Big Data Computing

Master's Degree in Computer Science

2025-2026

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SAPIENZA
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Similarity: Why Bother?

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- Each metric may be suitable for specific task(s) in a particular domain
- **Clustering** is one of these tasks!

CLUSTERING

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- A standard problem in many (big) data applications:
  - Categorizing documents by their topics
  - Grouping customers by their behaviors
  - ...

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- A typical example of **unsupervised learning** technique

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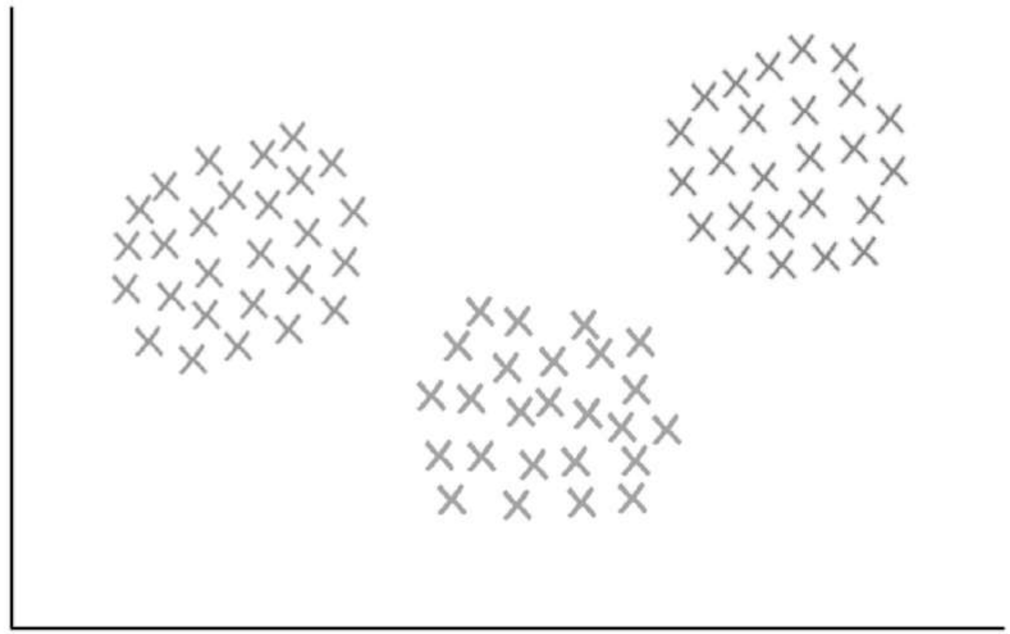
- A typical example of **unsupervised learning** technique
- A method of **data exploration**, i.e., a way of looking for patterns of interest in data

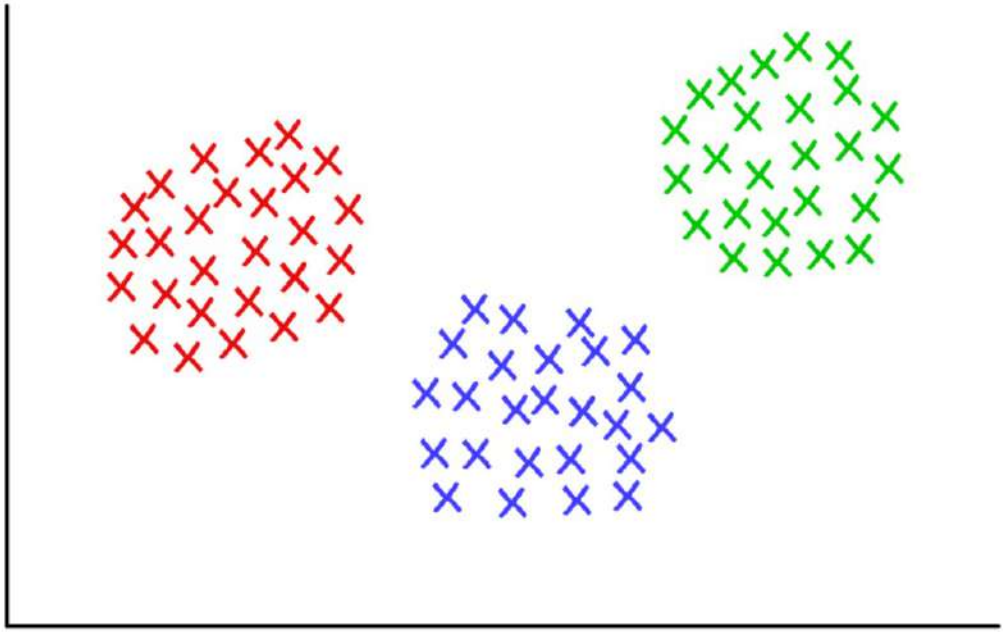
Clustering: Intuition

Given a set of 2-dimensional data points



Clustering: Intuition

We'd like to understand their "structure" to find groups of data points



Clustering: Formal Definition

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- Group the data points into some number of clusters so that:
  - Members of a cluster are close/similar to each other (i.e., **high intra-cluster similarity**)
  - Members of different clusters are dissimilar (i.e., **low inter-cluster similarity**)

Clustering: Practical Issues

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  - Data points may be in very high-dimensional spaces

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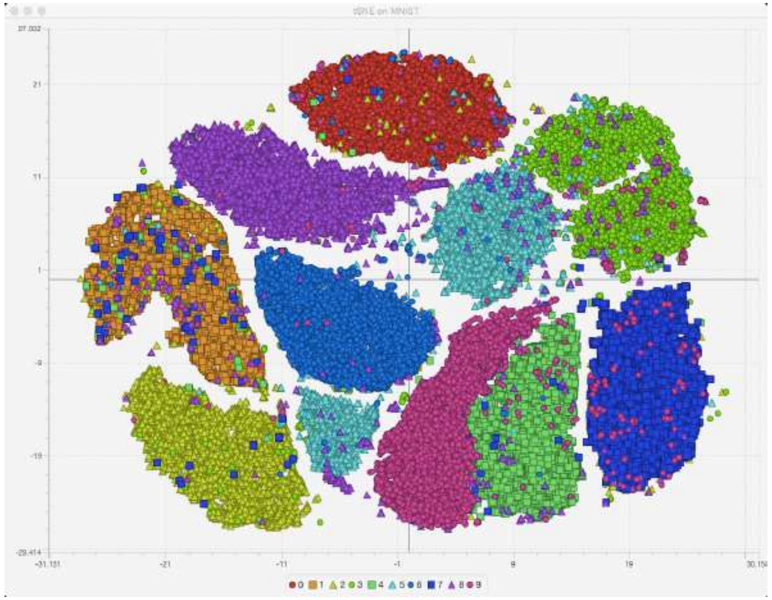
- Number of **output clusters**
  - Fixed apriori? Data-driven?

Clustering: A Hard Problem

Data points are not always easily and clearly separable



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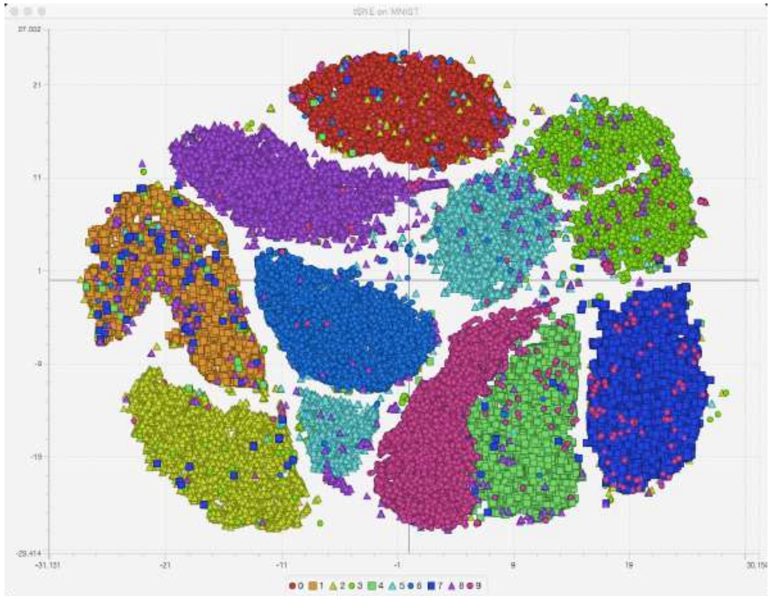

Finding a clear boundary between clusters may be hard in the real world

Clustering: A Hard Problem

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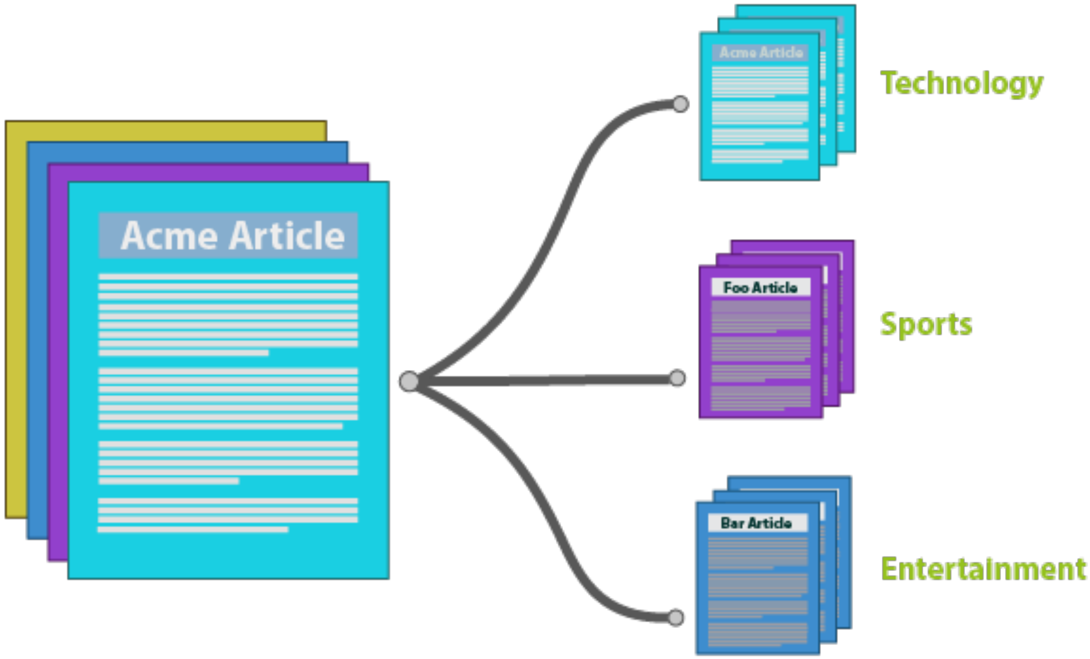
Many real-world applications involve 10s, 100s, or 1,000s of dimensions

In high-dimensional spaces almost all pairs of points are at the same (large) distance

Example: Text Document Clustering



source: https://towardsdatascience.com/applying-machine-learning-to-classify-an-unsupervised-text-document-e7bb6265f52

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- **Problem:** Group together documents on the same **topic**
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- **Key Issues:**
    - Representing documents (in the space of words)
    - Measuring document similarity (in the space of words)

Document Representation

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  - As a **set of words** (disregarding the order and multiplicity)
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  - As a **bag-of-*n*-grams** (i.e., the more general case of bag-of-words)
  - More advanced representations derived from (Large) Neural Language Models (e.g., word2vec, BERT, Transformers)
- The choice of document representation affects the similarity measure

Document Representation: Set of Words

doc 1

John likes to watch movies. Mary likes movies too.

doc 2

Mary also likes to watch football games.

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John likes to watch movies. Mary likes movies too.

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Mary also likes to watch football games.

{John, likes, to, watch, movies, Mary, too}

{Mary, also, likes, to, watch, football, games}

Document Representation: Bag-of-Words

We keep multiplicity

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John likes to watch movies. Mary likes movies too.

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Document Representation: Bag-of-Words

We keep multiplicity

doc 1

John likes to watch movies. Mary likes movies too.

{
John:1, likes:2, to:1, watch:1,
movies:2, Mary:1, too:1
}

doc 2

Mary also likes to watch football games.

{
Mary:1, also:1, likes:1, to:1,
watch:1, football:1, games:1
}

Document Representation: Bag-of-Words

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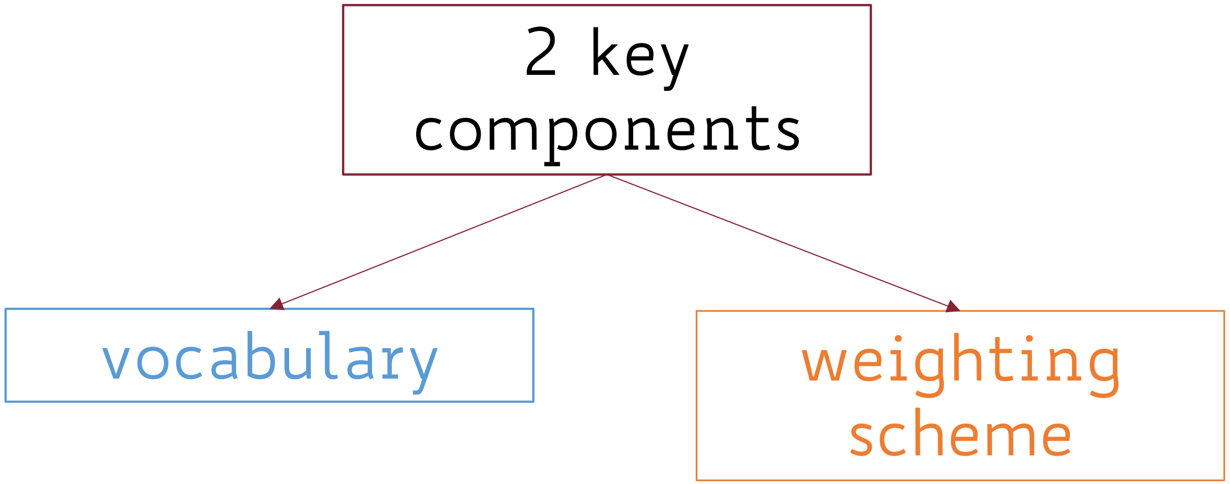

Bag-of-Words:Vocabulary

doc 1

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V = {also, football, games, John, likes, Mary, movies, to, too, watch}

Bag-of-Words: Weighting Scheme

doc 1

John likes to watch movies. Mary likes movies too.

A |V|-dimensional vector, where the i-th component indicates the multiplicity of the i-th word of the vocabulary

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Bag-of-Words: Weighting Scheme

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(0, 0, 0, 1, 2, 1, 2, 1, 1, 1)

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Bag-of-Words: Weighting Scheme

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Mary also likes to watch football games.

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Bag-of-Words: Weighting Scheme

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Mary also likes to watch football games.

A |V|-dimensional vector, where the i-th component indicates the multiplicity of the i-th word of the vocabulary

(1, 1, 1, 0, 1, 1, 0, 1, 0, 1)

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Bag-of-Words: A Formal Perspective

$D = \{d_1, \ldots, d_N\} =$ collection of N documents

$V = \{w_1, \ldots, w_{|V|}\} =$ **vocabulary** of $|V|$ words extracted from D

$\mathbf{d}_i = (f(w_1, i), \ldots, f(w_{|V|}, i)) = |V|$-dimensional vector representing d_i

$f : V \times D \longmapsto \mathbb{R}$ is a function that maps each word of a document to a real value (**weighting scheme**)

Bag-of-Words: A Formal Perspective

$\boxed{\text{One-Hot (binary) weighting scheme}}$

$$f(w_j, i) = \begin{cases} 1 & \text{if } w_j \text{ appears in } d_i \\ 0 & \text{otherwise} \end{cases}$$

Bag-of-Words: A Formal Perspective

Term-Frequency weighting scheme

$$f(w_j, i) = tf(w_j, i)$$

tf computes the number of times word w_j occurs in document d_i

Bag-of-Words: A Formal Perspective

$\boxed{\text{TF-IDF weighting scheme}}$

$$f(w_j, i) = tf(w_j, i) * idf(w_j)$$

$$idf(w_j) = \log\left(\frac{N}{n_j}\right)$$

n_j is the number of documents in D containing the word w_j

Bag-of-Words: A Formal Perspective

TF-IDF weighting scheme

$$f(w_j, i) = tf(w_j, i) * idf(w_j)$$

$$idf(w_j) = \log\left(\frac{N \boxed{+1}}{n_j \boxed{+1}}\right)$$

Any idea why?

n_j is the number of documents in D containing the word w_j

BoW: Limitations and Improvements

- **2 main limitations** of BoW model:
  - High dimensionality → sparseness
  - No sequential information nor semantics included → unigram model

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- **2 main limitations** of BoW model:
  - High dimensionality → sparseness
  - No sequential information nor semantics included → unigram model
- Possible improvements:
  - Use *n*-grams rather than unigrams to capture sequentiality between consecutive words (i.e., context)
  - Even better, use so-called Neural Language Models like word2vec, BERT, and, more recently, Transformers (LLMs)

Bag-of-*n*-grams

Example: bigrams (n=2)

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Bag-of-*n*-grams

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Mary also likes to watch football games.

{"John likes", "likes to", "to watch",
"watch movies", "Mary likes",
"likes movies", "movies too"}

{"Mary also", "also likes", "likes to",
"to watch", "watch football", "football games"}

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- Depending on those, several similarity measures can be used
- For example, if documents are represented as:
  - set of words → Jaccard coefficient
  - one-hot bag-of-words → Euclidean distance
  - tf or tf-idf bag-of-words → Cosine similarity

High-Dimensional Spaces

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- In the word space, the size of the vocabulary can be very high!
- Moreover, only few dimensions are non-zero
- Other domains like images, audio, etc. suffer from the same issue

High-Dimensional Spaces

- Data in a high-dimensional space tends to be **sparser** than in lower dimensions

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- Data in a high-dimensional space tends to be **sparser** than in lower dimensions
- Data points are **more dissimilar** to each other

High-Dimensional Spaces

- In Euclidean space, the distance between two points is large as long as they are far apart along **at least one** dimension

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⇩

The Curse of Dimensionality

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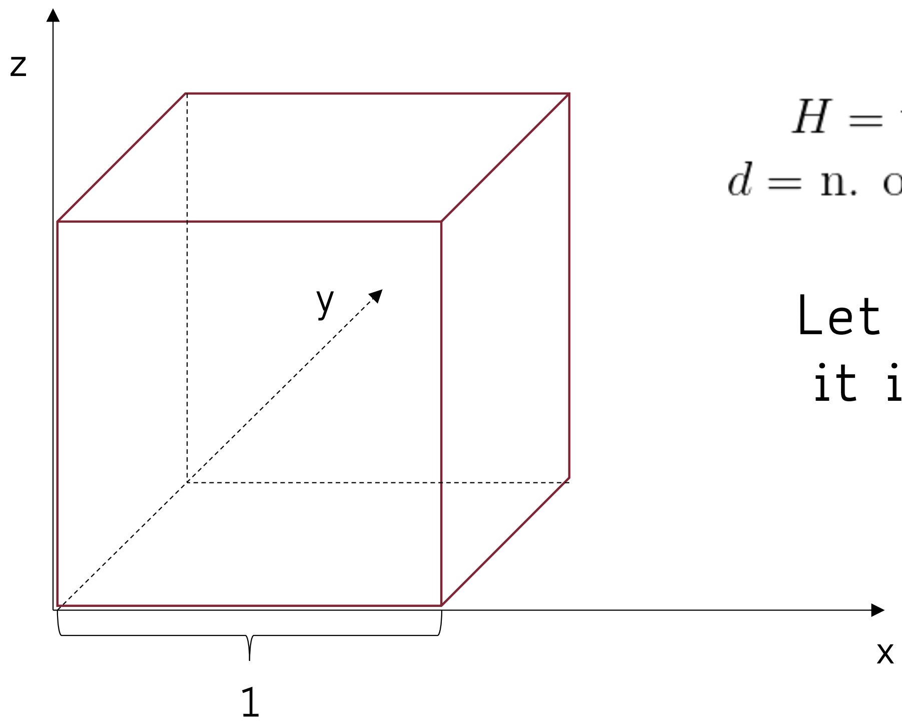
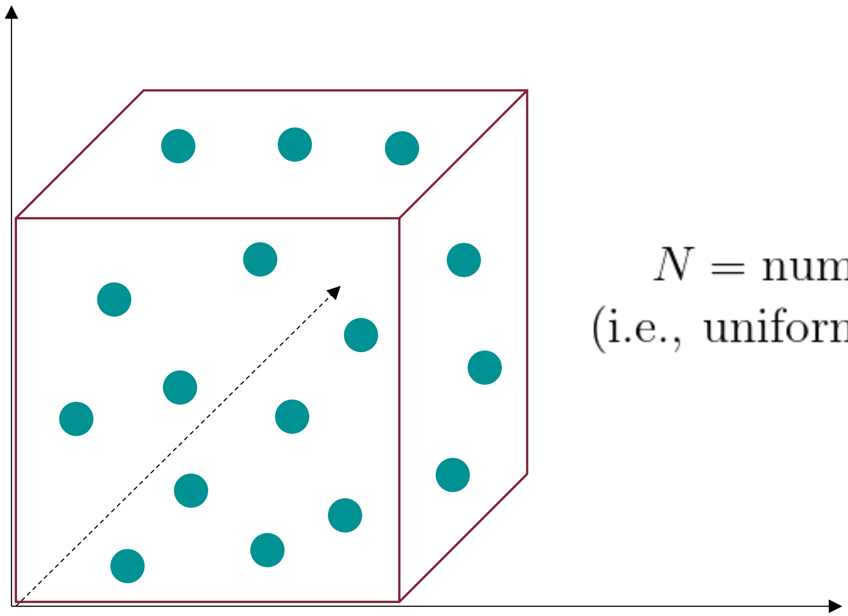


$$H = \text{unit-length hypercube in } \mathbb{R}^d$$
$$d = \text{n. of space dimensions}$$

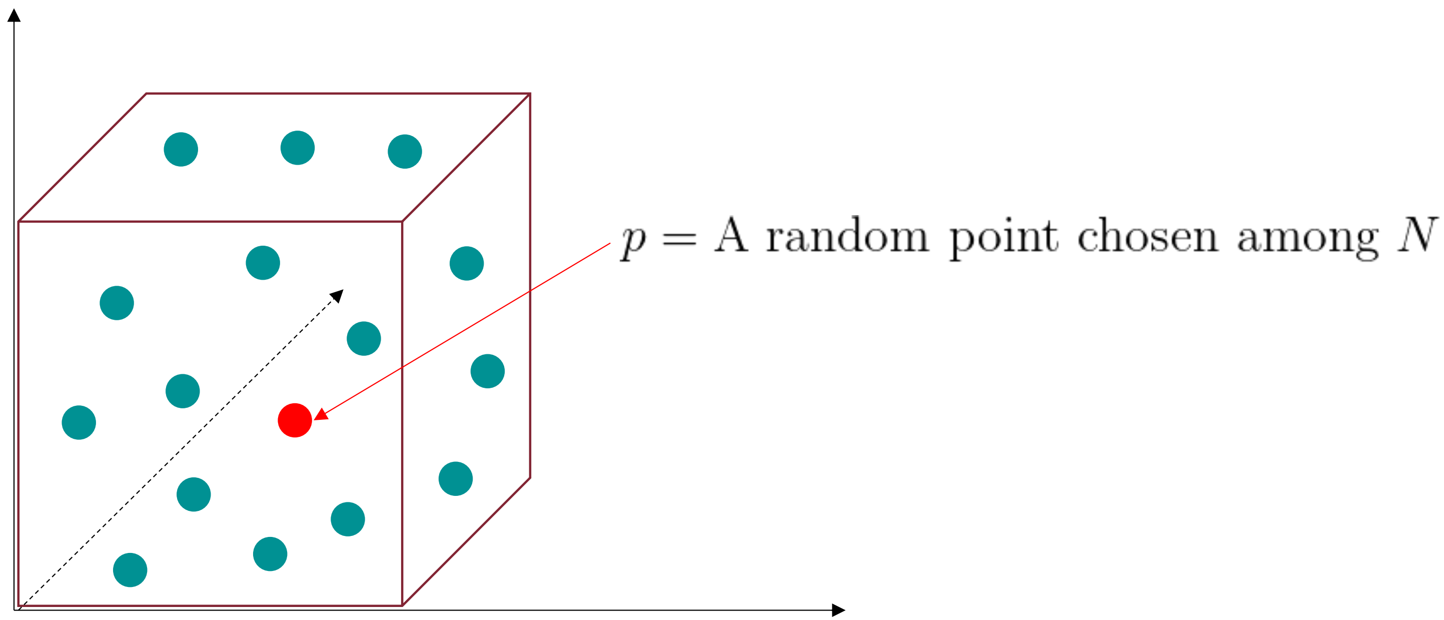
Let d=3 as beyond that it is hard to visualize the space

The Curse of Dimensionality



N = number of data points randomly (i.e., uniformly) distributed in H

The Curse of Dimensionality



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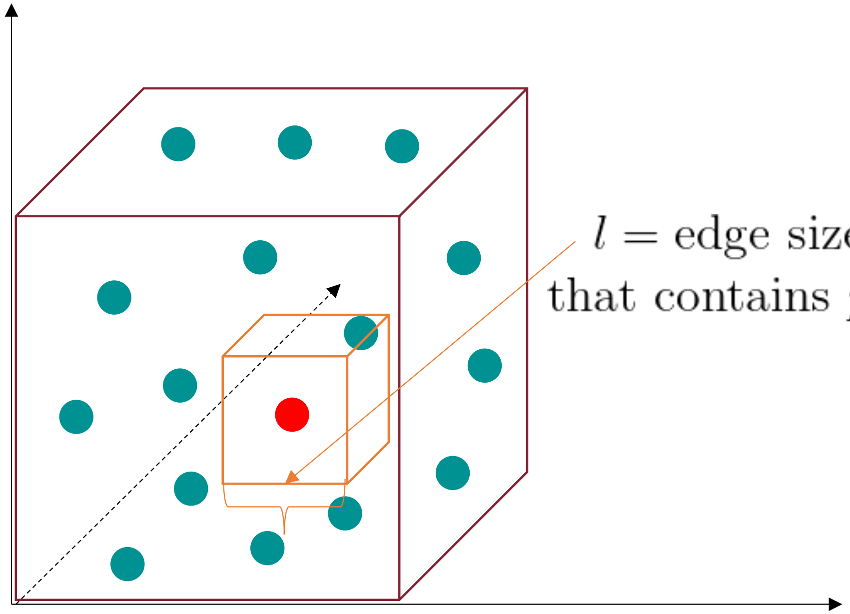
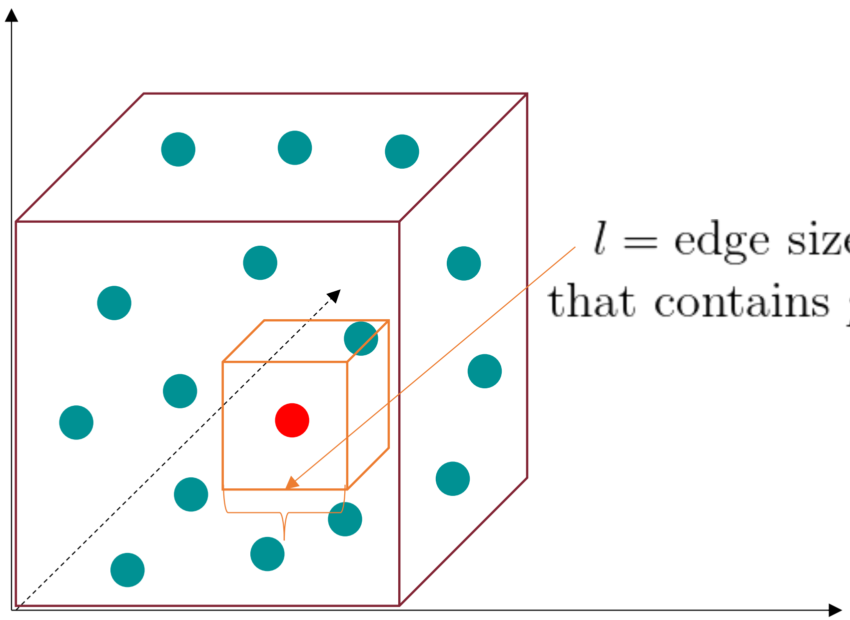


l = edge size of the hypercube h inscribed in H that contains p along with its k nearest points

The Curse of Dimensionality

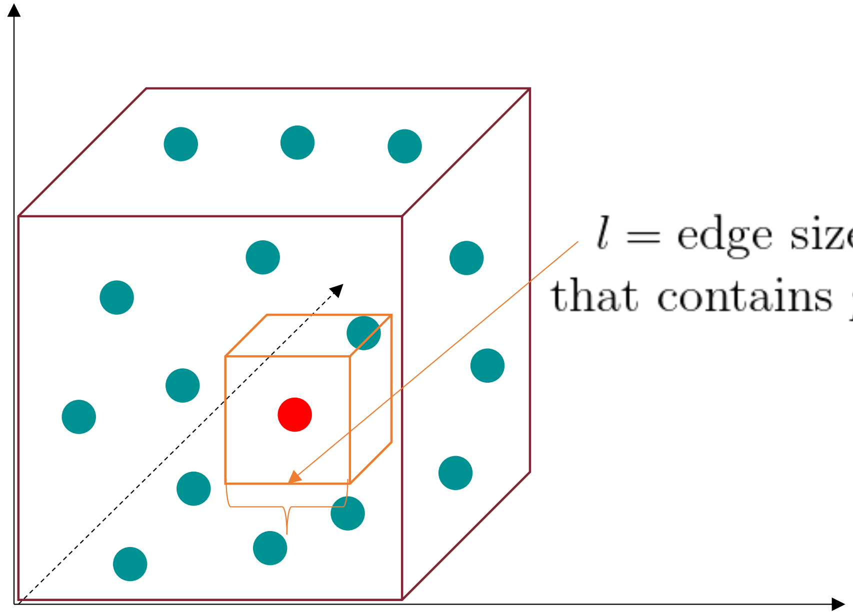


l = edge size of the hypercube h inscribed in H that contains p along with its k nearest points

We consider **edge points** whose distance from p is **at most** $\frac{l}{2}\sqrt{d}$

$$\boxed{\frac{l}{2}\sqrt{3}}$$

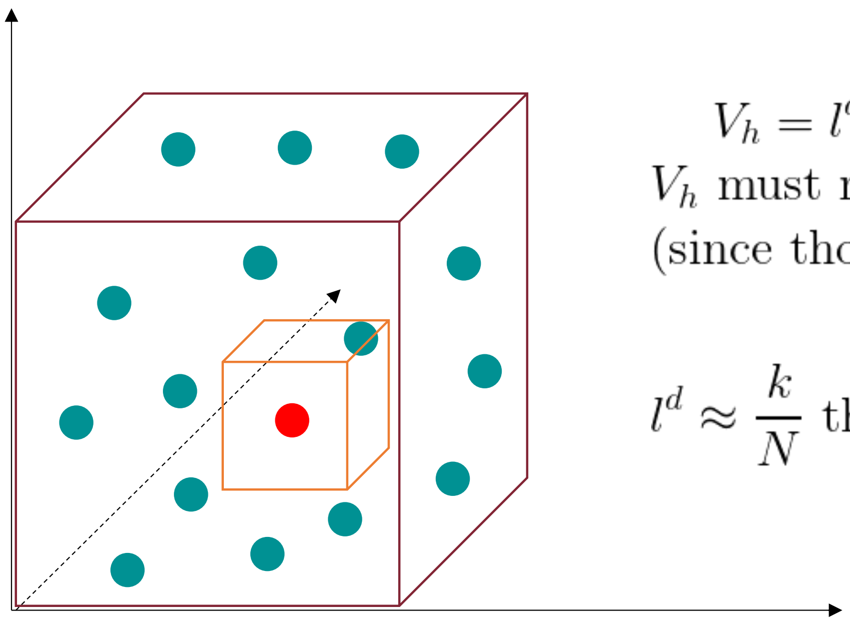
The Curse of Dimensionality



l = edge size of the hypercube h inscribed in H that contains p along with its k nearest points

The same question can be formulated in terms of the radius l of an inscribed hypersphere

The Curse of Dimensionality



$V_h = l^d$ volume of the hypercube h

V_h must roughly contain k/N points

(since those are randomly distributed)

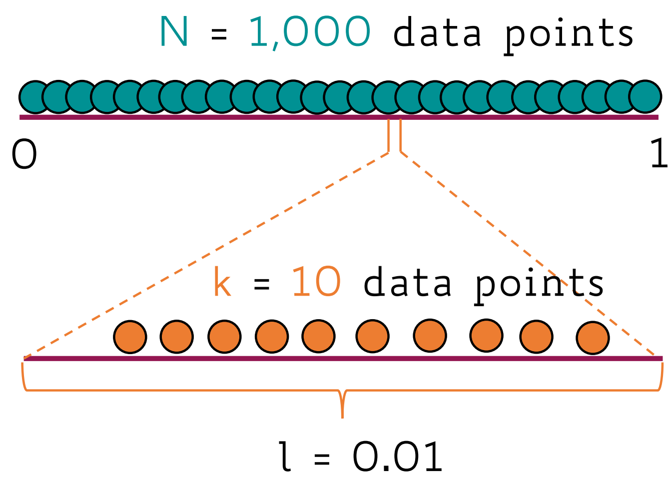
$$l^d \approx \frac{k}{N} \text{ therefore } l \approx \left(\frac{k}{N}\right)^{1/d}$$

The Curse of Dimensionality

A few numbers...

$$N = 1,000; k = 10 \quad l \approx \left(\frac{10}{1000}\right)^{1/d} = \left(\frac{1}{100}\right)^{1/d}$$

d	l
1	0.01



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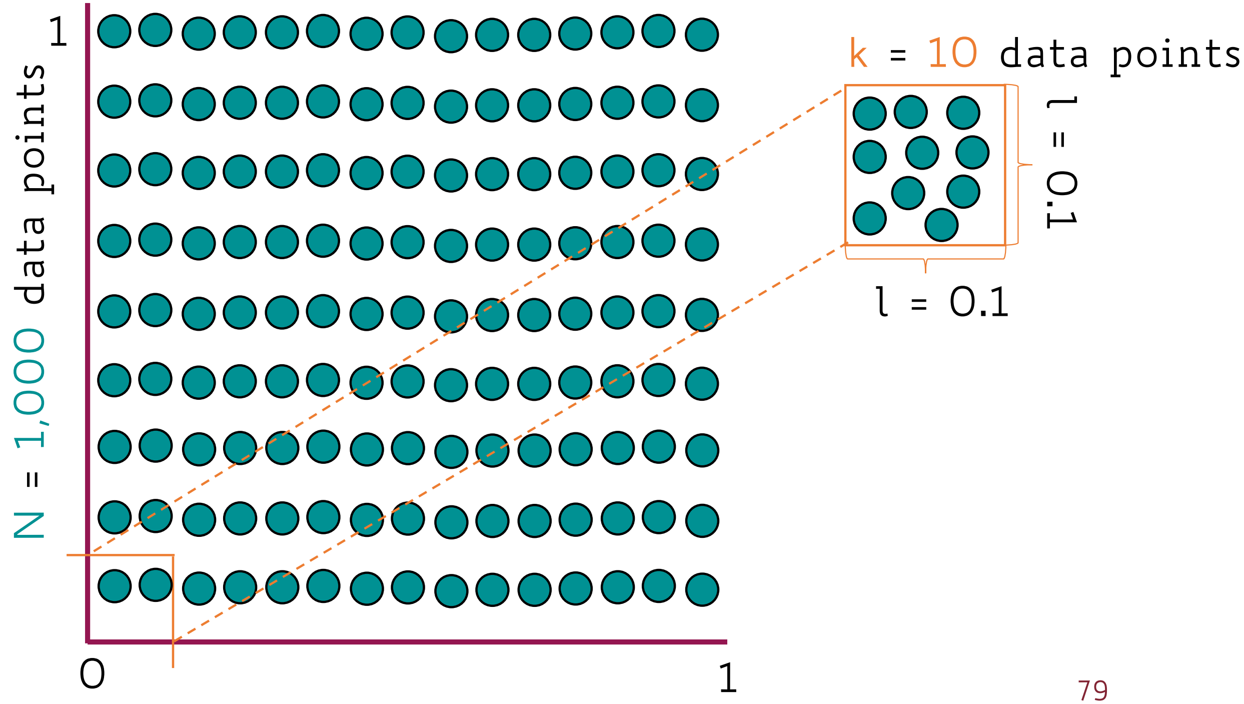
d	l
1	0.01
2	0.1



The Curse of Dimensionality

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d	l
1	0.01
2	0.1
3	0.215
...	...
10	0.631

When d is equal 10 the length of the edge of the inscribed hypercube is already about 63% of the largest hypercube

The Curse of Dimensionality

A few numbers… $N = 1,000; k = 10 \quad l \approx \left(\frac{10}{1000}\right)^{1/d} = \left(\frac{1}{100}\right)^{1/d}$

d	l
1	0.01
2	0.1
3	0.215
…	…
10	0.631
…	…
1000	0.995

When d is equal 1,000 there is basically no difference between the two hypercubes!

The Curse of Dimensionality: Why Bother?

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The Curse of Dimensionality: Why Bother?

- Points are more likely to be located at the edges of the region
- Nearest points are not close at all!
- Distance between points indistinguishable (**distance concentration**)
  - Hard to separate between nearest and furthest data points
  - Hard to find clusters among so many pairs that are all at approximately the same distance

The Curse of Dimensionality: The Edge

$\boxed{\text{Let } \varepsilon \text{ define the edge (i.e., border) of our space}}$

The Curse of Dimensionality: The Edge

Let ε define the edge (i.e., border) of our space

See how the probability of picking a data point that is not located at the edge changes as the number of dimensions grow

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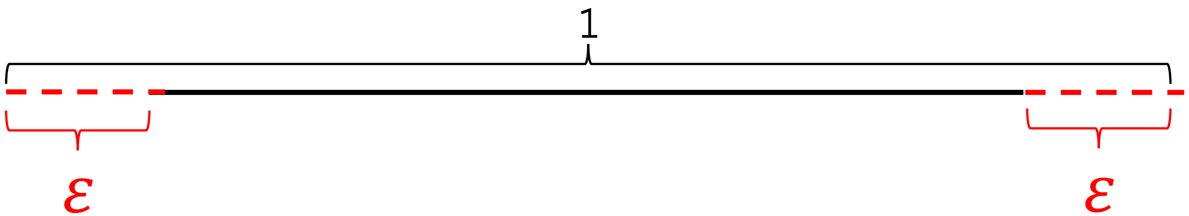
See how the probability of picking a data point that is not located at the edge changes as the number of dimensions grow

Remember:
We assume data points are uniformly distributed at random on the space

The Curse of Dimensionality: The Edge

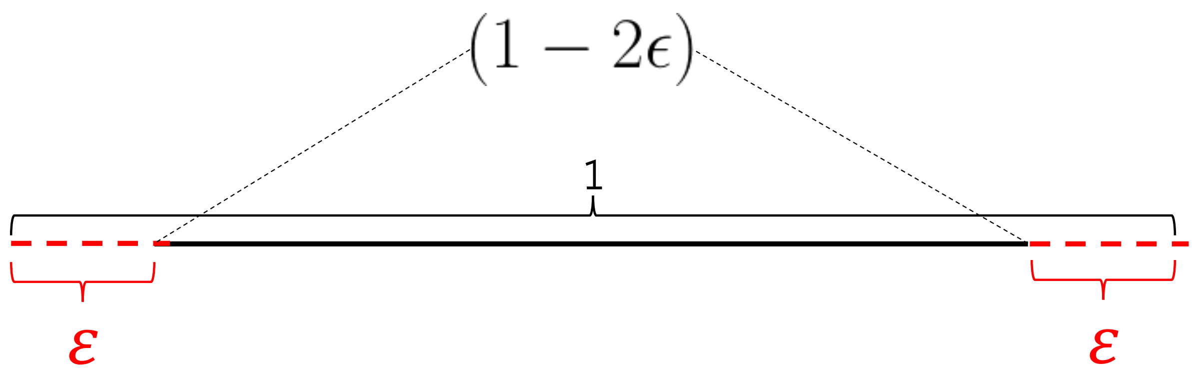
d = 1



The Curse of Dimensionality: The Edge

d = 1

The probability of being not at the edge is just



The Curse of Dimensionality: The Edge

$d > 1$

The probability of being not at the edge is the probability of being not at the edge on every single dimension

The Curse of Dimensionality: The Edge

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$$(1 - 2\epsilon)^d$$

assuming each dimension is independent from each other

The Curse of Dimensionality: The Edge

d > 1

The probability of being not at the edge is the probability of being not at the edge on every single dimension

$$(1-2\epsilon)^d$$

assuming each dimension is independent from each other

$$\lim_{d\to\infty}(1-2\epsilon)^d = 0$$

The Curse of Dimensionality

A Notebook where the Curse of Dimensionality is (visually) explained is available at the following link:

https://github.com/gtolomei/big-data-computing/blob/master/notebooks/The_Curse_of_Dimensionality.ipynb

So What Can We Do?

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- Luckily, though, real-world (interesting) data have patterns underneath (i.e., they are **not random**!)
- Lower intrinsic dimensionality

So What Can We Do?

The Manifold Hypothesis

- High dimensional data (e.g., images) lie on low-dimensional manifolds (i.e., sub-space) embedded in the high-dimensional space

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The Manifold Hypothesis

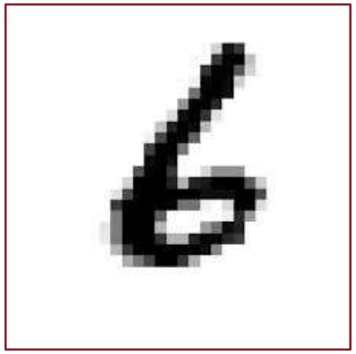
- High dimensional data (e.g., images) lie on low-dimensional manifolds (i.e., sub-space) embedded in the high-dimensional space
- Dimensionality reduction techniques (more on this later…)

Modeled vs. True Dimensionality

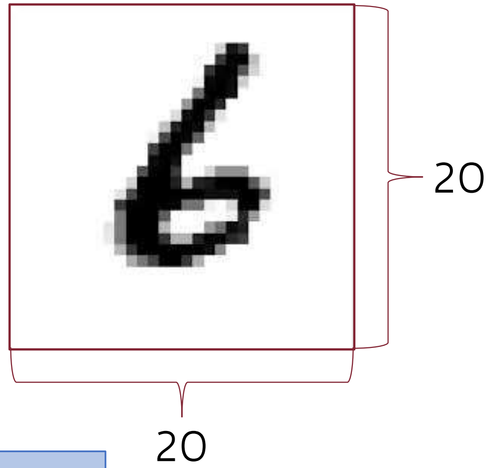
<u>Example</u>

Handwritten digit recognition

Modeled vs. True Dimensionality



Modeled vs. True Dimensionality

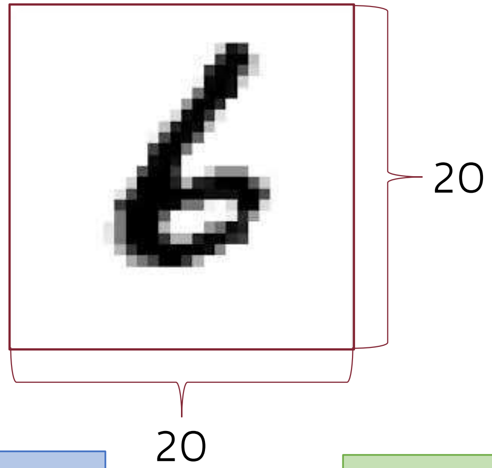


Modeled dimensionality

Each digit represented by
20x20 bitmap

400-dimensional binary vector

Modeled vs. True Dimensionality



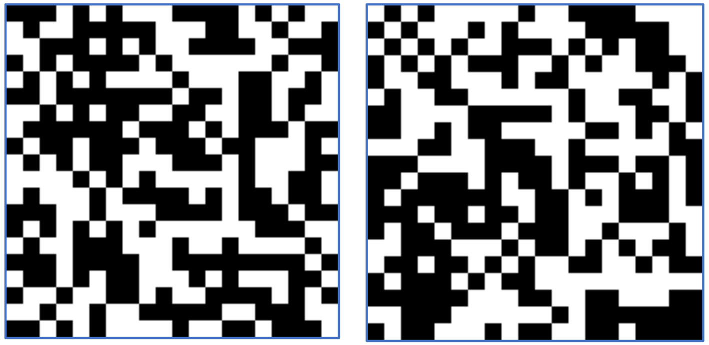
Modeled dimensionality	True dimensionality
Each digit represented by 20x20 bitmap	Actual digits just cover a tiny fraction of all this huge space
400-dimensional binary vector	Small variations of the pen-stroke

Modeled vs. True Dimensionality

Random samples from 400-d space

Modeled vs. True Dimensionality

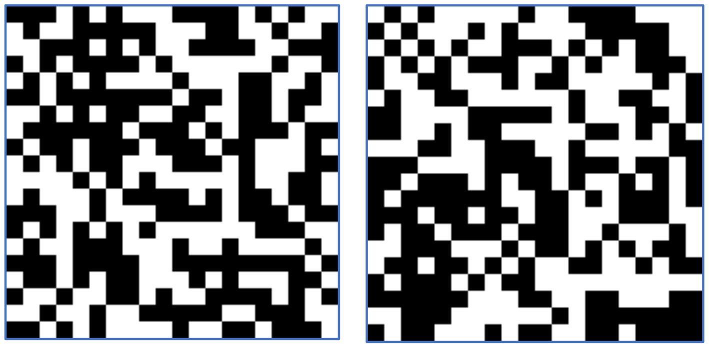
Random samples
from 400-d space



True digits living
in a
400-d space

Modeled vs. True Dimensionality

Random samples from 400-d space



True digits living in a 400-d space

We model data (i.e., digits) as very high dimensional…

… In fact, they are not so

Take-Home Message of Today

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- For example, clustering is an unsupervised learning technique to group "similar" objects together
- Depends on:
  - object representation
  - similarity measure

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- In the Euclidean space, when data dimensionality gets large, similarity/distance becomes meaningless!
- Any set of random data points are far away from each other → **curse of dimensionality**
- Luckily, real-data may live in lower-dimensional spaces