Near-Optimal Hashing Algorithms for Approximate Near(est) Neighbor Problem

Piotr Indyk MIT

Joint work with: Alex Andoni, Mayur Datar, Nicole Immorlica, Vahab Mirrokni

Definition

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



 \bigcirc

Nearest Neighbor: Motivation

- Learning: nearest neighbor rule
- Database retrieval
- Vector quantization, a.k.a. compression





Brief History of NN

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 $p \in P$, $||p-q|| \le r$
 - 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
- \rightarrow can solve exact near neighbor problem
- Other apps: c-approximate Minimum Spanning Tree, clustering, etc.



 \bigcirc

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/ε²}	d * logn / ϵ^2 or 1	c=1+ ε	Hamm, I ₂	[KOR'98, IM'98]
	$n^{\Omega(1/\epsilon^2)}$	O(1)			[AIP'0?]
	dn+n ^{1+p(c)}	dn ^{ρ(c)}	ρ(c)=1/c	Hamm, I ₂	[IM'98], [Cha'02]
			ρ(c)<1/c	l ₂	[DIIM'04]
	dn * logs	dn ^{σ(c)}	$\sigma(c)=O(\log c/c)$	Hamm, I ₂	[Ind'01]
			σ(c)=O(1/c)	l ₂	[Pan'06]
→	dn+n ^{1+p(c)}	dn ^{ρ(c)}	$\rho(c)=1/c^2 + o(1)$	₂	[Al'06]
	dn * logs	dn ^{σ(c)}	$\sigma(c)=O(1/c^2)$	I ₂	[Al'06]

Locality-Sensitive Hashing

- Idea: construct hash functions g: $\mathbb{R}^{d} \rightarrow \mathbb{U}$ such that $^{\circ_{p}}$ • for any points p,q:
 - If ||p-q|| ≤ r, then Pr[g(p)=g(q)] is <u>"high</u>" "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 → U is called (P₁,P₂,r,cr)-sensitive, if for any p,q:
 – if ||p-q|| <r then Pr[h(p)=h(q)] > P₁
 – if ||p-q|| >cr then Pr[h(p)=h(q)] < P₂
- Example: 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

p=10010010 q=11010110

LSH Algorithm

- We use functions of the form $g(p) = \langle h_1(p), h_2(p), \dots, h_k(p) \rangle$
- Preprocessing:
 - Select $g_1 \dots g_L$
 - For all $p \in P$, hash p to buckets $g_1(p) \dots g_L(p)$
- 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^{ρ}, ρ =log(1/P1)/log(1/P2)
 - E.g., for the Hamming distance we have $\rho=1/c$
 - Constant success probability per query q
- Questions:
 - Can we extend this beyond Hamming distance ?
 - Yes:
 - embed I_2 into I_1 (random projections)
 - $-I_1$ into Hamming (discretization)
 - Can we reduce the exponent ρ ?

Projection-based LSH

[Datar-Immorlica-Indyk-Mirrokni'04]

- Define $h_{X,b}(p) = \lfloor (p^*X+b)/w \rfloor$:
 - w ≈ r
 - X=(X₁...X_d), where X_i is chosen from:
 - Gaussian distribution (for I₂ norm)
 - "s-stable" distribution* (for I_s norm)
 - b is a scalar
- Similar to the $I_2 \rightarrow I_1 \rightarrow Hamming$ route



^{*} I.e., p^*X has same distribution as $||p||_s$ Z, where Z is s-stable

Analysis

- Need to:
 - Compute Pr[h(p)=h(q)] as a function of ||p-q|| and w; this defines P₁ and P₂
 - For each c choose w that minimizes

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

W

- Method:
 - For I₂: computational
 - For general I_s: analytic













New LSH scheme

[Andoni-Indyk'06]

- Instead of projecting onto R¹, project onto R^t, for constant t
- Intervals \rightarrow 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/c²+o(1)}
- [Motwani-Naor-Panigrahy'06]: LSH in I_2 must have $\rho \ge 0.45/c^2$





Connections to



- [Charikar-Chekuri-Goel-Guha-Plotkin'98]
 - Consider partitioning of R^d using balls of radius R
 - Show that $Pr[Ball(p) \neq Ball(q)] \leq ||p-q||/R * d^{1/2}$
 - Linear dependence on the distance same as Hamming
 - Need to analyze R≈||p-q|| to achieve non-linear behavior! (as for the projection on the line)
- [Karger-Motwani-Sudan'94]
 - Consider partitioning of the sphere via random vectors u from N^d(0,1) :

p is in Cap(u) if $u^*p \ge T$

- Showed $Pr[Cap(p) = Cap(q)] \le exp[-(2T/||p+q||)^2/2]$
 - Large relative changes to ||p-q|| can yield only small relative changes to ||p+q||



Proof idea

- Claim: $\rho = \log(P1)/\log(P2) \rightarrow 1/c^2$
 - P1=Pr(1), P2=Pr(c)
 - Pr(z)=prob. of collision when distance z
- Proof idea:
 - Assumption: ignore effects of mapping into R^t
 - Pr(z) is proportional to the volume of the cap
 - Fraction of mass in a cap is proportional to the probability that the x-coordinate of a random point u from a ball exceeds x
 - Approximation: the x-coordinate of u has approximately normal distribution

 \rightarrow Pr(x) \approx exp(-A x²)

 $- \rho = \log[\exp(-A1^2)] / \log[\exp(-Ac^2)] = 1/c^2$





New LSH scheme, ctd.

- How does it work in practice ?
- The time t^{O(t)}dn^{1/c²+f(t)} is not very practical
 - Need t \approx 30 to see some improvement
- Idea: a different decomposition of R^t
 - Replace random balls by Voronoi diagram of a lattice
 - For specific lattices, finding a cell containing a point can be very fast
 →fast hashing



Leech Lattice LSH

- Use Leech lattice in R²⁴, t=24
 - Largest kissing number in 24D: 196560
 - Conjectured largest packing density in 24D
 - 24 is 42 in reverse...
- Very fast (bounded) decoder: about 519 operations [Amrani-Beery'94]

• Performance of that decoder for c=2:

- $1/c^2$ 0.25 - 1/c 0.50
- Leech LSH, any dimension: $\rho \approx 0.36$
- Leech LSH, any unnension. $p \approx 0$
- Leech LSH, 24D (no projection): $\rho \approx 0.26$

Conclusions

- We have seen:
 - Algorithm for c-NN with $dn^{1/c^2+o(1)}$ query time
 - (and reasonable space)
 - Exponent tight up to a constant
 - (More) practical algorithms based on Leech lattice
- We haven't seen:
 - Algorithm for c-NN with $dn^{O(1/c^2)}$ query time and $dn \log n$ space
- Immediate questions:
 - Get rid of the o(1)
 - ...or came up with a really neat lattice...
 - Tight lower bound
- Non-immediate questions:
 - Other ways of solving proximity problems

Advertisement

- See LSH web page (linked from my web page for):
 - Experimental results (for the '04 version)
 - Pointers to code

Experiments

Experiments (with '04 version)

- E²LSH: 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 et al)
 - 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 $\varepsilon = 1000\%$ 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