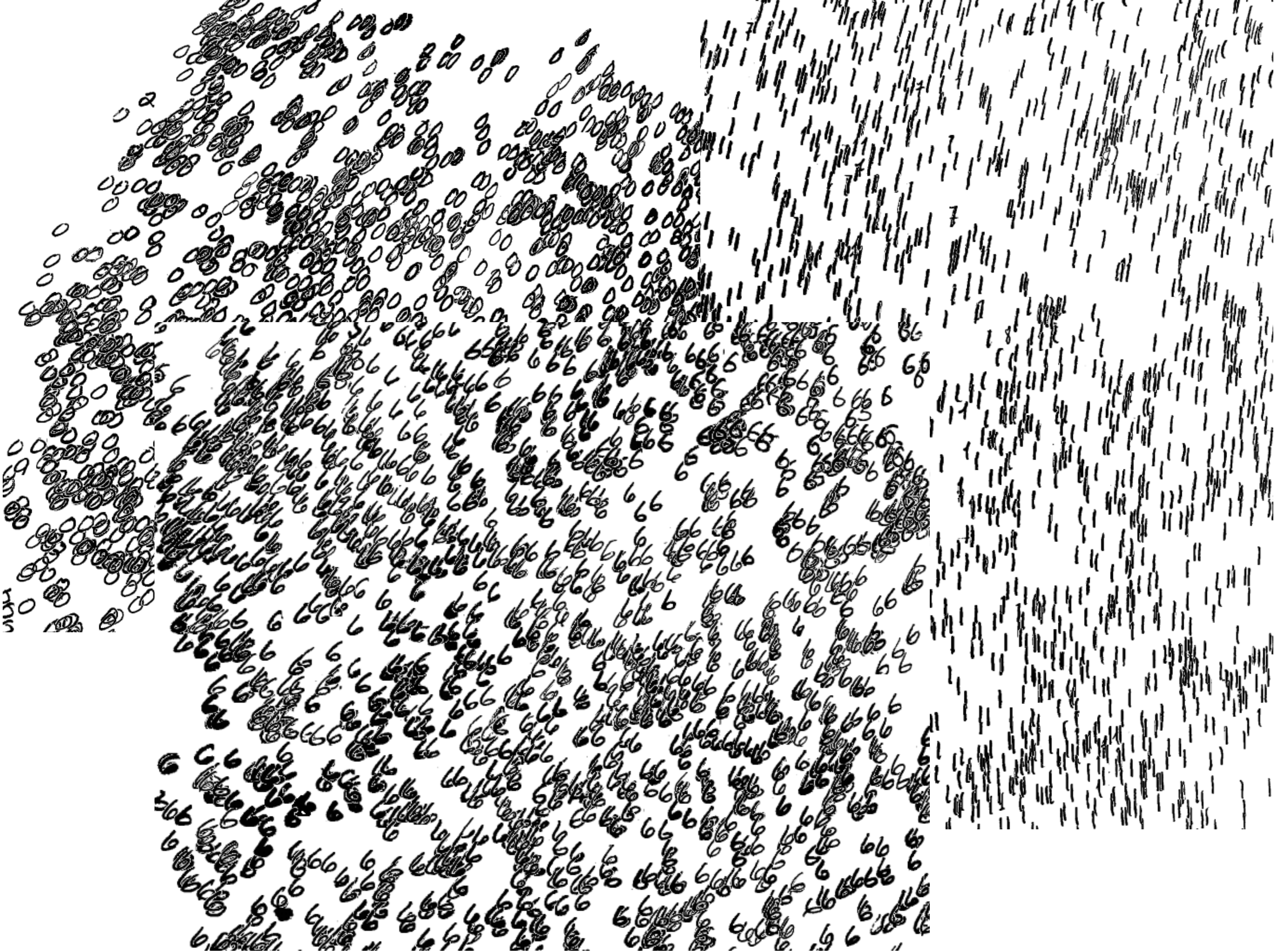

* Word map made by Joseph Turian at University of Montreal.

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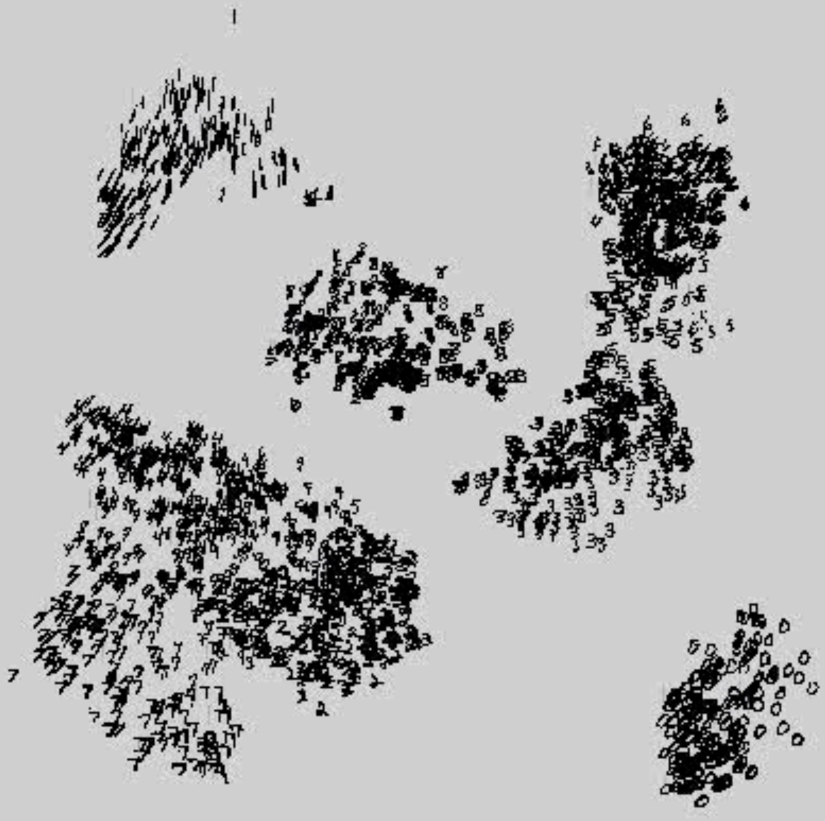
- t-SNE has already been successfully applied in a range of domains:
    - Bioinformatics, computer security, climate research, cancer research, *etc.*



QUESTIONS?

Try it out yourself! Code and papers are available on http://lvdmaaten.github.io/tsne
Shorter version of this talk is available on: http://www.youtube.com/user/GoogleTechTalks/videos