Hashing, sketching, and other approximate algorithms for high-dimensional data

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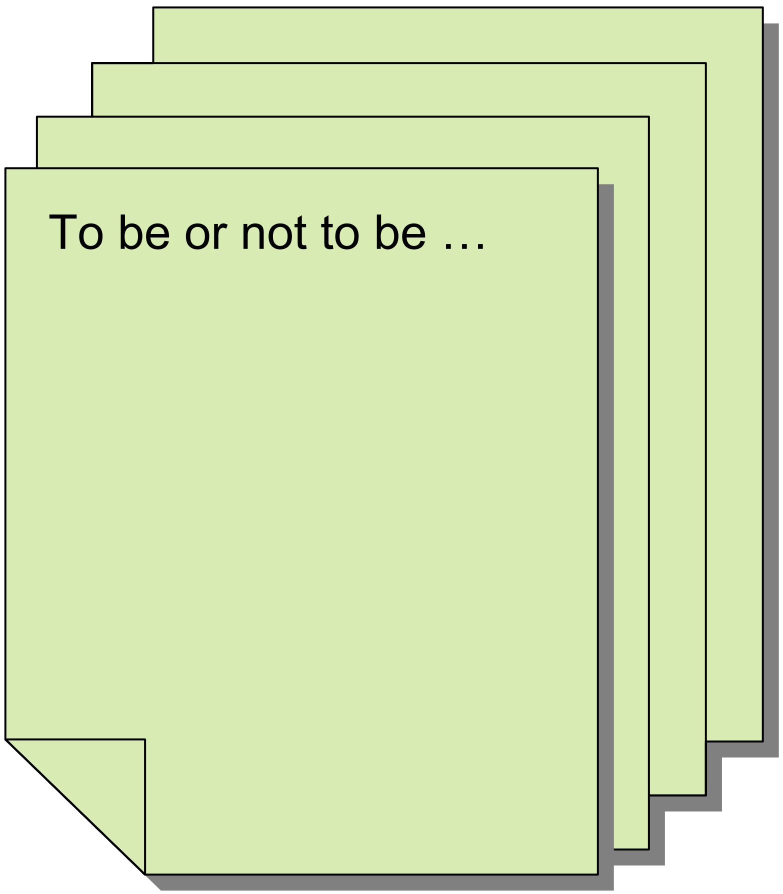
Plan

- Intro
  - High dimensionality
  - Problems
- Technique: randomized projection
  - Intuition
  - Proofoid
- Applications:
  - Sketching/streaming
  - Nearest Neighbor Search
- Conclusions
- Refs

High-Dimensional Data



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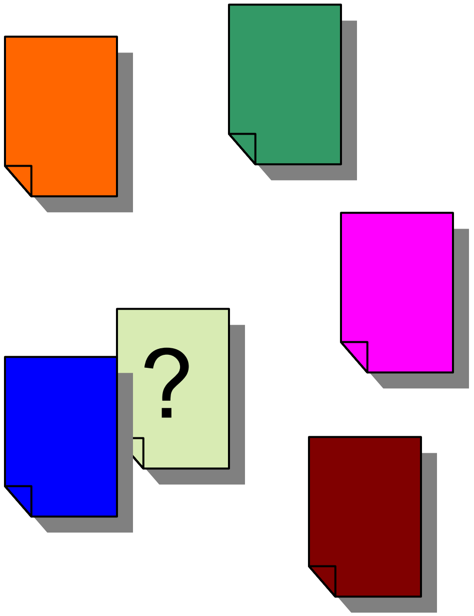
to be or not

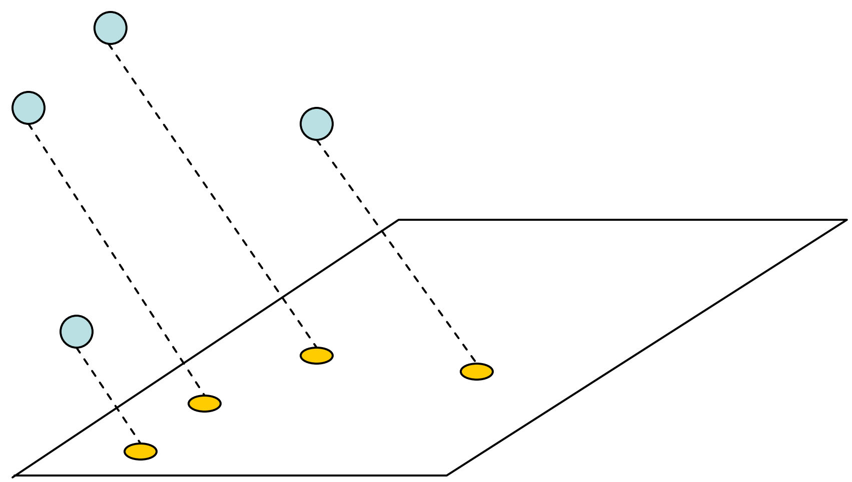
Problems

- Storage
  - How to represent the data "accurately" using "small" space
- Search
  - How to find "similar" documents
- Learning, etc…



Randomized Dimensionality Reduction

Randomized Dimensionality Reduction (a.k.a. "Flattening Lemma")



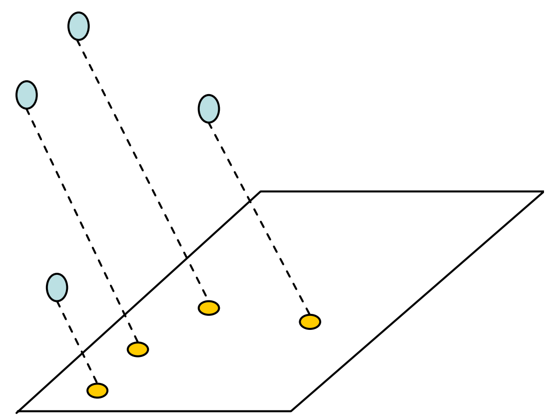
- Johnson-Lindenstrauss lemma (1984)
  - Choose the projection plane "at random"
  - The distances are "approximately" preserved with "high" probability

Dimensionality Reduction, Formally

- **JL:** For any set of n points X in R^d under Euclidean norm, there is a $(1+\varepsilon)$-distortion embedding of X into $R^{d'}$, for $d'=O(\log n / \varepsilon^2)$

- **JL':** There is a distribution over random linear mappings $A: R^d \rightarrow R^{d'}$, such that for any vector x we have $\|Ax\| = (1\pm\varepsilon)\|x\|$ with probability

$$1 - e^{-Cd'\varepsilon^2}$$



- Questions:
  - What is the distribution ?
  - Why does it work ?

Normal Distribution

- Normal distribution:
  - Range: $(-\infty, \infty)$
  - Density: $f(x)=e^{-x^2/2} / (2\pi)^{1/2}$
  - Mean=0, Variance=1
- Basic facts:
  - If X and Y independent r.v. with normal distribution, then $X+Y$ has normal distribution
  - $Var(cX)=c^2 Var(X)$
  - If X,Y independent, then $Var(X+Y)=Var(X)+Var(Y)$

Back to the Embedding

- We use mapping Ax where each entry of A has normal distribution
- Let $a^1,\ldots,a^{d'}$ be the rows of A
- Consider $Z=a^i*x = a*x=\sum_i a_i x_i$
- Each term $a_i x_i$
  - Has normal distribution
  - With variance x_i^2
- Thus, Z has normal distribution with variance $\sum_i x_i^{\,2} =||x||^2$
- This holds for each a^j

What is $||Ax||_2$

- $||Ax||^2 = (a^1 * x)^2+\ldots+(a^{d'} * x)^2 = Z_1^2+\ldots+Z_{d'}^2$ where:
  - All Z_i's are independent
  - Each has normal distribution with variance $||x||^2$

- Therefore, $E[\ ||Ax||^2\ ]=d'*E[Z_1^2]=d'\ ||x||^2$
- By "law of large numbers" (quantitive):

$$\Pr[\ |\ ||Ax||^2 - d'\ ||x||^2\ | > \varepsilon d'] < e^{-C\ d'\ \varepsilon\text{^}2}$$

for some constant C

Streaming/sketching implications

- Can replace d-dimensional vectors by d'-dimensional ones
  - Cost: $O(dd')$ per vector
  - Faster method known [Ailon-Chazelle'06]
- Can avoid storing the original d-dimensional vectors in the first place

(thanks to linearity of the mapping A)
  - Suppose:
    - x is the histogram of a document
    - We are receiving a stream of document words $w1, w2, w3$,..
  - For each word w, we want to update Ax to Ax' where $x'_w=x_w+1$ (and the rest of x stays the same)
  - Can be done via $Ax'=A(x+e_w) = Ax+Ae_w$
  - Streaming algorithms [Alon-Matias-Szegedy'96]

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to be or not

More Streaming/Sketching

- Generalizes to L_p norms, $p \in [0,2]$
  - Generate matrix A from p-stable distribution
    - E.g., for $p=1$ we have Cauchy distribution
  - Estimate $||x||_p$ using
    - median$(|a^1 x|,\ldots,|a^{d'} x|)$ [Indyk'00]
    - geometric mean, harmonic mean [Church-Hastie-Li'05..07]
- Can handle "Jaccard coefficient" [Broder'97]
  - For two sets A, B, define $J(A,B)=|A \cap B|/|A u B|$
  - "Min-wise hashes": functions h such that

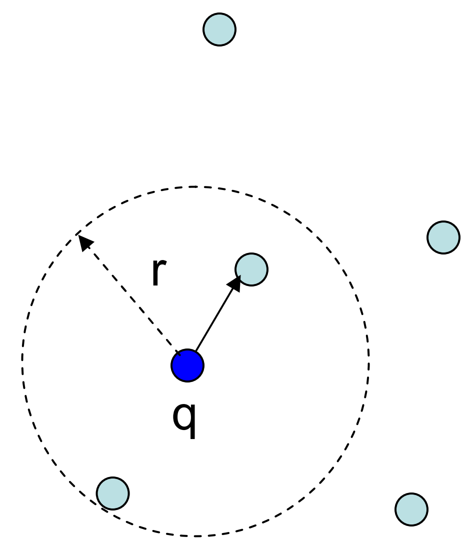
$$\Pr[h(A)=h(B)]=J(A,B)$$

  - Can sketch set A into $<h_1(A),\ldots,h_k(A)>$
- Can reconstruct approximation of x from Ax

Nearest neighbors

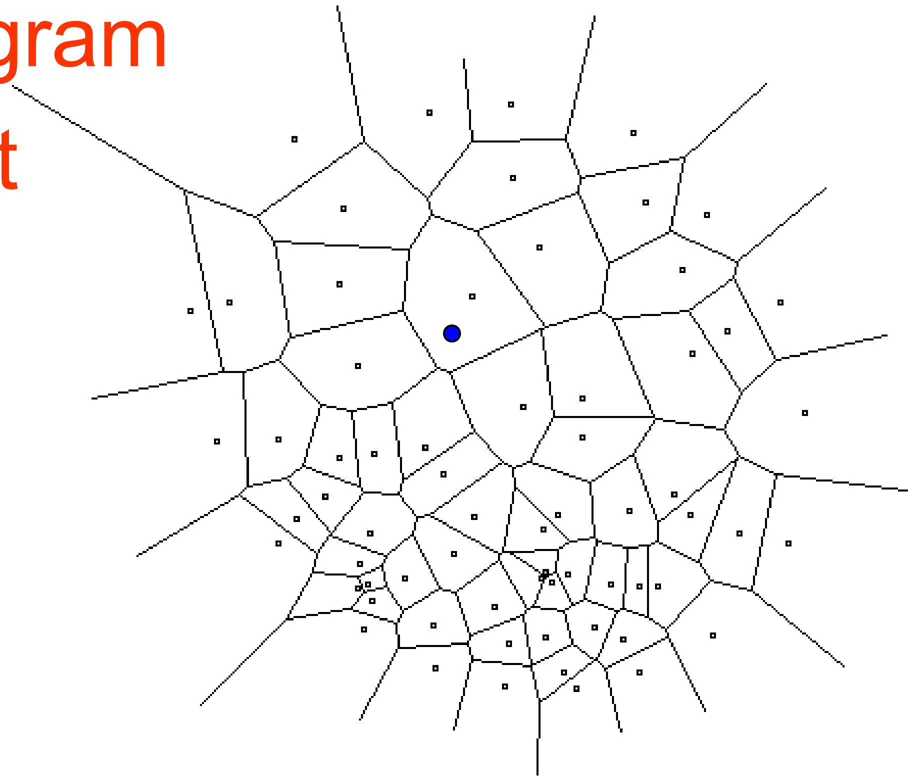
Near(est) neighbor

- Given: a set P of points in R^d
- Nearest Neighbor: for any query q, returns a point $p \in P$ minimizing $||p-q||$
- r-Near Neighbor: for any query q, returns a point $p \in P$ s.t. $||p-q|| \leq r$ (if it exists)



The case of d=2

- Compute Voronoi diagram
- Given q, perform point location
- Performance:
  - Space: O(n)
  - Query time: O(log n)

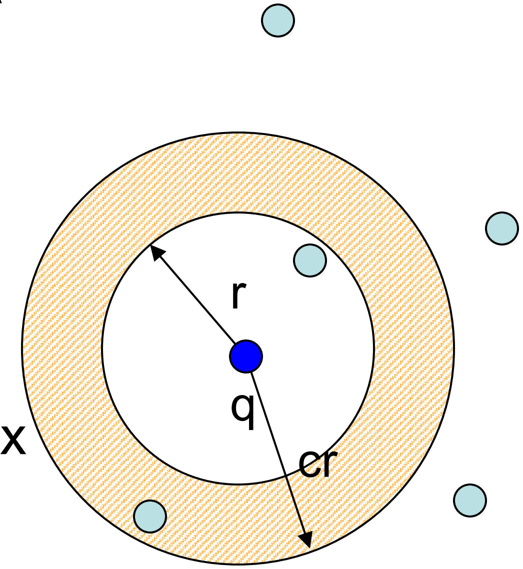


The case of d>2

- Voronoi diagram has size $n^{O(d)}$
- We can also perform a linear scan: $O(dn)$ time
- That is pretty much all what known for exact algorithms with theoretical guarantees
- In practice:
  - kd-trees work “well” in “low-medium” dimensions
  - Near-linear query time for high dimensions

Approximate Near Neighbor

- c-Approximate r-Near Neighbor: build data structure which, for any query q:
  - If there is a point $p \in P$, $||p-q|| \leq r$
  - it returns $p' \in P$, $||p-q|| \leq cr$



- Reductions:
  - c-Approx Nearest Neighbor reduces to c-Approx Near Neighbor

    (log overhead)
  - One can enumerate all approx near neighbors

    → can solve exact near neighbor problem
  - Other apps: c-approximate Minimum Spanning Tree, clustering, etc.

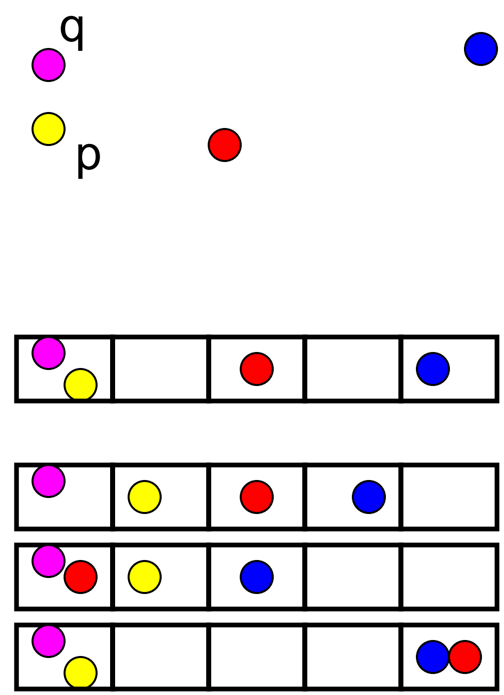
Approximate algorithms

- Space/time exponential in d [Arya-Mount-et al], [Kleinberg'97], [Har-Peled'02], [Arya-Mount-…]
- Space/time polynomial in d [Kushilevitz-Ostrovsky-Rabani'98], [Indyk-Motwani'98], [Indyk'98], [Gionis-Indyk-Motwani'99], [Charikar'02], [Datar-Immorlica-Indyk-Mirrokni'04], [Chakrabarti-Regev'04], [Panigrahy'06], [Ailon-Chazelle'06]…

Space	Time	Comment	Norm	Ref
$dn+n^{4/\varepsilon^2}$	$d * \log n / \varepsilon^2$ or 1	$c=1+\varepsilon$	Hamm, l_2	[KOR'98, IM'98]
$n^{\Omega(1/\varepsilon^2)}$	O(1)			[AIP'06]
$dn+n^{1+\rho(c)}$	$dn^{\rho(c)}$	$\rho(c)=1/c$	Hamm, l_2	[IM'98], [Cha'02]
		$\rho(c)<1/c$	l_2	[DIIM'04]
$dn * \log s$	$dn^{\sigma(c)}$	$\sigma(c)=O(\log c/c)$	Hamm, l_2	[Ind'01]
		$\sigma(c)=O(1/c)$	l_2	[Pan'06]
$dn+n^{1+\rho(c)}$	$dn^{\rho(c)}$	$\rho(c)=1/c^2 + o(1)$	l_2	[AI'06]
$dn * \log s$	$dn^{\sigma(c)}$	$\sigma(c)=O(1/c^2)$	l_2	[AI'06]

Locality-Sensitive Hashing

- Idea: construct hash functions $g: R^d \rightarrow U$ such that for any points p,q:
  - If $||p-q|| \leq r$, then $Pr[g(p)=g(q)]$ is ~~“high”~~ “not-so-small”
  - If $||p-q|| > cr$, then $Pr[g(p)=g(q)]$ is “small”
- Then we can solve the problem by hashing



LSH [Indyk-Motwani'98]

- A family H of functions $h: R^d \rightarrow U$ is called (P_1,P_2,r,cr)-sensitive, if for any p,q:
  - if $||p-q|| < r$ then $\Pr[\, h(p)=h(q)\,] > P_1$
  - if $||p-q|| > cr$ then $\Pr[\, h(p)=h(q)\,] < P_2$

- Examples:
  - Hamming distance
    - LSH functions: $h(p)=p_i$, i.e., the i-th bit of p
    - Probabilities: $\Pr[\, h(p)=h(q)\,] = 1-D(p,q)/d$
  - Jaccard coefficient
    - Min-wise hashing (slide 12)

p=10010010
q=11010110

LSH Algorithm

- We use functions of the form

  $g(p)=<h_1(p),h_2(p),\ldots,h_k(p)>$
- Preprocessing:
  - Select $g_1\ldots g_L$
  - For all $p\in P$, hash p to buckets $g_1(p)\ldots g_L(p)$

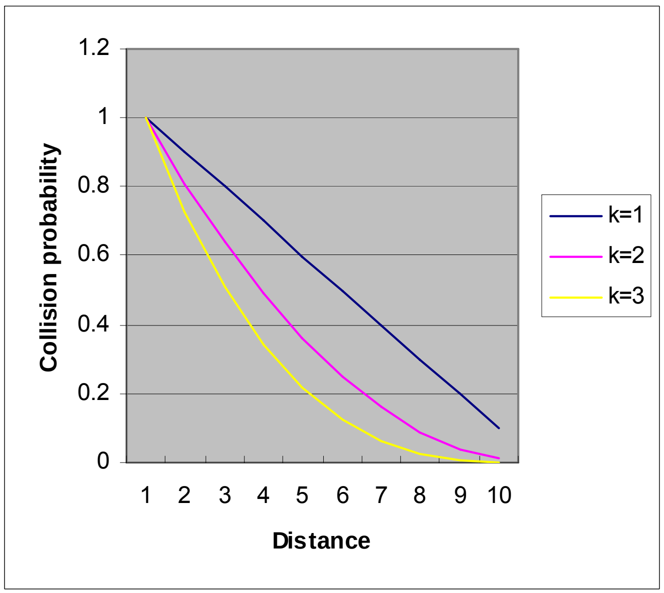
- Query:
  - Retrieve the points from buckets $g_1(q)$, $g_2(q)$, … , until
    - Either the points from all L buckets have been retrieved, or
    - Total number of points retrieved exceeds $2L$
  - Answer the query based on the retrieved points
  - Total time: $O(dL)$

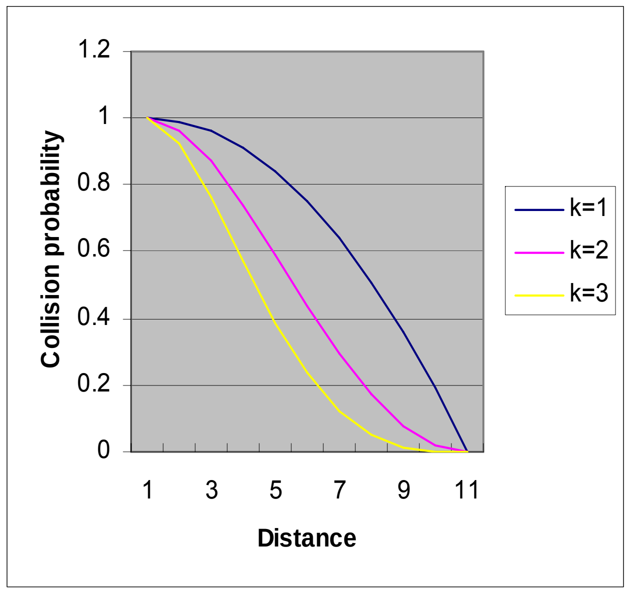
Analysis

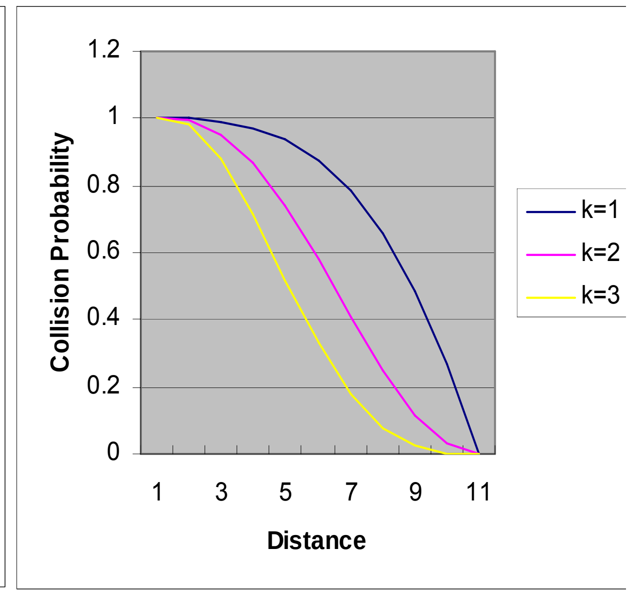
- LSH solves c-approximate NN with:
  - Number of hash fun: $L=n^{\rho}$, $\rho=\log(1/P1)/\log(1/P2)$
  - E.g., for the Hamming distance we have $\rho=1/c$
  - Constant success probability per query q

Proof by picture

- Hamming distance
- Collision prob. for k=1..3, L=1..3 (recall: L=#indices, k=#h's)
- Distance ranges from 0 to 10 (max)







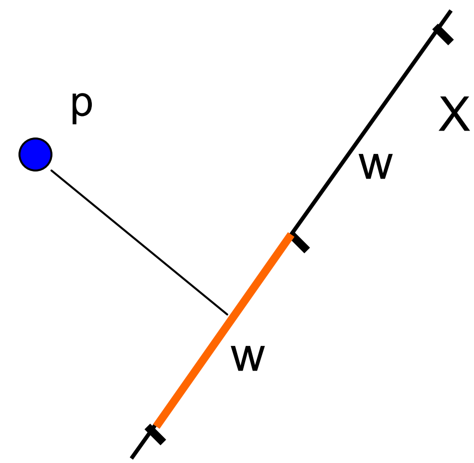
- The argument can be massaged to show that

  $L=n^{\rho}$, $\rho = \log_{1/P_2}(1/P_1)$

  works with constant probability.

Projection-based LSH
[Datar-Immorlica-Indyk-Mirrokni'04]

- Define $h_{X,b}(p)=\lfloor (p*X+b)/w \rfloor$:
  - $w \approx r$
  - $X=(X_1 \ldots X_d)$, where X_i is chosen from:
    - Gaussian distribution (for l_2 norm)
    - "s-stable" distribution* (for l_s norm)
  - b is a scalar

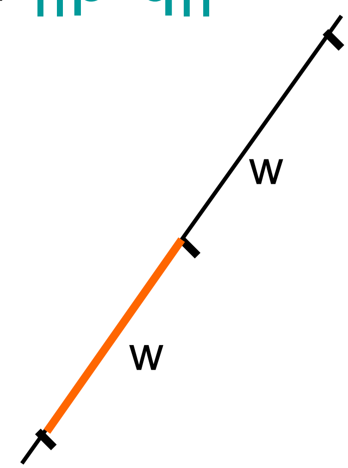


- Simple enough
- Code available [Andoni-Indyk'05]

Analysis

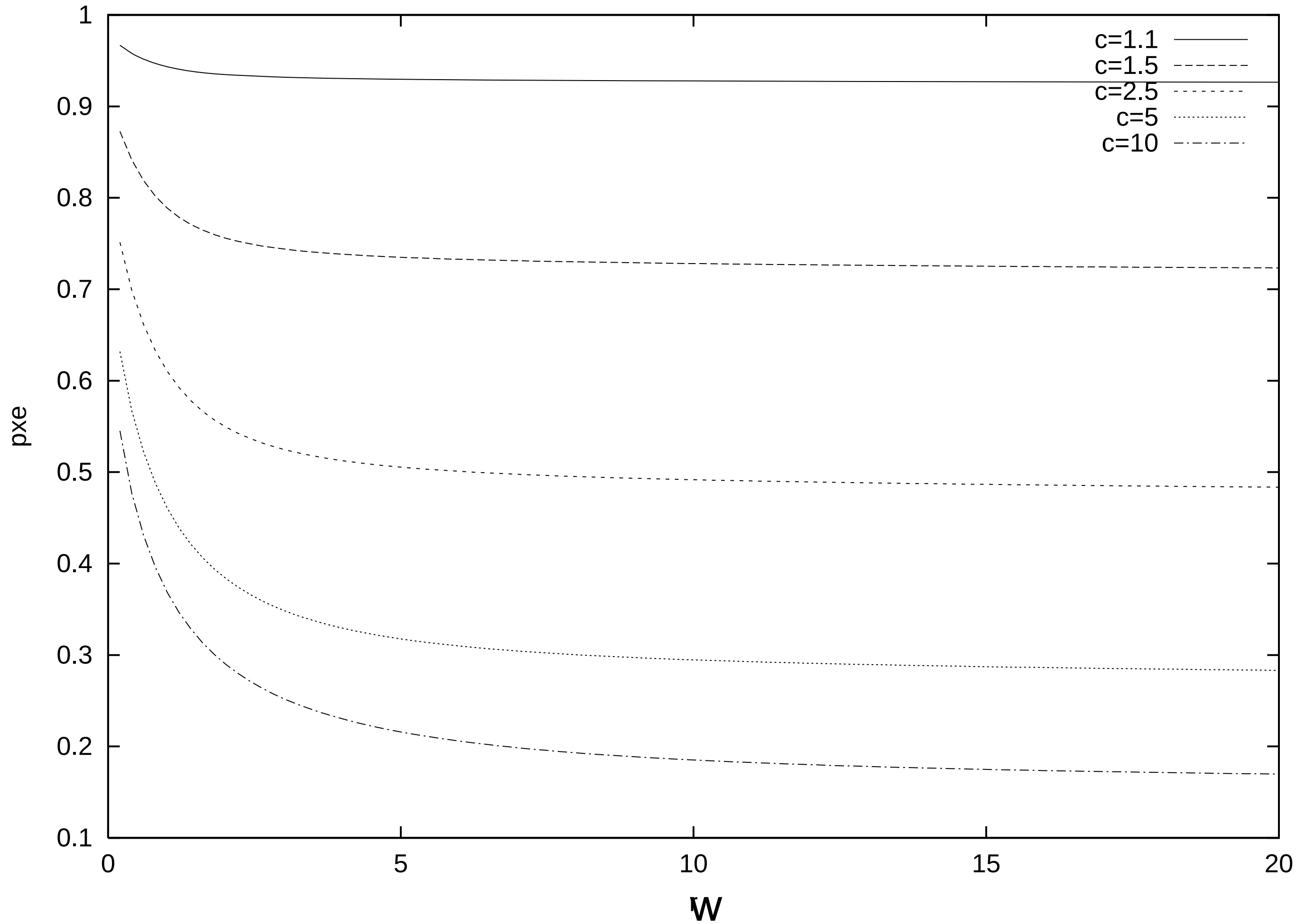
- Need to:
  - Compute $Pr[h(p)=h(q)]$ as a function of $||p-q||$ and w; this defines P_1 and P_2
  - For each c choose w that minimizes

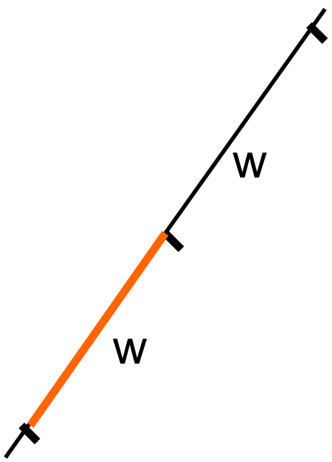
$$\rho=\log_{1/P2}(1/P_1)$$



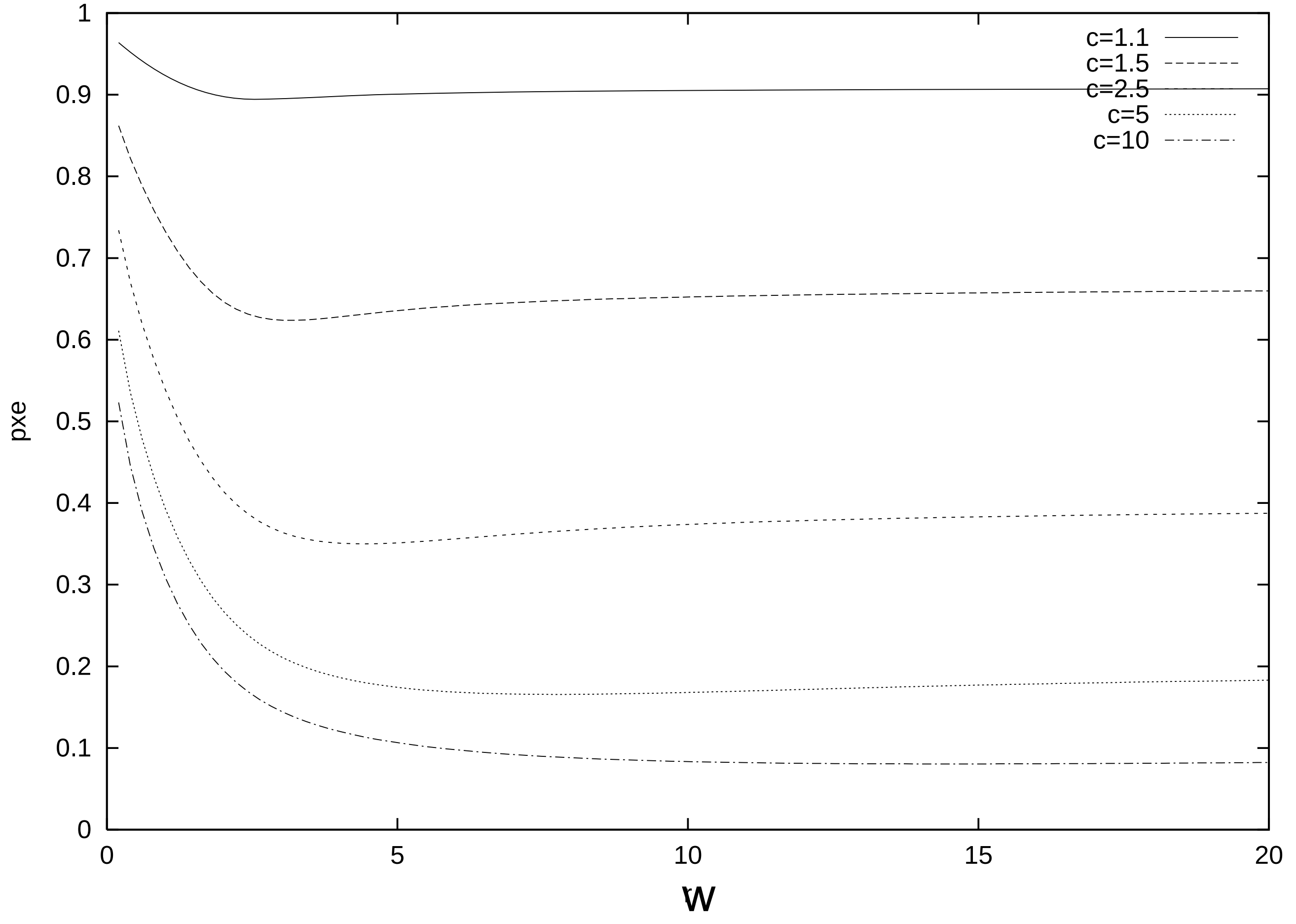
- Method:
  - For l_2: computational
  - For general l_s: analytic

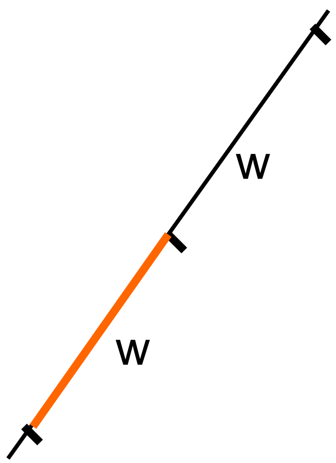
$\rho(w)$ for various c's: l_1



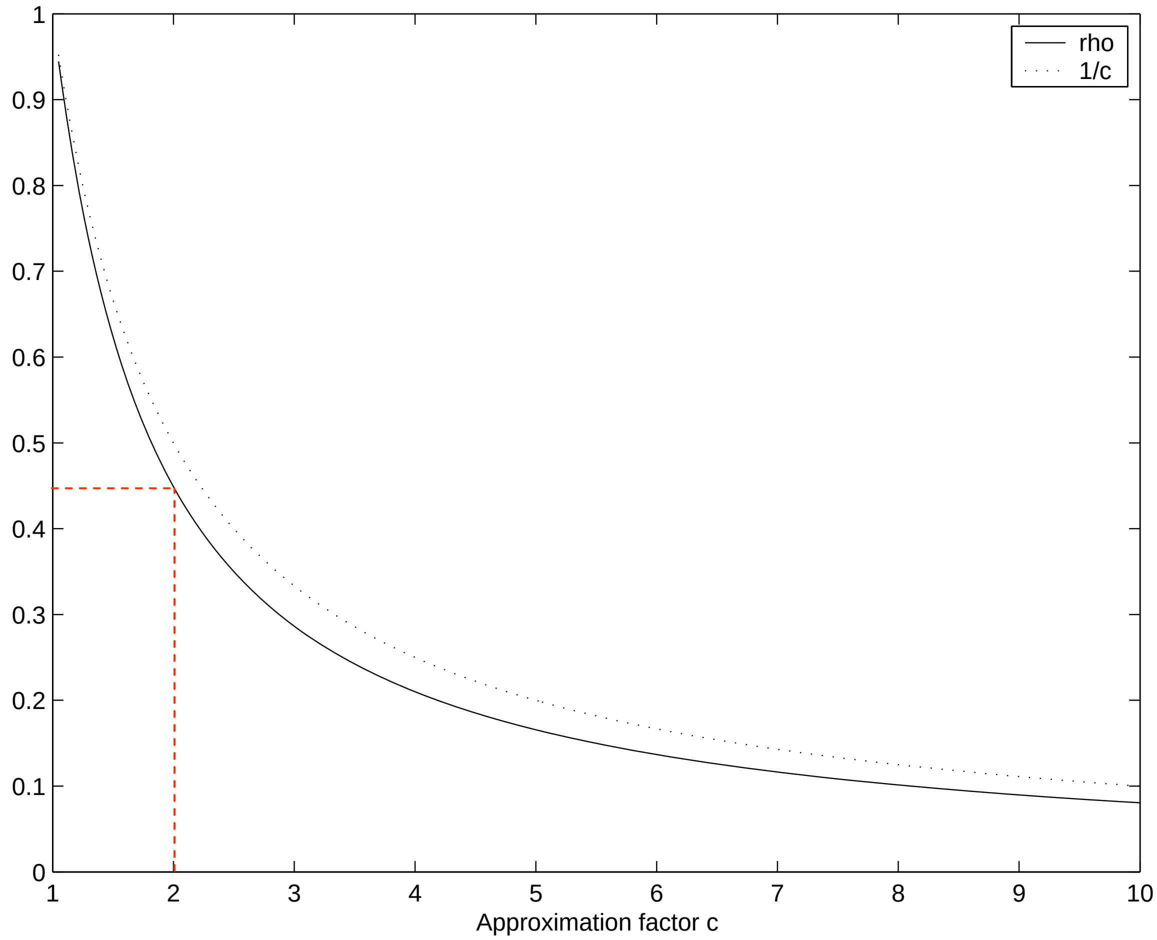


$\rho(w)$ for various c's: l_2





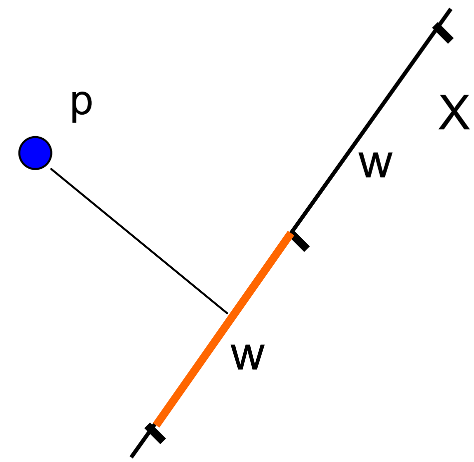
$\rho(c)$ for l_2

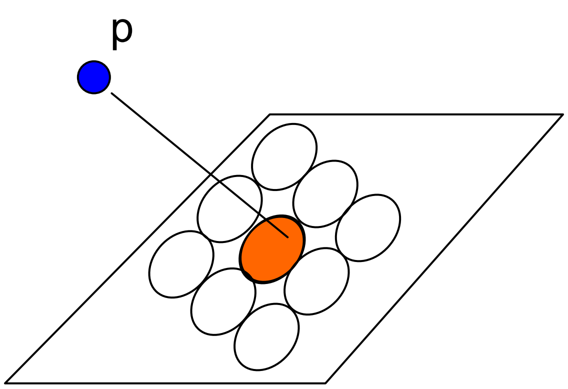

rho
1/c
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1
2
3
4
5
6
7
8
9
10
Approximation factor c

New LSH scheme

[Andoni-Indyk'06]

- Instead of projecting onto R^1, project onto R^t, for constant t
- Intervals → lattice of balls
  - Can hit empty space, so hash until a ball is hit
- Analysis:
  - $\rho = 1/c^2 + O(\log t / t^{1/2})$
  - Time to hash is $t^{O(t)}$
  - Total query time: $dn^{1/c^2+o(1)}$
- [Motwani-Naor-Panigrahy'06]: LSH in l_2 must have $\rho \geq 0.45/c^2$





Conclusions

- Overview of randomized approximate approximate algorithms for high-dimensional data
  - Reduce space
  - Reduce time
- Randomized dimensionality reduction plays important role
  - Source of randomization and approximation

If you would like to RTFM

- Random projections: monograph by S. Vempala
- Nearest neighbor in high dimensions:
  - CRC Handbook’03 (my web page)
  - CACM Survey (draft, on request)
- Streaming:
  - Survey: S. Muthu Muthukrishnan (see his web page)
  - Summer school +materials: Google “Madalgo”
- Streaming for CL: [Church-Hastie-Li, ACL’05]
- LSH for CL: [Ravichandran-Pantel-Hovy, ACL’05]

  (use related algorithm by [Charikar’02])
- LSH for web clustering: [Broder et al, WWW’97], [Gionis et al, WebDB’00, WWW’02]
- Code available (see my web page)

Thanks!

- To the organizers
- To Mike and Regina
- To you ☺

PCA vs JL

- Technical differences: average square error (PCA) vs maximum error (JL)
- PCA advantage:
  - Data dependent
  - Can adjust to distribution
- PCA disadvantage:
  - Data dependent
  - Requires linear storage, and linear update time if data set changes

Experiments

LSH Experiments (with ’04 version)

- E^2LSH: Exact Euclidean LSH (with Alex Andoni)
  - Near Neighbor
  - User sets r and P = probability of NOT reporting a point within distance r (=10%)
  - Program finds parameters k,L,w so that:
    - Probability of failure is at most P
    - Expected query time is minimized
- Nearest neighbor: set radius (radiae) to accommodate 90% queries (results for 98% are similar)
  - 1 radius: 90%
  - 2 radiae: 40%, 90%
  - 3 radiae: 40%, 65%, 90%
  - 4 radiae: 25%, 50%, 75%, 90%

Data sets

- MNIST OCR data, normalized (LeCun)
  - d=784
  - n=60,000
- Corel_hist
  - d=64
  - n=20,000
- Corel_uci
  - d=64
  - n=68,040
- Aerial data (Manjunath)
  - d=60
  - n=275,476

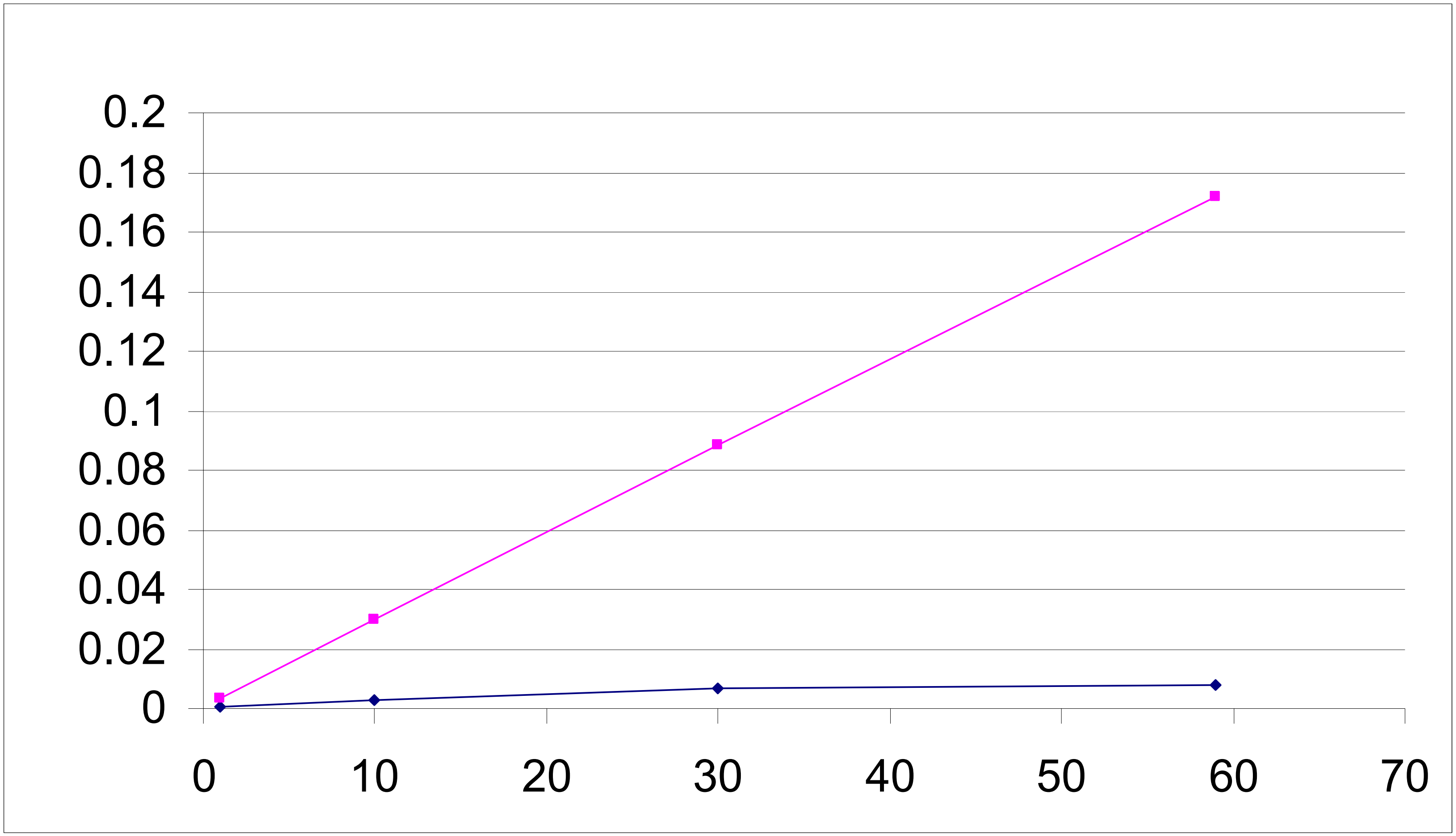
Other NN packages

- ANN (by Arya & Mount):
  - Based on kd-tree
  - Supports exact and approximate NN
- Metric trees (by Moore et al):
  - Splits along arbitrary directions (not just x,y,..)
  - Further optimizations

Running times

	MNIST	Speedup	Corel_hist	Speedup	Corel_uci	Speedup	Aerial	Speedup
E2LSH-1	0.00960							
E2LSH-2	0.00851		0.00024		0.00070		0.07400	
E2LSH-3			0.00018		0.00055		0.00833	
E2LSH-4							0.00668	
ANN	0.25300	29.72274	0.00018	1.011236	0.00274	4.954792	0.00741	1.109281
MT	0.20900	24.55357	0.00130	7.303371	0.00650	11.75407	0.01700	2.54491

LSH vs kd-tree (MNIST)



Caveats

- For ANN (MNIST), setting ε=1000% results in:
  - Query time comparable to LSH
  - Correct NN in about 65% cases, small error otherwise
- However, no guarantees
- LSH eats much more space (for optimal performance):
  - LSH: 1.2 GB
  - Kd-tree: 360 MB