# VLDB 2020 Tutorial

# Similarity Query Processing for High-Dimensional Data


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# Outline



- Introduction
- Exact Query Processing
- Approximate Query Processing
- Selectivity Estimation
- Open Problems

# Introduction

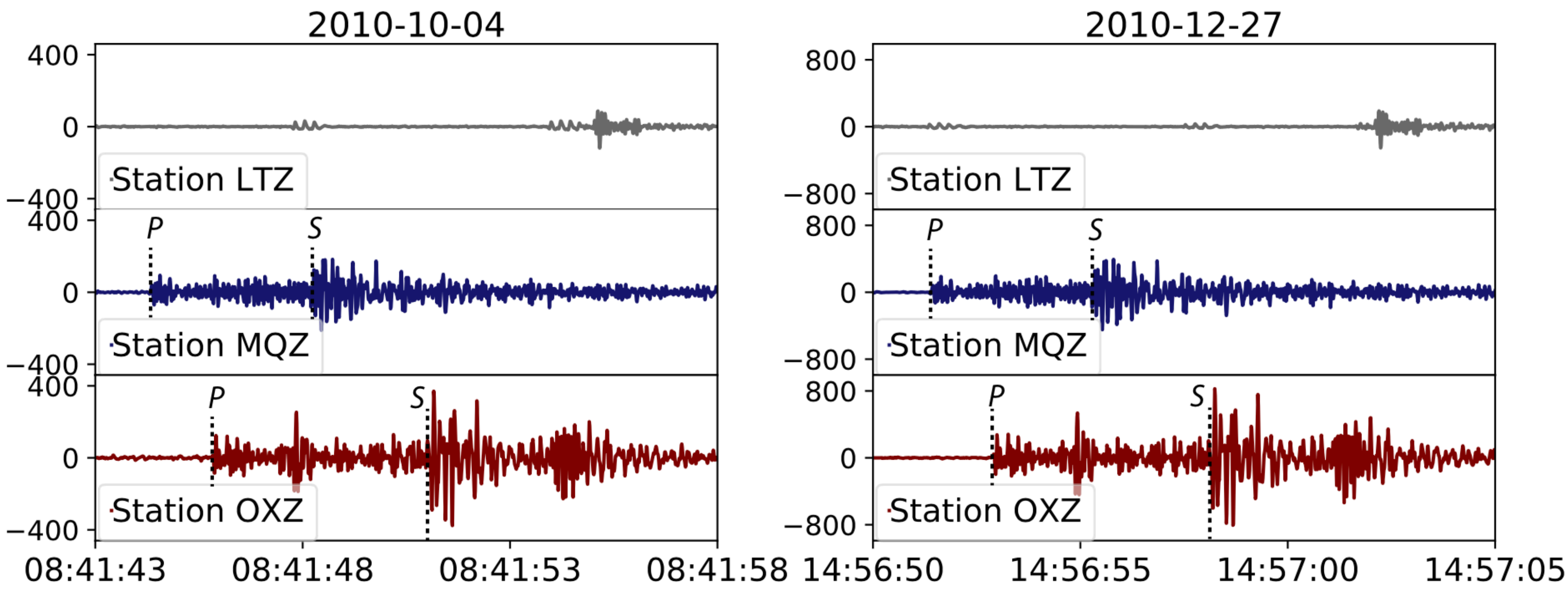


- High-dimensional data is abundant
  - Traditional sources:
    - **Time-series** [EZPB19], scientific applications
    - Document, multimedia, strings, feature vectors
  - New data sources:
    - Embedding from deep learning models
- Growing size and complexity
  - Web, social network, IoT
  - NOAA (USA) collects 100TB sensing data / day for weather forecasting
  - A variety of similarity/distance functions concerned

# Example: Scientific Applications



- High-dimensional data in huge volumes in scientific domains [YHEB17, RYBE+18]

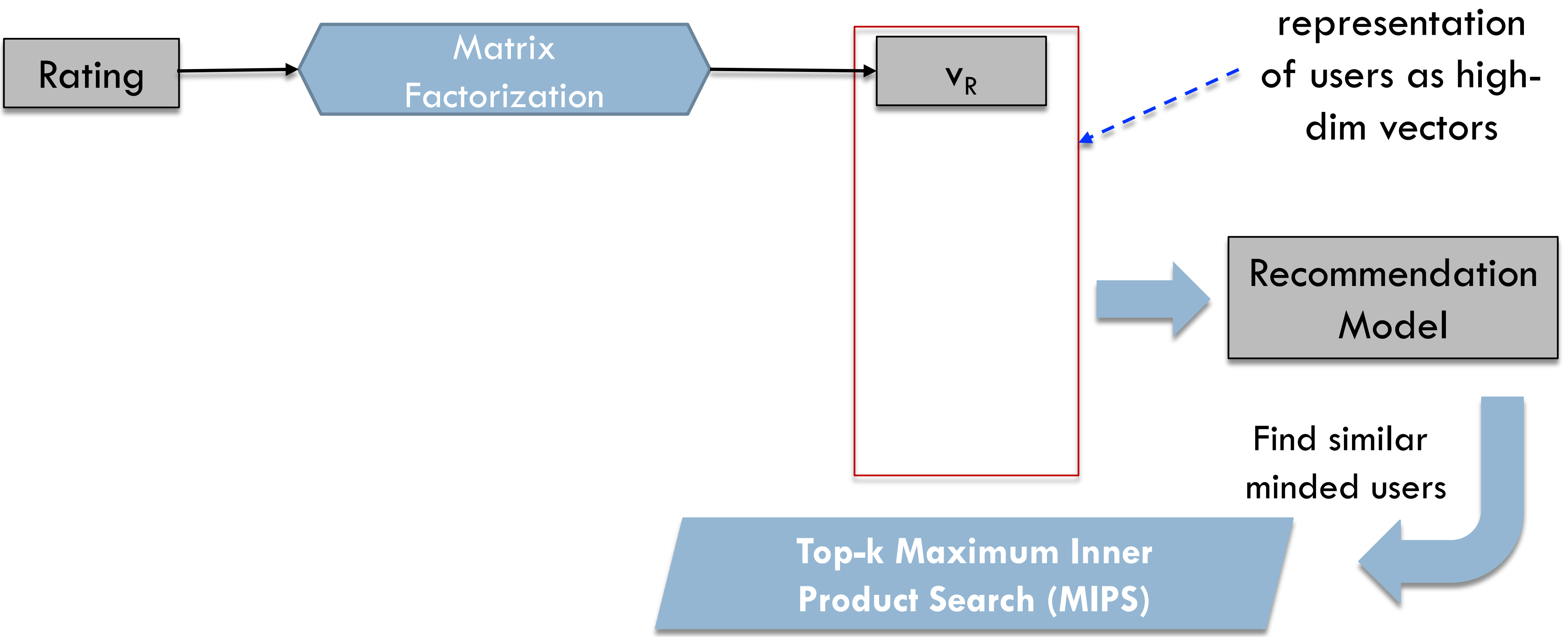



**Research Question**: Whether the magnitude 4.7 earthquake in Arkansa 2011 was caused by wastewater injection

# Example: Embedding Vectors



- DL presents a unified and engineering-friendly way to handle various information sources
  - Representation learning: e.g., embedding



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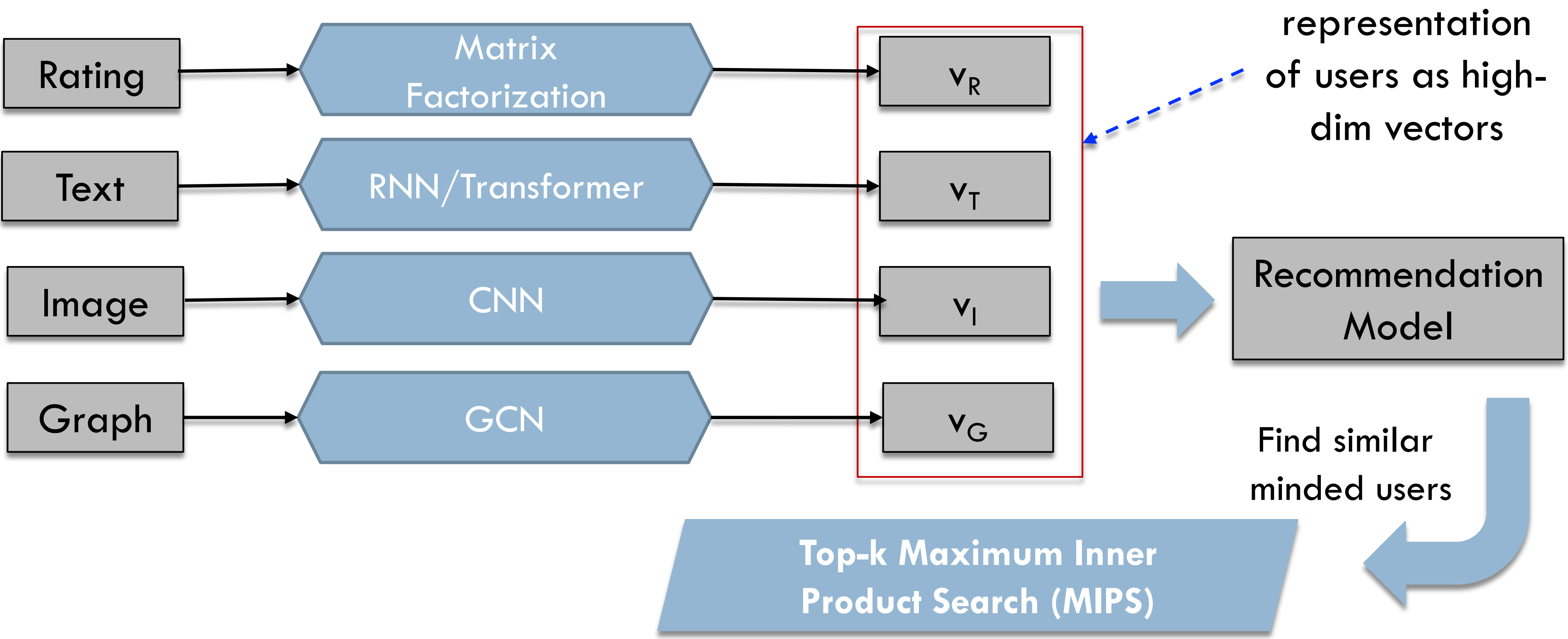


# Example: Usage in Machine/Deep Learning



- Kernel trick
  - $\varphi$: mapping low-dim feature vectors to high-dim vectors

$$\langle \varphi(x), \varphi(x') \rangle = \mathcal{K}(x, x')$$

- Feature hashing trick
  - $\varphi$: **random** mapping high-dim feature vectors to low-dim vectors

$$\mathbb{E}\left[\langle \varphi(x), \varphi(x') \rangle\right] = \langle x, x' \rangle$$

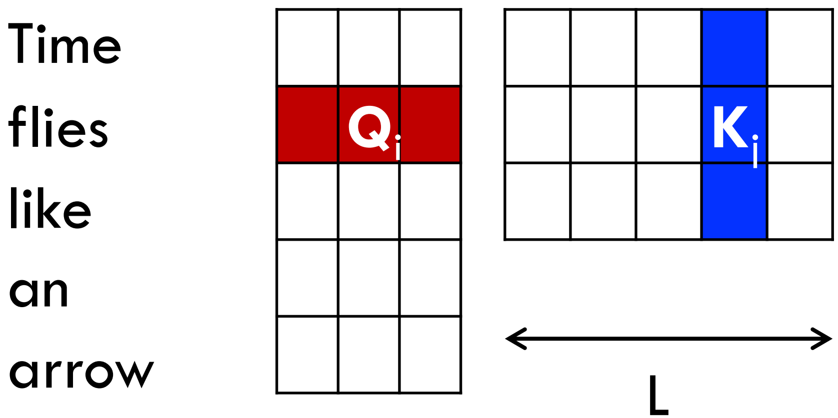
Improves efficiency, scalability and sometimes effectiveness

# Example: Usage in Machine/Deep Learning



- Reformer [KKL20]
  - Speed up self-attention

$$\mathrm{Attention}(\mathbf{Q},\mathbf{K},\mathbf{V}) = \mathrm{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}}\right)\mathbf{V}$$




Find batch top-k $\mathbf{K}_i$'s for each $\mathbf{Q}_i$

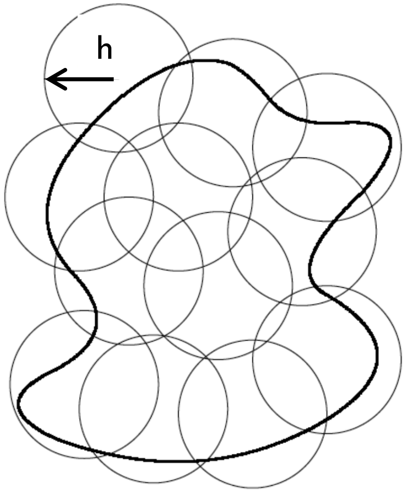
Scale to long sequences, $O(L \log L)$ instead of $O(L^2)$

# Usage in Machine/Deep Learning



- Q-learning with nearest neighbor [SX18]
  - Idea:
    - quantization of the state space X into $\{c_i\}_{i=1}^N$
    - (non-parametric) kernel ridge regression for new (x, a) values

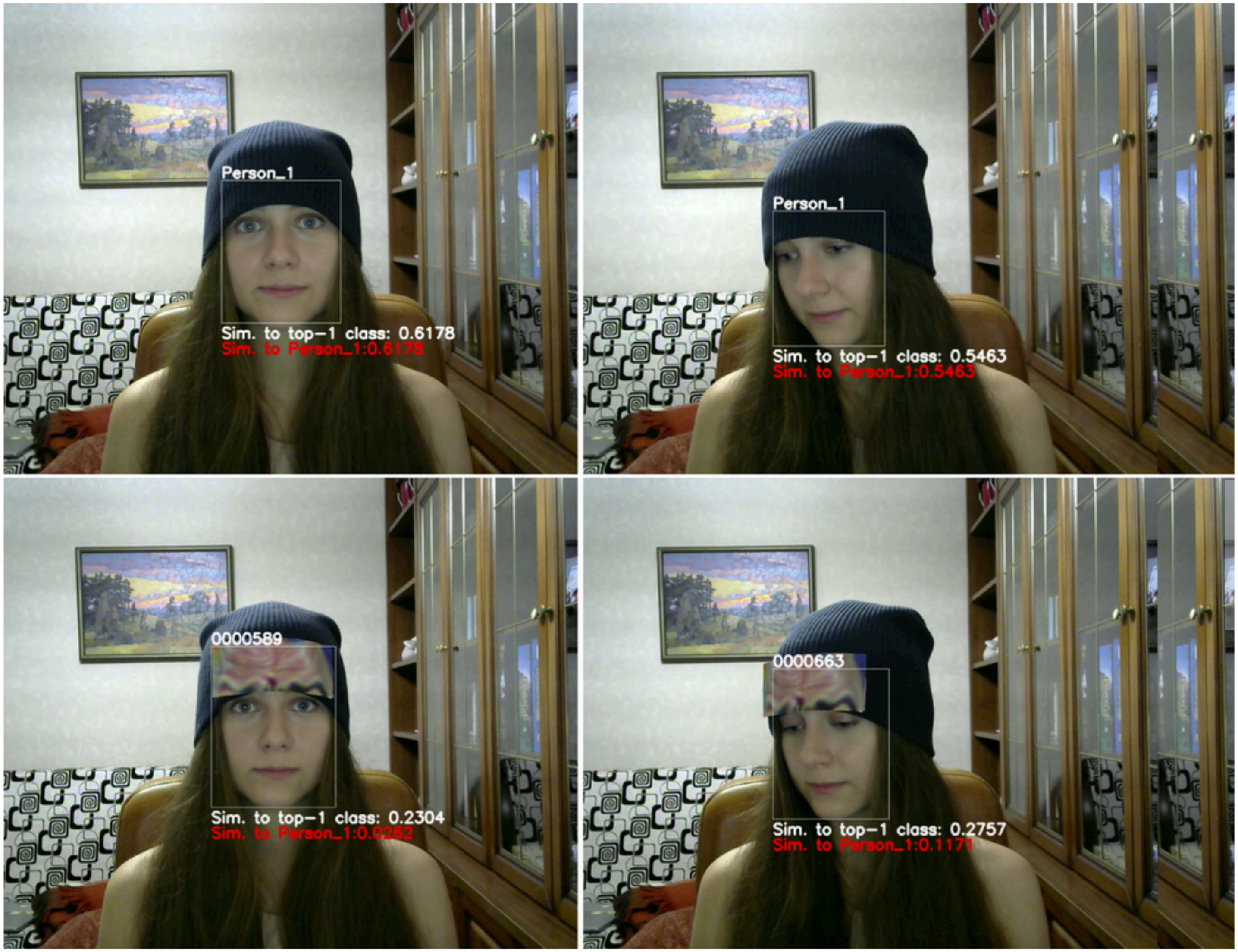
$$\hat{q}(x,a) = \sum_{i=1}^{n} K(x, c_i)\, q(c_i, a)$$
$$= \sum_{K(c,x) \le h} K(x, c)\, q(c, a)$$




Reinforcement Learning has been used in several DB problems, including Neo query optimizer [MNMZ+19]

# Example: Adversarial Machine Learning






sim ≥ 0.54

Adversarial sticker on the forehead

sim ≤ 0.28

[KP19]

# Example: Adversarial Machine Learning



- Local intrinsic dimensionality (LID) is an important feature to detect adversarial examples [MLWE+18]

$$\widehat{\mathrm{LID}}(x) = -\left(\frac{1}{k}\sum_{i=1}^{k}\log\frac{r_i(x)}{r_k(x)}\right)^{-1}$$

- High-dimensional geometry explains the existence of adversarial examples [GMFS+18]

require kNN queries

kNN queries are also useful in

- outlier/novelty detection
- kNN classification
- zero/few-shot learning

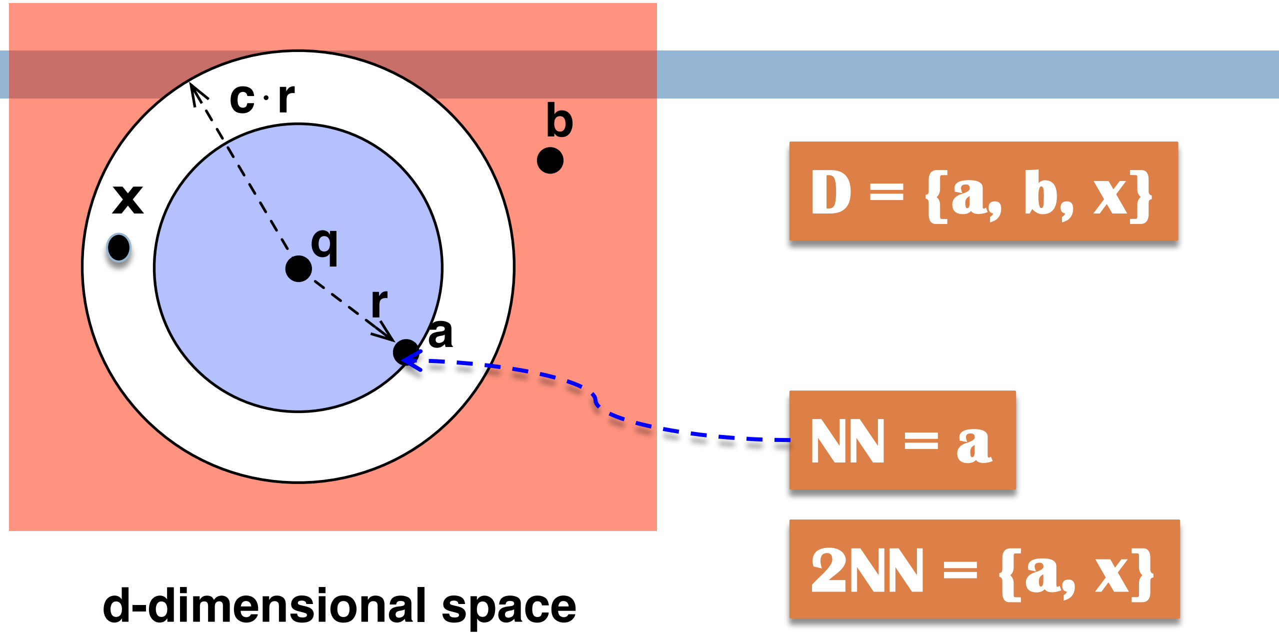
# Problem Definitions



- Database object & the query
  - d-dimensional point/vectors $\in R^d$
- Distance or similarity functions
  - dist(u, v) — $L_p$ distance ($0<p\leq 2$, $\infty$), Hamming dist, edit dist …
  - sim(u, v) — cosine similarity/inner product, Jaccard
- Query types
  - k-nearest neighbor queries (kNN)
  - range queries
  - conjunctive queries
  - similarity/distance join queries (top-k, range, closest pair, containment, …)

# NN and kNN



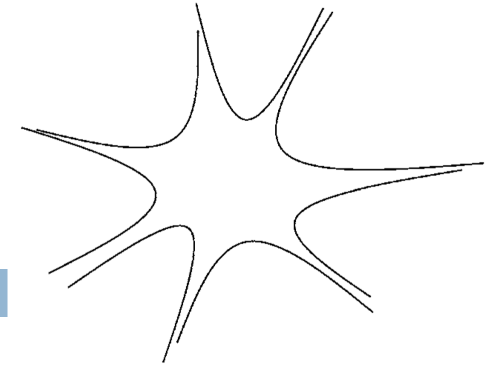



dist() is typically $L_2$ distance

- Nearest Neighbor (of q): o*
  - dist(o*, q) = min {dist(o, q), o ∈ D}
  - Generalizes to k-NN
- c-Approximate NN: o
  - dist(o, q) ≤ c * dist(o*, q)

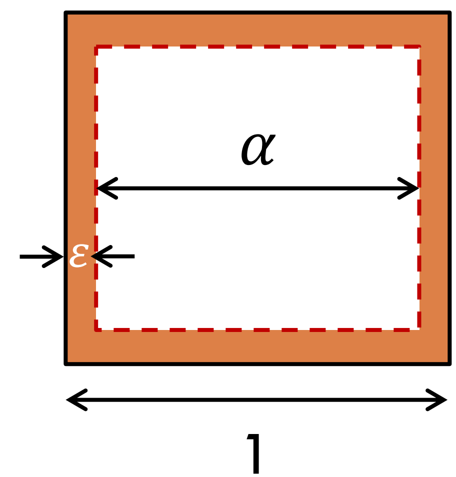
# Challenges /1

high-dimensional convex body





- Non-intuitive high-dimensional Geometry
  - Sampling uniformly within a unit hypercube ➔ samples are within a thin $\varepsilon$ 'shell'
    - Vol(r) = $\alpha^d \approx e^{-2\varepsilon d} \rightarrow 0$ ($\alpha < 1$)
  - Angle between two vectors
    - random Radamacher vectors ➔





$$\Pr\left[|\cos(\theta_{x,y})| > \sqrt{\frac{\log c}{d}}\right] < \frac{1}{c}$$

orthogonal w.h.p

Mohammed J. Zaki, Wagner Meira Jr. Data Mining and Analysis: Fundamental Concepts and Algorithms.

# Challenges /1



- Curse of Dimensionality / Concentration of Measure
  - Under some assumptions, maxdist(q, D)/mindist(q, D) converges to 1
    - Key assumption: independent distribution in each dimension
    - k-NN is still meaningful for real datasets

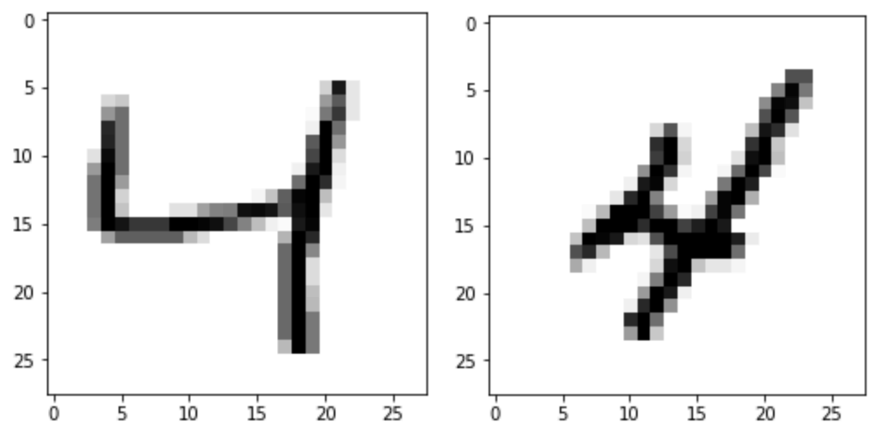
  - Hard to find algorithms sub-linear in *n* (# of points) and polynomial in d (# of dimensions)
  - Approximate version (c-ANN) is not much easier

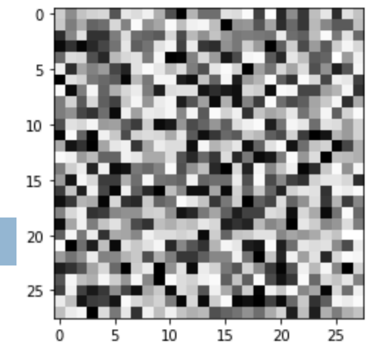
Asymptotic Geometric Analysis, Part I. Shiri Artstein-Avidan, Apostolos Giannopoulos, and Vitali Milman

# Challenges /2

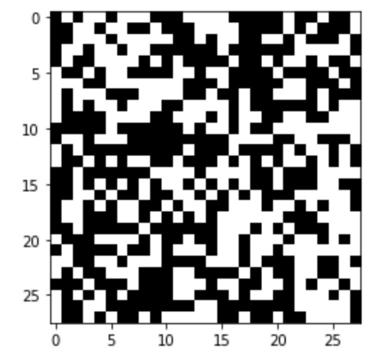


- No idea of the distribution of real data
  - Manifold hypothesis

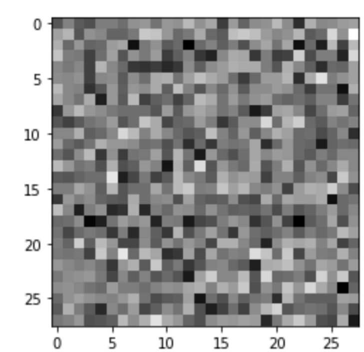




uniform



Radamacher



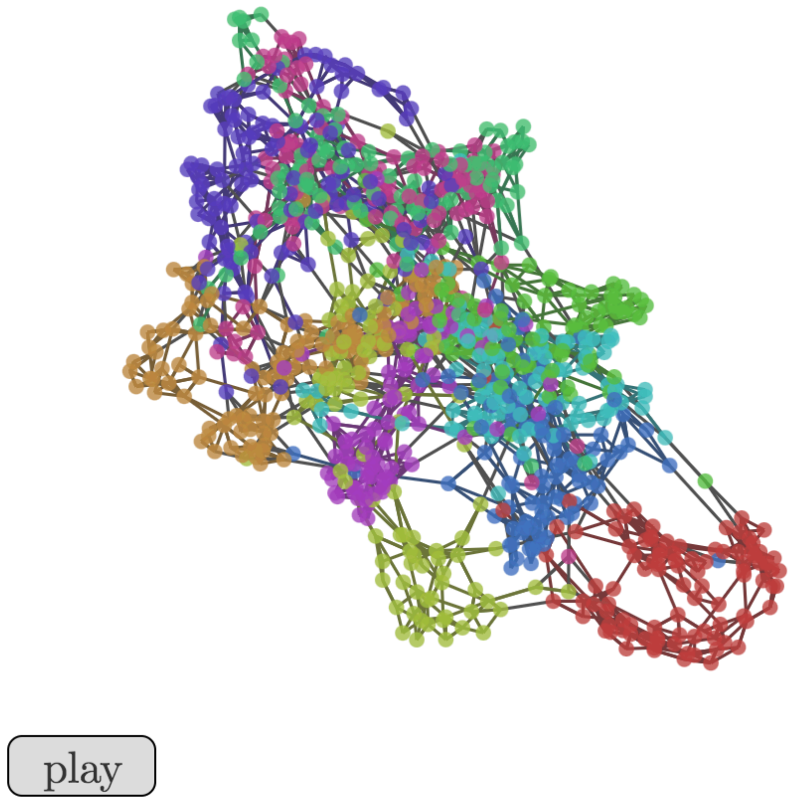
Gaussian

https://deepai.org/machine-learning-glossary-and-terms/manifold-hypothesis

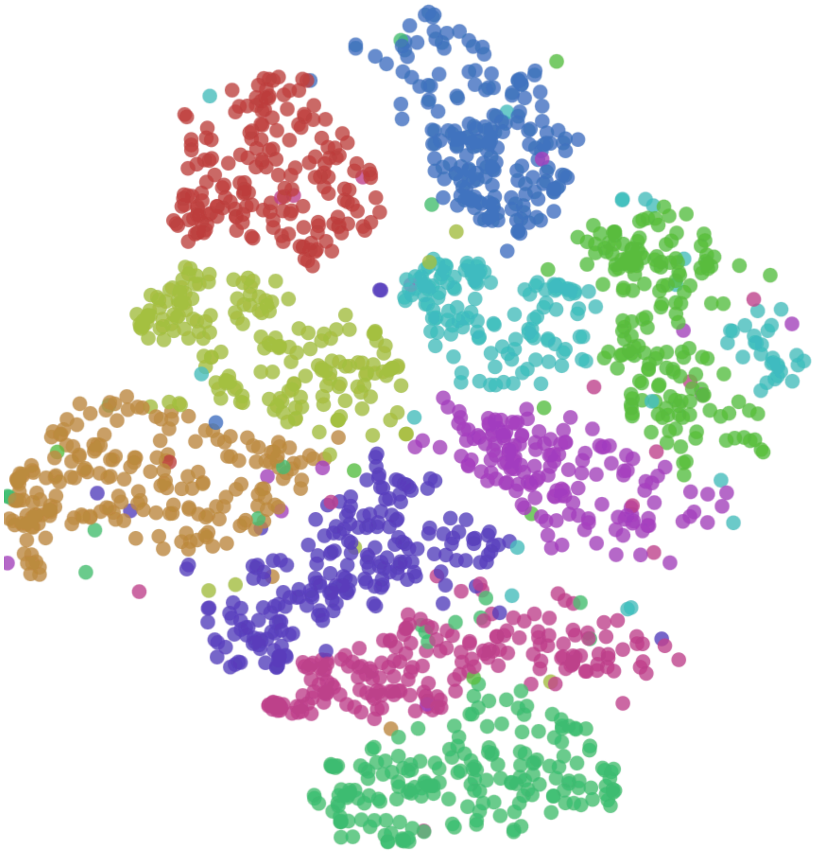
# Challenges /2



- Distribution of Real Data
  - Manifold hypothesis




Visualizing MNIST as a Graph



A t-SNE plot of MNIST

# Challenges /3



- Large data size
  - 1KB for a single point with 256 dims → 1B pts = 1TB
    - ~100 SIFT vectors per image
  - High-dimensionality (e.g., documents → millions of dimensions)
- Variety of distance/similarity functions
  - Less of an issue in the DL era