Distance Geometry in Data Science

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My line of reasoning

(Weighted) graphs are appropriate tools to model data

1. Computers can "reason by analogy"
   un/supervised ML: clustering, artificial neural networks…
2. Clustering on vectors allows more flexibility
   ANNs need vector input
3. Need to embed (weighted) graphs into Euclidean spaces
4. High dimensions make clustering expensive/unstable
5. Lower-dimensional projections improve efficiency/stability

Outline

Clustering

"Machine intelligence":
analogy based on proximity

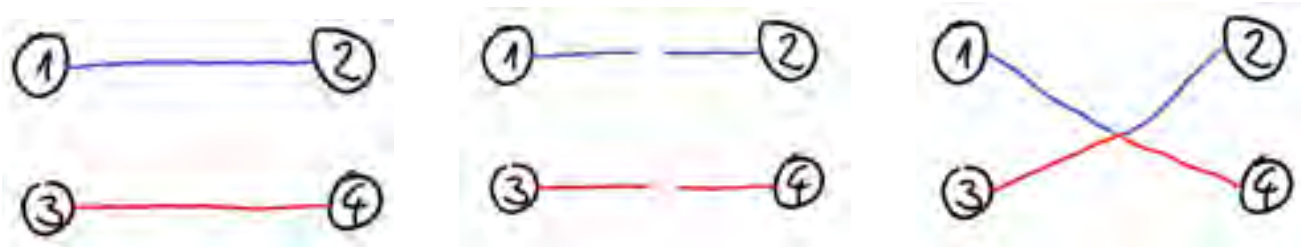
Subsection 1

Clustering in graphs

Modularity clustering

"Modularity is the fraction of the edges that fall within a cluster minus the expected fraction if edges were distributed at random."

- *"at random"* = random graphs over same degree sequence
- *degree sequence* $= (k_1, \ldots, k_n)$ where $k_i = |N(i)|$
- *"expected"* = all possible "half-edge" recombinations



- expected edges between u, v: $k_u k_v/(2m)$ where $m = |E|$
- $\mathsf{mod}(u, v) = (A_{uv} - k_u k_v/(2m))$
- $\mathsf{mod}(G) = \sum_{\{u,v\} \in E} \mathsf{mod}(u, v) x_{uv}$

  $x_{uv} = 1$ if u, v in the same cluster and 0 otherwise
- *"Natural extension" to weighted graphs:* $k_u = \sum_v A_{uv}$, $m = \sum_{uv} A_{uv}$

[Girvan & Newman 2002]

Use modularity to define clustering

- What is the "best clustering"?
- *Maximize discrepancy between actual and expected*
  "as far away as possible from average"

$$\left.\begin{array}{rl} \max & \sum_{\{u,v\}\in E} \mathsf{mod}(u,v)x_{uv} \\ \forall u \in V, v \in V & x_{uv} \in \{0,1\} \end{array}\right\}$$

- Issue: trivial solution $x = 1$ "one big cluster"
- Idea: *treat clusters as cliques*
  then clique partitioning constraints for transitivity

$$\begin{array}{lrcl} \forall i<j<k & x_{ij} + x_{jk} - x_{ik} & \leq & 1 \\ \forall i<j<k & x_{ij} - x_{jk} + x_{ik} & \leq & 1 \\ \forall i<j<k & -x_{ij} + x_{jk} + x_{ik} & \leq & 1 \\ \forall \{i,j\} \notin E & x_{ij} & = & 0 \end{array}$$

if $i, j \in C$ and $j, k \in C$ then $i, k \in C$

[Aloise et al. 2010]

Maximizing the modularity of a graph

- Modularity Maximization MP is a MILP
- *MILP is* **NP***-hard but* $\exists$ *technologically advanced solvers*
- Otherwise, use (fast) heuristics
- Unlike other methods, *this decides the number of clusters*

[Cafieri et al. 2014]

Subsection 2

Clustering in Euclidean spaces

Minimum sum-of-squares clustering

- MSSC, a.k.a. the *k-means problem* (k =#clusters)
- Given points $p_1, \ldots, p_n \in \mathbb{R}^m$, find clusters $C_1, \ldots, C_k$

$$\min \sum_{j \leq k} \sum_{i \in C_j} \|p_i - \mathsf{centroid}(C_j)\|_2^2$$

where $\mathsf{centroid}(C_j) = \frac{1}{|C_j|} \sum_{i \in C_j} p_i$

- k-means alg.: given initial clustering $C_1, \ldots, C_k$
  vars $x_{ij} = 1$ if i assigned to j (0 othw)
  1: $\forall j \leq k$ compute $y_j = \mathsf{centroid}(C_j)$
  2: $\forall i \leq n, j \leq k$ if y_j is the closest centroid to p_i let $x_{ij} = 1$ else 0
  3: $\forall j \leq k$ update $C_j \leftarrow \{p_i \mid x_{ij} = 1 \wedge i \leq n\}$
  4: repeat until stability

note that k is given (unlike modularity clustering)

[MacQueen 1967, Aloise et al. 2012]

MP formulation

$$
\left.
\begin{array}{lrcl}
\min\limits_{x,y,s} & \sum\limits_{i\le n}\sum\limits_{j\le k} \|p_i - y_j\|_2^2\, x_{ij} & & \\
\forall j \le k & \frac{1}{s_j}\sum\limits_{i\le n} p_i x_{ij} & = & y_j \\
\forall i \le n & \sum\limits_{j\le k} x_{ij} & = & 1 \\
\forall j \le k & \sum\limits_{i\le n} x_{ij} & = & s_j \\
\forall j \le k & y_j & \in & \mathbb{R}^m \\
& x & \in & \{0,1\}^{nk} \\
& s & \in & \mathbb{N}^k
\end{array}
\right\} \text{(MSSC)}
$$

MINLP: nonconvex terms; continuous, binary and integer variables

Reformulation

The (MSSC) formulation has the same optima as:

$$
\left.
\begin{array}{rrcl}
\min\limits_{x,y,P} & \sum\limits_{i\le n}\sum\limits_{j\le k} P_{ij}\, x_{ij} & & \\
\forall i \le n, j \le k & \|p_i - y_j\|_2^2 & \le & P_{ij} \\
\forall j \le k & \sum\limits_{i\le n} p_i x_{ij} & = & \sum\limits_{i\le n} y_j x_{ij} \\
\forall i \le n & \sum\limits_{j\le k} x_{ij} & = & 1 \\
\forall j \le k & y_j & \in & ([\min\limits_{i\le n} p_{ih}, \max\limits_{i\le n} p_{ih}] \mid h \le k) \\
& x & \in & \{0,1\}^{nk} \\
& P & \in & [0, P^U]^{nk}
\end{array}
\right\}
$$

- The only nonconvexities are
  products of binary by continuous bounded variables

Products of binary and continuous vars.

- Suppose term xy appears in a formulation
- Assume $x \in \{0, 1\}$ and $y \in [0, 1]$ is bounded
- means "either $z = 0$ or $z = y$"
- *Replace xy by a new variable z*
- Adjoin the following constraints:

$$\begin{aligned} z &\in [0, 1] \\ y - (1 - x) \leq z &\leq y + (1 - x) \\ -x \leq z &\leq x \end{aligned}$$

- $\Rightarrow$ Everything's linear now!

[Fortet 1959]

Products of binary and continuous vars.

- Suppose term xy appears in a formulation
- Assume $x \in \{0, 1\}$ and $y \in [y^L, y^U]$ is bounded
- means "either $z = 0$ or $z = y$"
- *Replace xy by a new variable z*
- Adjoin the following constraints:

$$\begin{aligned} z &\in [\min(y^L, 0), \max(y^U, 0)] \\ y - (1-x)\max(|y^L|, |y^U|) \leq z &\leq y + (1-x)\max(|y^L|, |y^U|) \\ -x\max(|y^L|, |y^U|) \leq z &\leq x\max(|y^L|, |y^U|) \end{aligned}$$

- $\Rightarrow$ Everything's linear now!

[L. et al. 2009]

MSSC is a convex MINLP

$$
\begin{array}{rrcll}
 & \min\limits_{x,y,P,\chi,\xi} \sum\limits_{i\le n}\sum\limits_{j\le k} \chi_{ij} & & & \\
\forall i \le n, j \le k & 0 \le \chi_{ij} & \le P_{ij} & & \\
\forall i \le n, j \le qquad & P_{ij} - (1 - x_{ij})P^U \le \chi_{ij} & \le x_{ij} P^U & & \\
\forall i \le n, j \le k & \|p_i - y_j\|_2^2 \le P_{ij} & & \Leftarrow \text{ convex} & \\
\forall j \le k & \sum\limits_{i\le n} p_i x_{ij} = \sum\limits_{i\le n} \xi_{ij} & & & \\
\forall i \le n, j \le k & y_j - (1 - x_{ij})\max(|y^L|,|y^U|) \le \xi_{ij} & \le y_j + (1 - x_{ij})\max(|y^L|,|y^U|) & & \\
\forall i \le n, j \le k & -x_{ij}\max(|y^L|,|y^U|) \le \xi_{ij} & \le x_{ij}\max(|y^L|,|y^U|) & & \\
\forall i \le n & \sum\limits_{j\le k} x_{ij} = 1 & & & \\
\forall j \le k & y_j \in [y^L, y^U] & & & \\
 & x \in \{0,1\}^{nk} & & & \\
 & P \in [0, P^U]^{nk} & & & \\
 & \chi \in [0, P^U]^{nk} & & & \\
\forall i \le n, j \le k & \xi_{ij} \in [\min(y^L, 0), \max(y^U, 0)] & & &
\end{array}
$$

y_j, ξ_{ij}, y^L, y^U are vectors in $\mathbb{R}^m$

Solving the MSSC

- k-means
  - heuristic (optimum not guaranteed)
  - fast, well-known, lots of analyses
  - scales reasonably well
  - implemented in practically all languages
- convex MINLP
  - exact (guaranteed global optima)
  - reasonably fast only for small sizes
  - scales exponentially
  - Solvers: KNITRO (commercial), Bonmin (free)
    need an MP language interpreter (AMPL)

Outline

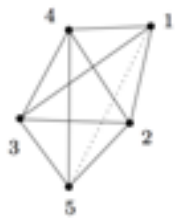
Euclidean Distance Geometry

Embedding weighted graphs in ℓ_2

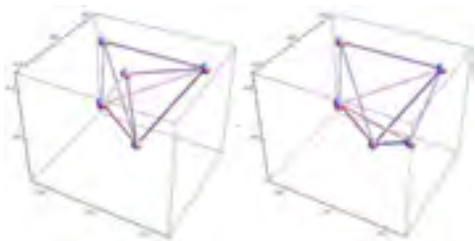
Distance Geometry Problem (DGP)

Given $K \in \mathbb{N}$ *and* $G = (V, E, d)$ *with* $d : E \to \mathbb{R}_+$,
find $x : V \to \mathbb{R}^K$ *s.t.*

$$\forall \{i, j\} \in E \quad \|x_i - x_j\|_2^2 = d_{ij}^2$$

Given a weighted graph 

, draw it so edges are drawn as segments

with lengths = weights 

[Cayley 1841, Menger 1928, Schoenberg 1935, Yemini 1978]

Subsection 1

Applications

Some applications

- clock synchronization ($K = 1$)
- sensor network localization ($K = 2$)
- molecular structure from distance data ($K = 3$)
- autonomous underwater vehicles ($K = 3$)
- distance matrix completion (whatever K)

Clock synchronization

From [Singer, *Appl. Comput. Harmon. Anal.* 2011]

Determine a set of unknown timestamps from a partial measurements of their time differences

- $K = 1$
- V: timestamps
- $\{u, v\} \in E$ if known time difference between u, v
- d: values of the time differences

Used in time synchronization of distributed networks

Sensor network localization

From [Yemini, *Proc. CDSN*, 1978]

The positioning problem arises when it is necessary to locate a set of geographically distributed objects using measurements of the distances between some object pairs

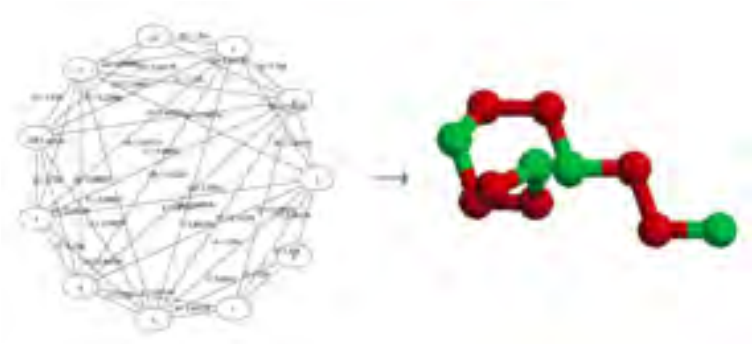
- $K = 2$
- V: (mobile) sensors
- $\{u, v\} \in E$ iff distance between u, v is measured
- d: distance values

Used whenever GPS not viable (e.g. underwater)

$d_{uv} \propto$ battery consumption in P2P communication betw. u, v

Molecular structure from distance data

From [L. et al., *SIAM Rev.*, 2014]



- $K = 3$
- V: atoms
- $\{u, v\} \in E$ iff distance between u, v is known
- d: distance values

Used whenever X-ray crystallography does not apply (e.g. liquid)

Covalent bond lengths and angles known precisely

Distances $\lesssim 5.5$ measured approximately by NMR

Subsection 2

Computational complexity

Complexity class

- DGP$_1$ with $d : E \to \mathbb{Q}_+$ is in **NP**
  - if instance YES $\exists$ realization $x \in \mathbb{R}^{n \times 1}$
  - if some component $x_i \notin \mathbb{Q}$ translate x so $x_i \in \mathbb{Q}$
  - consider some other x_j
  - let $\ell = (\text{length sh. path } p : i \to j) = \sum_{\{u,v\} \in p} d_{uv} \in \mathbb{Q}$
  - then $x_j = x_i \pm \ell \to x_j \in \mathbb{Q}$
  - $\Rightarrow$ verification of

$$\forall \{i, j\} \in E \quad |x_i - x_j| = d_{ij}$$

    in polytime
- DGP$_K$ may not be in **NP** for $K > 1$

  don't know how to verify $\|x_i - x_j\|_2 = d_{ij}$ for $x \notin \mathbb{Q}^{nK}$

Hardness

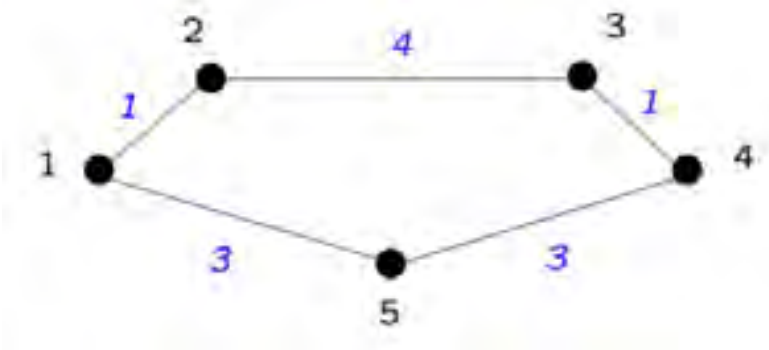
- DGP_1 is **NP**-hard by reduction from PARTITION

  Given $a = (a_1, \ldots, a_n) \in \mathbb{N}^n$, $\exists\, I \subseteq \{1, \ldots, n\}$ s.t. $\sum_{i \in I} a_i = \sum_{i \notin I} a_i$?

- $a \longrightarrow$ cycle C

  $$V(C) = \{1, \ldots, n\}, E(C) = \{\{1, 2\}, \ldots, \{n, 1\}\}$$

- For $i < n$ let $d_{i,i+1} = a_i$ and $d_{n,n+1} = d_{n1} = a_n$
- *E.g. for* $a = (1, 4, 1, 3, 3)$, *get cycle graph:*



- Argue DGP_1 is YES iff PARTITION is YES

  choose x_i *right/left of* $x_{i-1} \Leftrightarrow i \in I$ *or* $\notin I$

[Saxe, 1979]

Subsection 3

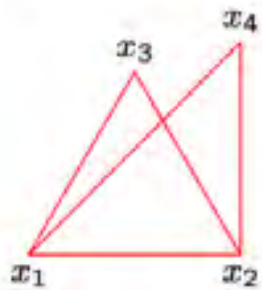
Number of solutions modulo congruences

Examples

$V^1 = \{1, 2, 3\}$
$E^1 = \{\{u, v\} \mid u < v\}$
$d^1 = 1$

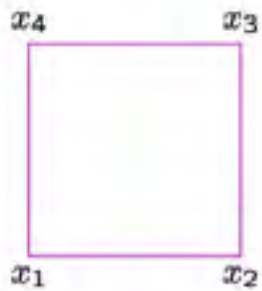
ρ congruence in $\mathbb{R}^2$
$\Rightarrow \rho x$ valid realization
$|X| = 1$

$V^2 = V^1 \cup \{4\}$
$E^2 = E^1 \cup \{\{1, 4\}, \{2, 4\}\}$
$d^2 = 1 \wedge d_{14} = \sqrt{2}$



ρ reflects x_4 wrt $\overline{x_1, x_2}$
$\Rightarrow \rho x$ valid realization
$|X| = 2$ (△, ◁)

$V^3 = V^2$
$E^3 = \{\{u, u+1\} | u \leq 3\} \cup \{1, 4\}$
$d^1 = 1$



ρ rotates $\overline{x_2x_3}$, $\overline{x_1x_4}$ by θ
$\Rightarrow \rho x$ valid realization
$|X|$ is uncountable
(□, ▱, ▱, ▱, ...)

Rigidity, flexibility and $|X|$

- infeasible $\Leftrightarrow |X| = 0$
- rigid graph $\Leftrightarrow |X| < \aleph_0$
- globally rigid graph $\Leftrightarrow |X| = 1$
- flexible graph $\Leftrightarrow |X| = 2^{\aleph_0}$
- DMDGP graphs $\Leftrightarrow |X|$ a power of 2
- $|X| = \aleph_0$: impossible by Milnor's theorem

[Milnor 1964, L. et al. 2013]

Milnor's theorem implies $|X| \neq \aleph_0$

- System S of polynomial equations of degree 2

$$\forall i \leq m \quad p_i(x_1, \ldots, x_{nK}) = 0$$

- Let X be the set of $x \in \mathbb{R}^{nK}$ satisfying S
- Number of connected components of X is $O(3^{nK})$
  [Milnor 1964]
- If $|X|$ is countably ∞ then G cannot be flexible
  $\Rightarrow$ *incongruent elts of X are separate connected components*
  $\Rightarrow$ by Milnor's theorem, there's finitely many of them

Subsection 4

MP based solution methods

Unconstrained Global Optimization

$$\min_x \sum_{\{u,v\} \in E} (\|x_u - x_v\|_2^2 - d_{uv}^2)^2 \qquad (1)$$

Globally optimal obj. fun. value of (1) is 0 iff x solves DGP

Computational experiments in [L. et al., 2006]*:*

- GO solvers from 10 years ago
- randomly generated protein data: ≤ 50 atoms
- cubic crystallographic grids: ≤ 64 atoms

Constrained global optimization

- $\min_x \sum_{\{u,v\}\in E} |\|x_u - x_v\|_2^2 - d_{uv}^2|$ exactly reformulates DGP
- Relax objective f to concave part, remove constant term, rewrite $\min -f$ as $\max f$
- Reformulate convex part of obj. fun. to convex constraints
- *Exact reformulation*

$$\left.\begin{array}{rl} \max_x & \sum_{\{u,v\}\in E} \|x_u - x_v\|_2^2 \\ \forall \{u,v\} \in E & \|x_u - x_v\|_2^2 \leq d_{uv}^2 \end{array}\right\} \quad (2)$$

[Mencarelli et al. 2017]

Linearization

$$\forall \{i,j\} \in E \quad \|x_i - x_j\|_2^2 = d_{ij}^2$$

$$\Rightarrow \quad \forall \{i,j\} \in E \quad \|x_i\|_2^2 + \|x_j\|_2^2 - 2x_i \cdot x_j = d_{ij}^2$$

$$\Rightarrow \quad \begin{cases} \forall \{i,j\} \in E & X_{ii} + X_{jj} - 2X_{ij} = d_{ij}^2 \\ & X = x\,x^\top \end{cases}$$

$$X = x\,x^\top \Leftrightarrow \forall i,j\ X_{ij} = x_i x_j$$

Relaxation

$$\begin{aligned} X &= x\,x^\top \\ \Rightarrow \quad X - x\,x^\top &= 0 \end{aligned}$$

$$\begin{aligned} \text{(relax)} \quad \Rightarrow \quad X - x\,x^\top &\succeq 0 \end{aligned}$$

$$\mathsf{Schur}(X,x) = \begin{pmatrix} I_K & x^\top \\ x & X \end{pmatrix} \succeq 0$$

If x does not appear elsewhere $\Rightarrow$ get rid of it (e.g. choose $x = 0$):

replace $\mathsf{Schur}(X,x) \succeq 0$ *by* $X \succeq 0$

Reason for this "weird" relaxation: there are efficient solvers for Semidefinite Programming (SDP)

SDP relaxation

$$\begin{aligned} & \min F \bullet X \\ \forall \{i,j\} \in E \quad X_{ii} + X_{jj} - 2X_{ij} &= d_{ij}^2 \\ X &\succeq 0 \end{aligned}$$

How do we choose F?

- For protein conformation:

$$\max \sum_{\{i,j\} \in E} (X_{ii} + X_{jj} - 2X_{ij})$$

with $=$ changed to $\leq$ in constraints *(or* min *and* $\geq$*)* [Dias & L. 2016]
"push-and-pull" the realization

When SDP solvers hit their size limit

- SDP solver: technological bottleneck
- How can we best use an LP solver?
- Diagonally Dominant (DD) matrices are PSD
- Not *vice versa*: inner approximate PSD cone $Y \succeq 0$
- *Idea by A.A. Ahmadi and co-authors*

[Ahmadi & Majumdar 2014, Ahmadi & Hall 2015]

Diagonally dominant matrices

$n \times n$ matrix X is DD if

$$\forall i \leq n \quad X_{ii} \geq \sum_{j \neq i} |X_{ij}|.$$

E.g.
$$\begin{pmatrix} 1 & 0.1 & -0.2 & 0 & 0.04 & 0 \\ 0.1 & 1 & -0.05 & 0.1 & 0 & 0 \\ -0.2 & -0.05 & 1 & 0.1 & 0.01 & 0 \\ 0 & 0.1 & 0.1 & 1 & 0.2 & 0.3 \\ 0.04 & 0 & 0.01 & 0.2 & 1 & -0.3 \\ 0 & 0 & 0 & 0.3 & -0.3 & 1 \end{pmatrix}$$

DD Linearization

$$\forall i \leq n \quad X_{ii} \geq \sum_{j \neq i} |X_{ij}| \qquad (*)$$

- introduce "sandwiching" variable T
- write $|X|$ as T
- add constraints $-T \leq X \leq T$
- by $\geq$ constraint sense, write $(*)$ as

$$X_{ii} \geq \sum_{j \neq i} T_{ij}$$

DD Programming (DDP) formulation

$$
\left.
\begin{array}{rrcl}
\min & \sum_{\{i,j\}\in E} (X_{ii} + X_{jj} - 2X_{ij}) & & \\
\forall \{i,j\} \in E & X_{ii} + X_{jj} - 2X_{ij} & \geq & d_{ij}^2 \\
\forall i \leq n & \sum_{\substack{j \leq n \\ j \neq i}} T_{ij} & \leq & X_{ii} \\
& -T \leq X & \leq & T \\
& T & \geq & 0
\end{array}
\right\}
$$

This is just an LP, much more efficient to solve than SDP!

[Dias & L., 2016]

Outline

Distance resolution limit

Clustering in high dimensions is unstable

Nearest Neighbours

k-NEAREST NEIGHBOURS (*k*-NN). *Given:*

- $k \in \mathbb{N}$
- *a distance function* $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}_+$
- *a set* $\mathcal{X} \subset \mathbb{R}^n$
- *a point* $z \in \mathbb{R}^n \setminus \mathcal{X}$,

find the subset $\mathcal{Y} \subset \mathcal{X}$ *such that:*

(a) $|\mathcal{Y}| = k$

(b) $\forall y \in \mathcal{Y}, x \in \mathcal{X} \setminus \mathcal{Y} \quad (d(z, y) \leq d(z, x))$

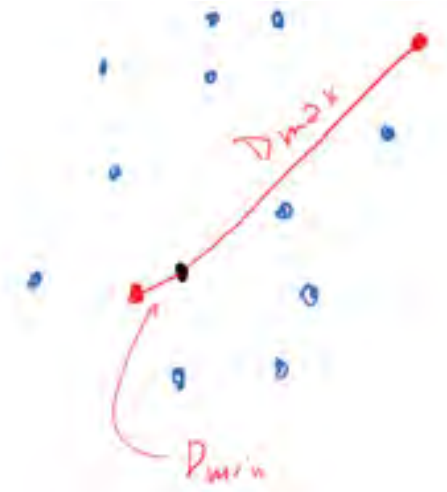
- basic problem in data science
- pattern recognition, computational geometry, machine learning, data compression, robotics, recommender systems, information retrieval, natural language processing and more
- Example: Used in Step 2 of k-means:

  assign points to closest centroid

  the two ks in k-means and k-NN are *not the same*

[Cover & Hart 1967]

With random variables



- Consider 1-NN
- Let $\ell = |\mathcal{X}|$
- Distance function family
  $\{d^m : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}_+\}_m$
- For each m:
  - random variable Z^m with some distribution over $\mathbb{R}^n$
  - for $i \leq \ell$, random variable X_i^m with some distrib. over $\mathbb{R}^n$
  - X_i^m iid w.r.t. i, Z^m independent of all X_i^m
  - $D_{\min}^m = \min_{i \leq \ell} d^m(Z^m, X_i^m)$
  - $D_{\max}^m = \max_{i \leq \ell} d^m(Z^m, X_i^m)$

Distance Instability Theorem

- Let $p > 0$ be a constant
- If

$$\exists i \leq \ell \quad (d^m(Z^m, X_i^m))^p \textit{ converges as } m \to \infty$$

then, for any $\varepsilon > 0$,

closest and furthest point are at about the same distance

Note "$\exists i$" suffices since $\forall m$ we have X_i^m iid w.r.t. i

Meaning of m: e.g. dimension

[Beyer et al. 1999]

Distance Instability Theorem

- Let $p > 0$ be a constant
- If

$$\exists i \leq \ell \quad \lim_{m \to \infty} \mathsf{Var}((d^m(Z^m, X_i^m))^p) = 0$$

then, for any $\varepsilon > 0$,

$$\lim_{m \to \infty} \mathbb{P}(D_{\text{max}}^m \leq (1 + \varepsilon) D_{\text{min}}^m) = 1$$

Note "$\exists i$" suffices since $\forall m$ we have X_i^m iid w.r.t. i

Meaning of m: e.g. dimension

[Beyer et al. 1999]

Subsection 1

When to start worrying

When the limit applies

- iid random variables from any distribution
- Particular forms of correlation
  e.g. $U_i \sim \mathsf{Uniform}(0, \sqrt{i})$, $X_1 = U_1$, $X_i = U_i + (X_{i-1}/2)$ for $i > 1$
- Variance tending to zero
  e.g. $X_i \sim \mathsf{N}(0, 1/i)$
- Discrete uniform distribution on m-dimensional hypercube
  for both data and query
- Computational experiments: instability already with $n > 15$

. . . and when it doesn't

- Complete linear dependence on all distributions
  can be reduced to NN in 1D
- Exact and approximate matching
  query point = (or ≈) data point
- Query point in a well-separated cluster in data
- Implicitly low dimensionality
  project; but NN must be stable in lower dim.

Outline

Approximate projections

Losing dimensions but not too much information

Lower dimensional (approximate) embeddings

- Given distance matrix, find approximate Euclidean embedding
- Application: visualize a metric space
  e.g. embed genealogy tree in $\mathbb{R}^3$ *(some errors allowed)*
- For visualization purposes, $K \in \{1, 2, 3\}$
  for other purposes, $K < n$

Classical methods

- Multi-Dimensional Scaling (MDS)
- Principal Component Analysis (PCA)

Subsection 1

Classic Multidimensional Scaling

Gram in function of EDM

- $x = (x_1, \ldots, x_n) \subseteq \mathbb{R}^K$, written as $n \times K$ matrix
- matrix $G = xx^\top = (x_i \cdot x_j)$ is the *Gram matrix* of x
- Schoenberg's theorem: *relation between EDMs and Gram matrices*

$$G = -\frac{1}{2} J D^2 J \qquad (\S)$$

- $D^2 = (d_{ij}^2)$, $J = I_n - \frac{1}{n}\mathbf{1}\mathbf{1}^\top$

Multidimensional scaling (MDS)

- Often get approximate EDMs $\tilde{D}$ from raw data
  (dissimilarities, discrepancies, differences)
- $\tilde{G} = -\frac{1}{2} J \tilde{D}^2 J$ is an approximate Gram matrix
- Approximate Gram $\Rightarrow$ spectral decomposition $P\tilde{\Lambda}P^\top$ has $\tilde{\Lambda} \not\geq 0$
- Let Λ be closest PSD diagonal matrix to $\tilde{\Lambda}$:
  zero the negative components of $\tilde{\Lambda}$
- $x = P\sqrt{\Lambda}$ is an "approximate realization" of $\tilde{D}$
- Dimensionality of x is $|\{\Lambda_{ii} > 0 \mid i \leq n\}|$

Subsection 2

Principal Component Analysis

Principal Component Analysis (PCA)

- *MDS with fixed K*
- Motivation: "draw" $x = P\sqrt{\Lambda}$ in 2D or 3D
  but $\mathsf{rank}(\Lambda) = K > 3$
- Only keep 2 or 3 largest components of Λ
  zero the rest
- Get realization in desired space

[Pearson 1901]

Getting primal solutions from SDP/DDP

- SDP is a *relaxation* of the original problem
- DDP is an *inner approximation* of SDP
- Both return realizations in $\mathbb{R}^n$
- We need them in $\mathbb{R}^K$
- *Use PCA to lower dimension*

Computational evaluation

- Download protein files from Protein Data Bank (PDB)

  they contain atom realizations
- Mimick a Nuclear Magnetic Resonance experiment

  Keep only pairwise distances < 5.5
- Try and reconstruct the protein shape from those weighted graphs
- Quality evaluation of results:
  - $\mathrm{LDE}(x) = \max\limits_{\{i,j\}\in E} \left| \|x_i - x_j\|_2 - d_{ij} \right|$
  - $\mathrm{MDE}(x) = \frac{1}{|E|} \sum\limits_{\{i,j\}\in E} \left| \|x_i - x_j\|_2 - d_{ij} \right|$

SDP vs. DDP: tests

SDP solved with Mosek, DDP with CPLEX

SDP/DDP + PCA

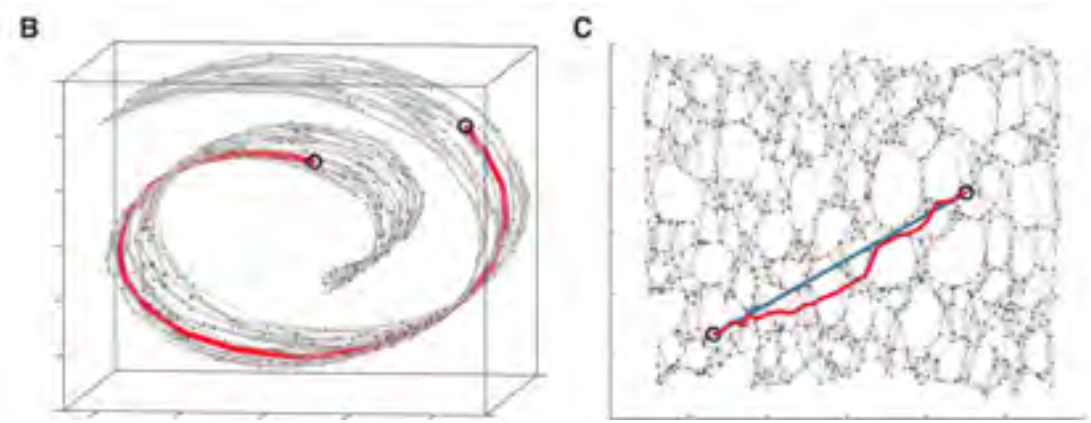
	SDP			DDP		
Instance	*LDE*	*MDE*	*CPU modl/soln*	*LDE*	*MDE*	*CPU modl/soln*
`C0700odd.1`	0.79	0.34	0.06/0.12	0.38	0.30	0.15/0.15
`C0700.odd.G`	2.38	0.89	0.57/1.16	1.86	0.58	1.11/0.95
`C0150alter.1`	1.48	0.45	0.73/1.33	1.54	0.55	1.23/1.04
`C0080create.1`	2.49	0.82	1.63/7.86	0.98	0.67	3.39/4.07
`1guu-1`	0.50	0.15	6.67/684.89	1.00	0.85	37.74/153.17

Subsection 3

Isomap for the DGP

Isomap for the DGP

1. Let D' be the (square) weighted adjacency matrix of G
2. Complete D' to *approximate* EDM $\tilde{D}$
3. MDS/PCA on $\tilde{D} \Rightarrow$ obtain embedding $x \in \mathbb{R}^K$ *for given* K



Vary Step 2 to generate Isomap heuristics

[Tenenbaum et al. 2000, L. & D'Ambrosio 2017]

Variants for Step 2

A. Floyd-Warshall all-shortest-paths algorithm on G
(classic Isomap)

B. Find a spanning tree (SPT) of G, compute any embedding $\bar{x} \in \mathbb{R}^K$ for STP, use its EDM

C. Solve a push-and-pull SDP relaxation, get soln. $\bar{x} \in \mathbb{R}^n$, use its EDM
seen previously

D. SDP with "Barvinok objective", sol. $\bar{x} \in \mathbb{R}^r$ with $r \leq \lfloor (\sqrt{8|E|+1} - 1)/2 \rfloor$, use its EDM
haven't really talked about this, sorry

Post-processing: $\tilde{x}$ *as starting point for NLP descent in GO formulation*

[L. & D'Ambrosio 2017]

Results

Comparison with `dgsol` [Moré, Wu 1997]

Instance			mde						lde						CPU					
Name	n	$\|E\|$	Isomap	IsoNLP	SPT	SDP	Barvinok	DGSol	Isomap	IsoNLP	SPT	SDP	Barvinok	DGSol	Isomap	IsoNLP	SPT	SDP	Barvinok	DGSol
C0700odd.1	15	39	0.585	0.001	0.190	0.068	**0.000**	0.135	0.989	0.004	0.896	0.389	**0.001**	0.634	**0.002**	1.456	1.589	0.906	1.305	1.747
C0700odd.2	15	39	0.599	**0.000**	0.187	0.086	**0.000**	0.128	0.985	**0.002**	0.956	0.389	0.009	1.000	**0.003**	1.370	1.226	1.002	1.063	0.887
C0700odd.3	15	39	0.599	**0.000**	0.060	0.086	**0.000**	0.128	0.985	**0.002**	0.326	0.389	0.009	1.000	**0.003**	1.259	1.256	0.861	1.167	0.877
C0700odd.4	15	39	0.599	**0.000**	0.283	0.086	0.001	0.128	0.985	**0.002**	2.449	0.389	0.008	1.000	**0.003**	1.347	1.222	0.976	1.063	1.033
C0700odd.5	15	39	0.599	**0.000**	0.225	0.086	0.000	0.128	0.985	**0.002**	0.867	0.389	0.007	1.000	**0.003**	1.284	1.157	0.987	1.100	0.709
C0700odd.6	15	39	0.599	**0.000**	0.283	0.086	0.000	0.128	0.985	**0.002**	1.520	0.389	**0.002**	1.000	**0.002**	1.372	1.196	0.998	1.305	0.909
C0700odd.7	15	39	0.585	0.001	0.080	0.068	**0.000**	0.135	0.989	0.004	0.361	0.389	**0.001**	0.634	**0.003**	1.469	1.322	0.894	1.093	1.719
C0700odd.8	15	39	0.585	0.001	0.056	0.068	**0.000**	0.135	0.989	0.004	0.275	0.389	**0.003**	0.634	**0.003**	1.408	1.300	0.692	1.079	1.744
C0700odd.9	15	39	0.585	0.001	0.057	0.068	**0.000**	0.135	0.989	0.004	0.301	0.389	**0.002**	0.634	**0.002**	1.430	1.172	0.791	1.093	1.745
C0700odd.A	15	39	0.585	0.001	0.043	0.068	**0.000**	0.135	0.989	**0.004**	0.316	0.389	**0.004**	0.634	**0.002**	1.294	1.269	0.722	1.220	1.523
C0700odd.B	15	39	0.585	0.001	0.151	0.068	**0.000**	0.135	0.989	**0.004**	1.022	0.389	**0.004**	0.634	**0.002**	1.297	1.279	0.871	1.111	1.747
C0700odd.C	15	39	0.835	**0.022**	0.033	0.039	0.031	0.025	1.012	**0.147**	0.393	0.211	0.294	0.167	**0.004**	6.803	6.369	7.371	7.030	7.000
C0700odd.D	36	242	0.835	**0.022**	0.041	0.039	0.042	0.025	1.012	**0.147**	0.423	0.211	0.268	0.167	**0.006**	6.806	6.575	7.422	7.603	7.095
C0700odd.E	36	242	0.835	**0.022**	0.064	0.039	0.031	0.025	1.012	**0.147**	0.894	0.211	0.260	0.167	**0.006**	6.911	6.638	7.365	6.979	7.008
C0700odd.F	36	242	0.599	**0.000**	0.047	0.086	**0.000**	0.128	0.985	**0.002**	0.308	0.389	0.005	1.000	**0.002**	1.299	1.310	1.008	1.100	1.040
C0150alter.1	37	335	0.786	0.058	0.066	0.014	0.015	**0.010**	0.992	0.571	0.693	0.256	0.285	**0.253**	**0.004**	9.492	9.456	10.276	10.120	9.272
C0080create.1	60	681	0.887	0.053	0.083	**0.024**	**0.024**	0.054	1.967	0.949	0.789	**0.511**	0.516	0.718	**0.012**	18.835	19.720	21.247	20.906	19.962
C0080create.2	60	681	0.887	0.053	0.047	**0.024**	**0.024**	0.054	1.967	0.949	0.585	**0.511**	0.512	0.718	**0.008**	18.791	20.009	21.728	20.885	19.740
C0020pdb	107	999	0.939	0.110	0.119	**0.059**	0.060	0.103	1.242	1.113	1.349	1.082	1.138	**0.798**	**0.035**	29.024	27.772	35.273	35.486	32.479
1guu	150	955	0.986	0.068	0.069	**0.057**	**0.057**	0.061	0.999	0.854	0.830	**0.735**	0.751	0.768	**0.048**	30.869	28.784	41.468	41.852	37.848
1guu-1	150	959	0.986	0.061	0.063	0.058	**0.057**	0.060	1.000	**0.711**	0.855	0.805	0.829	0.778	**0.053**	31.322	31.442	42.308	41.590	37.218
1guu-4000	150	968	0.974	0.081	0.080	0.072	**0.065**	0.079	1.000	0.901	**0.728**	0.760	0.961	0.826	**0.050**	30.352	29.856	42.330	39.832	42.015
C0030pkl	198	3247	0.961	0.112	0.160	**0.076**	0.077	0.137	**1.197**	1.354	2.230	1.995	2.054	1.401	**0.091**	105.175	104.775	149.192	146.360	111.859
1PPT	302	3102	0.984	**0.121**	0.129	0.128	0.129	0.123	**1.000**	1.519	1.219	1.944	1.956	1.224	**0.356**	112.448	110.345	185.815	187.182	118.681
100d	488	5741	0.987	0.146	0.146	0.155	0.157	**0.137**	**1.000**	1.577	1.397	1.764	1.749	1.358	**0.828**	229.809	213.136	659.638	659.280	233.115
GeoMean			0.74	**0.00**	0.09	0.06	**0.00**	0.08	1.07	**0.04**	0.73	0.50	0.06	0.66	**0.01**	6.30	6.04	5.93	6.63	6.30
Avg			0.76	0.04	0.11	0.07	**0.03**	0.10	1.09	**0.44**	0.88	0.63	0.47	0.77	**0.06**	36.12	25.21	49.69	49.55	27.96
StDev			0.17	0.05	0.07	**0.03**	0.04	0.04	**0.27**	0.55	0.57	0.52	0.65	0.34	**0.18**	51.69	48.82	135.08	134.97	53.26

Outline

Random projections

The mathematics of big data

Subsection 1

Barvinok's naive algorithm

Concentration of measure

From [Barvinok, 1997]

> *The value of a "well behaved" function at a random point of a "big" probability space X is "very close" to the mean value of the function.*

and

> *In a sense, measure concentration can be considered as an extension of the law of large numbers.*

Concentration of measure

Given Lipschitz function $f : X \to \mathbb{R}$ s.t.

$$\forall x, y \in X \quad |f(x) - f(y)| \leq L\|x - y\|_2$$

for some $L \geq 0$, there is *concentration of measure* if $\exists$ constants c, C s.t.

$$\forall \varepsilon > 0 \quad \mathsf{P}_x(|f(x) - \mathbb{E}(f)| > \varepsilon) \leq c\, e^{-C\varepsilon^2/L^2}$$

$\equiv$ *"discrepancy from mean is unlikely"*

Barvinok's theorem

Consider:

- for each $k \leq m$, manifolds $\mathcal{X}_k = \{x \in \mathbb{R}^n \mid x^\top Q^k x = a_k\}$
- a feasibility problem $x \in \bigcap_{k \leq m} \mathcal{X}_k$
- its SDP relaxation $\forall x \leq m \ (Q^k \bullet X = a_k)$ with soln. $\bar{X}$

Let $\boxed{T = \mathsf{factor}(\bar{X})}$, $\boxed{y \sim \mathcal{N}^n(0,1) \text{ and } x' = Ty}$

Then $\exists c$ and $n_0 \in \mathbb{N}$ s.t. if $n \geq n_0$,

$$\mathsf{Prob}\left(\forall k \leq m \ \mathsf{dist}(x', \mathcal{X}_k) \leq c\sqrt{\|\bar{X}\|_2 \ln n}\right) \geq 0.9.$$

IDEA: since x' is "close" to each $\mathcal{X}_k$
try local Nonlinear Programming (NLP)

Application to the DGP

- $\forall \{i,j\} \in E \quad \mathcal{X}_{ij} = \{x \in \mathbb{R}^{nK} \mid \|x_i - x_j\|_2^2 = d_{ij}^2\}$
- DGP can be written as $\bigcap_{\{i,j\} \in E} \mathcal{X}_{ij}$
- SDP relaxation $X_{ii} + X_{jj} - 2X_{ij} = d_{ij}^2 \wedge X \succeq 0$ with soln. $\bar{X}$

- Difference with Barvinok: $x \in \mathbb{R}^{Kn}$, $\mathrm{rk}(\bar{X}) \leq K$
- IDEA: sample $y \sim \mathcal{N}^{nK}(0, \frac{1}{\sqrt{K}})$
- Thm. Barvinok's theorem works in rank K

[L. & Vu, unpublished]

The heuristic

1. Solve SDP relaxation of DGP, get soln. $\bar{X}$
   use DDP+LP if SDP+IPM too slow

2. a. $T = \mathsf{factor}(\bar{X})$
   b. $y \sim \mathcal{N}^{nK}(0, \frac{1}{\sqrt{K}})$
   c. $x' = Ty$

3. Use x' as starting point for a local NLP solver on formulation

$$\min_x \sum_{\{i,j\} \in E} \left(\|x_i - x_j\|^2 - d_{ij}^2 \right)^2$$

and return improved solution x

[Dias & L., 2016]

SDP+Barvinok vs. DDP+Barvinok

	SDP			DDP		
Instance	*LDE*	*MDE*	*CPU*	*LDE*	*MDE*	*CPU*
C0700odd.1	0.00	0.00	0.63	0.00	0.00	1.49
C0700.odd.G	0.00	0.00	21.67	0.42	0.01	30.51
C0150alter.1	0.00	0.00	29.30	0.00	0.00	34.13
C0080create.1	0.00	0.00	139.52	0.00	0.00	141.49
1b03	0.18	0.01	132.16	0.38	0.05	101.04
1crn	0.78	0.02	800.67	0.76	0.04	522.60
1guu-1	0.79	0.01	1900.48	0.90	0.04	667.03

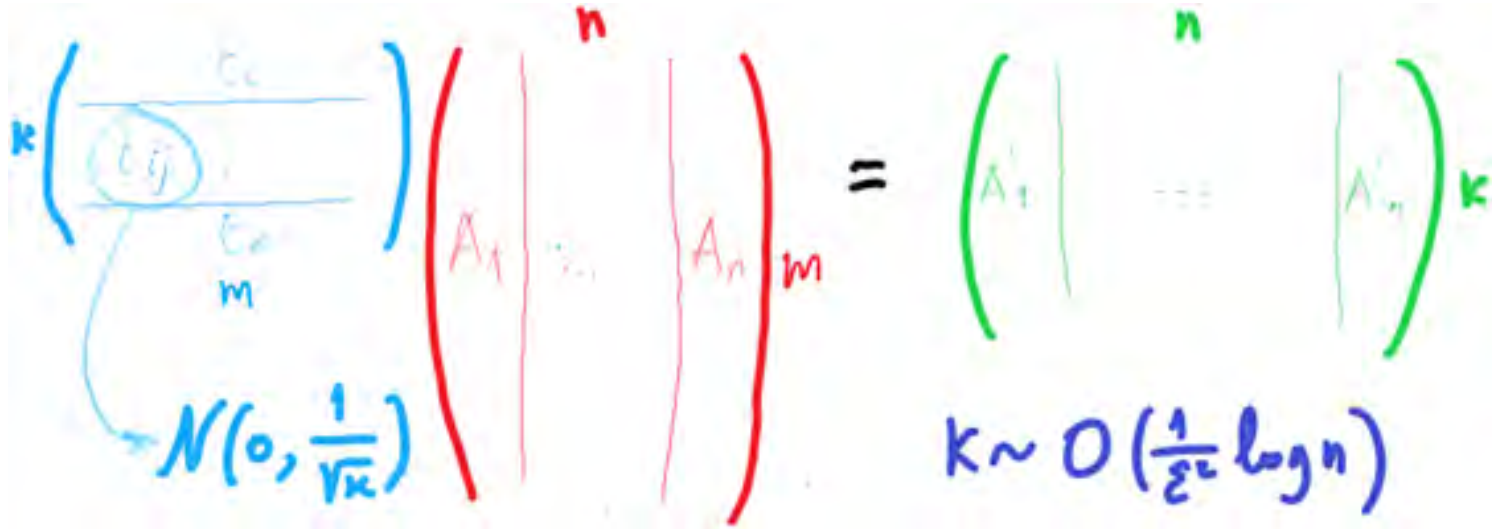
Most of the CPU time taken by local NLP solver

Subsection 2

Johnson-Lindenstrauss Lemma

Randomly losing dimensions

- *"Mathematics of big data"*
- In a nutshell



- *Clustering on* $\boxed{A'}$ *rather than* A
  yields approx. same results with arbitrarily high probability (wahp)

[Johnson & Lindenstrauss, 1984]

Randomly losing dimensions

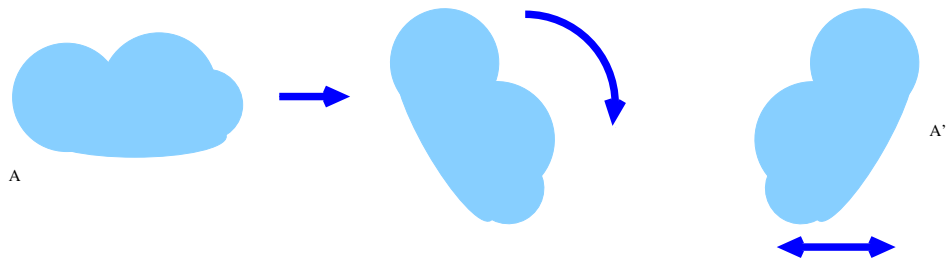
- *"Mathematics of big data"*
- In a nutshell
  1. Given points $A_i, \ldots, A_n \in \mathbb{R}^m$ with m large and $\varepsilon \in (0,1)$
  2. Pick "appropriate" $k \approx O(\frac{1}{\varepsilon^2} \ln n)$
  3. Sample $k \times d$ matrix T (*each comp. i.i.d.* $\mathcal{N}(0, \frac{1}{\sqrt{k}})$)
  4. Consider *projected* points $A'_i = TA_i \in \mathbb{R}^k$ for $i \leq n$
  5. With prob$\to$ 1 exponentially fast as $k \to \infty$

$$\forall i,j \leq n \quad (1-\varepsilon)\|A_i - A_j\|_2 \leq \|A'_i - A'_j\|_2 \leq (1+\varepsilon)\|A_i - A_j\|_2$$

[Johnson & Lindenstrauss, 1984]

The shape of a set of points

- Lose dimensions but not too much accuracy
  Given $A_1, \ldots, A_n \in \mathbb{R}^m$ find $k \ll m$ and points
  $A'_1, \ldots, A'_n \in \mathbb{R}^k$ s.t. A and A' "have almost the same shape"
- What is the shape of a set of points?



congruent sets have the same shape

- Approximate congruence $\Leftrightarrow$ distortion:
  A, A' have almost the same shape if

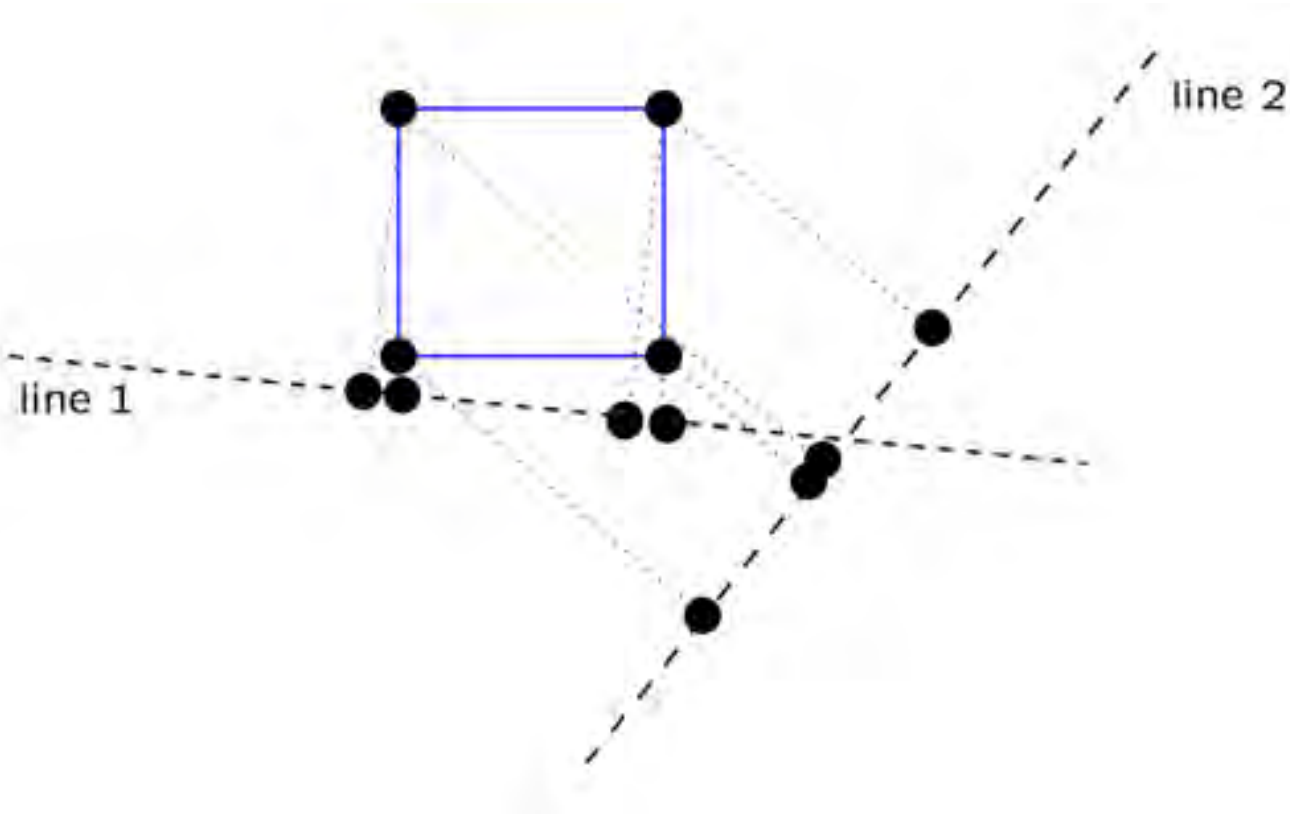
$$\forall i < j \leq n \quad (1-\varepsilon)\|A_i - A_j\| \;\leq\; \|A'_i - A'_j\| \;\leq\; (1+\varepsilon)\|A_i - A_j\|$$

  for some small $\varepsilon > 0$

Assume norms are all Euclidean

Losing dimensions = "projection"

In the plane, hopeless



In 3D: no better

Johnson-Lindenstrauss Lemma

Thm.

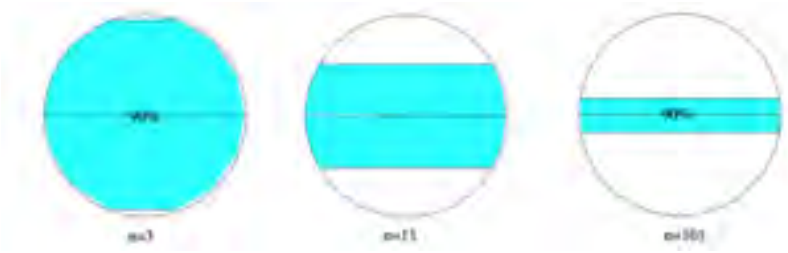
Given $A \subseteq \mathbb{R}^m$ with $|A| = n$ and $\varepsilon > 0$ there is $k \sim O(\frac{1}{\varepsilon^2} \ln n)$ and a $k \times m$ matrix T s.t.

$$\forall x, y \in A \quad (1-\varepsilon)\|x-y\| \;\leq\; \|Tx - Ty\| \;\leq\; (1+\varepsilon)\|x-y\|$$

If $k \times m$ matrix T is sampled componentwise from $\mathsf{N}(0, \frac{1}{\sqrt{k}})$, then A and TA have almost the same shape

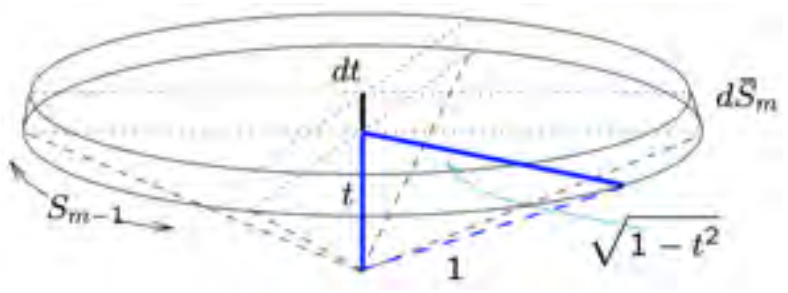
[Johnson & Lindenstrauss, 1984]

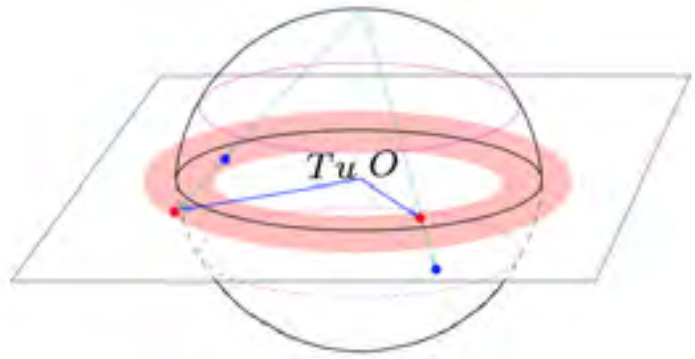
Sketch of a JLL proof by pictures

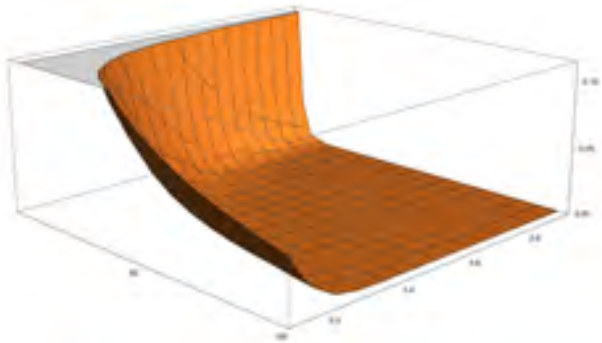


Thm.

Let T be a $k \times m$ rectangular matrix with each component sampled from $\mathsf{N}(0, \frac{1}{\sqrt{k}})$, and $u \in \mathbb{R}^m$ s.t. $\|u\| = 1$. Then $\mathbb{E}(\|Tu\|^2) = 1$







In practice

- Empirically, sample T very few times (e.g. once will do!)
  on average $\|Tx - Ty\| \approx \|x - y\|$, *and distortion decreases exponentially with* n

We only need a logarithmic number of dimensions in function of the number of points

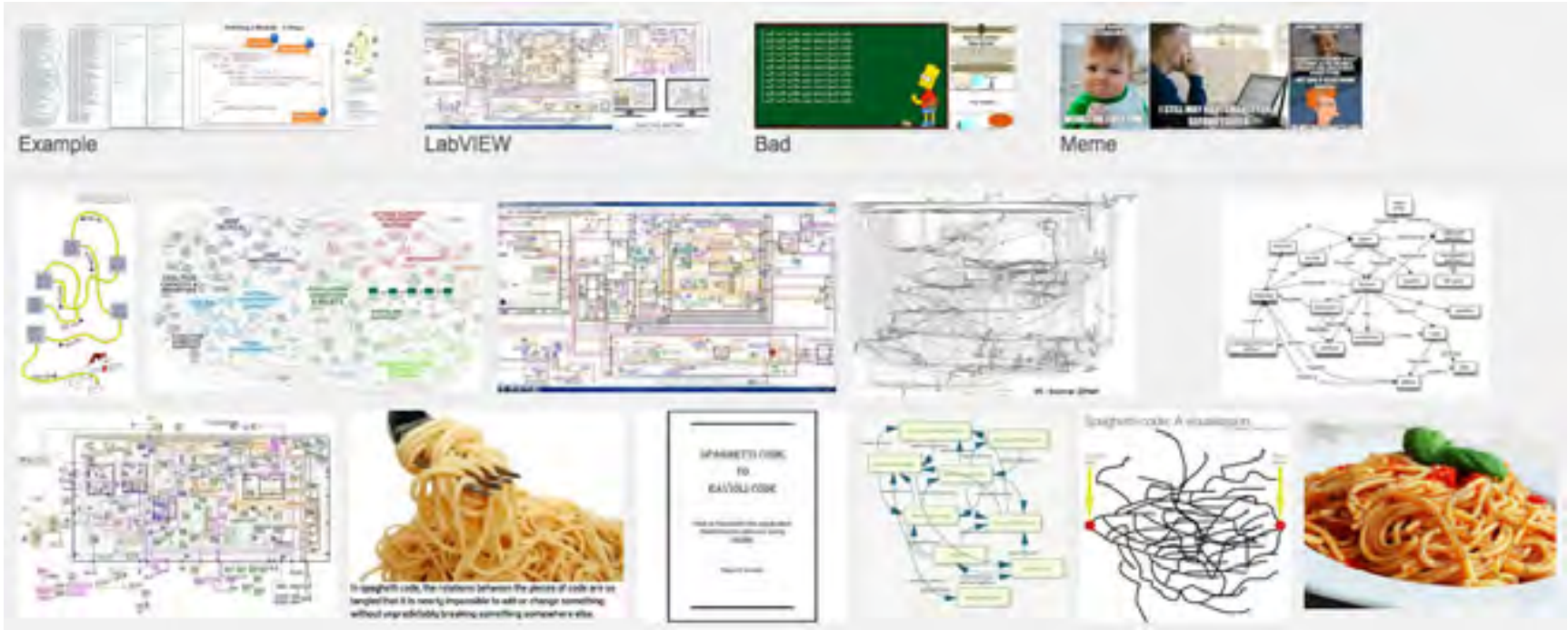
Surprising fact:

k is independent of the original number of dimensions m

Subsection 3

More efficient clustering

Clustering Google images



[L. & Lavor, *in press*]

k-means without random projections

```
VHimg = Map[Flatten[ImageData[#]] &, Himg];
```

Out[28]=

```
VHcl = Timing[ClusteringComponents[VHimg, 3, 1]]
Out[29]= {0.405908, {1, 2, 2, 2, 2, 2, 3, 2, 2, 2, 3}}
```

Too slow!

k-means with random projections

```
Get["Projection.m"];
VKimg = JohnsonLindenstrauss[VHimg, 0.1];
VKcl = Timing[ClusteringComponents[VKimg, 3, 1]]
Out[34]= {0.002232, {1, 2, 2, 2, 2, 2, 3, 2, 2, 2, 3}}
```

From 0.405s CPU time to 0.00232s

Same clustering

Works on the MSSC MP formulation too!

$$
\left.
\begin{array}{lrcl}
\min\limits_{x,y,s} & \sum\limits_{i\leq n}\sum\limits_{j\leq d} \|Tp_i - Ty_j\|_2^2\, x_{ij} & & \\
\forall j \leq d & \frac{1}{s_j}\sum\limits_{i\leq n} Tp_i x_{ij} & = & Ty_j \\
\forall i \leq n & \sum\limits_{j\leq d} x_{ij} & = & 1 \\
\forall j \leq d & \sum\limits_{i\leq n} x_{ij} & = & s_j \\
\forall j \leq d & y_j & \in & \mathbb{R}^m \\
& x & \in & \{0,1\}^{nd} \\
& s & \in & \mathbb{N}^d
\end{array}
\right\}
$$

where T is a $k \times m$ random projector
replace Ty by y'

Works on the MSSC MP formulation too!

$$
\left.
\begin{array}{lrcl}
\min\limits_{x,y',s} & \sum\limits_{i\le n}\sum\limits_{j\le d} \|Tp_i - y'_j\|_2^2\, x_{ij} & & \\
\forall j \le d & \frac{1}{s_j}\sum\limits_{i\le n} Tp_i x_{ij} & = & y'_j \\
\forall i \le n & \sum\limits_{j\le d} x_{ij} & = & 1 \\
\forall j \le d & \sum\limits_{i\le n} x_{ij} & = & s_j \\
\forall j \le d & y'_j & \in & \mathbb{R}^k \\
& x & \in & \{0,1\}^{nd} \\
& s & \in & \mathbb{N}^d
\end{array}
\right\} \quad (\text{MSSC}')
$$

- *where* $k = O(\frac{1}{\varepsilon^2}\ln n)$
- less data, $|y'| < |y| \Rightarrow$ get solutions faster
- Yields smaller cMINLP

Random projections in MP

- Random projections work in many more MP settings
  - Linear Programming [Vu, Poirion, L. MOR, to appear]
  - Trust-region subproblem formulations [working paper]
  - SDP and SOCP [working paper]

Summary

Graphs and weighted graphs necessary to model data

1. Computers can "reason by analogy" (clustering)
   Modularity clustering
2. Clustering on vectors allows more flexibility
   k-means, MSSC
3. Need to embed (weighted) graphs into Euclidean spaces
   Metric embeddings, Distance Geometry
4. High dimensions make clustering expensive/unstable
   Distance resolution limit
5. Use approximate projections to reduce dimensions
   MDS/PCA, random projections

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