Approximate Nearest Neighbor (ANN) Search - II

Sanjiv Kumar, Google Research, NY

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Two popular ANN approaches

Tree approaches

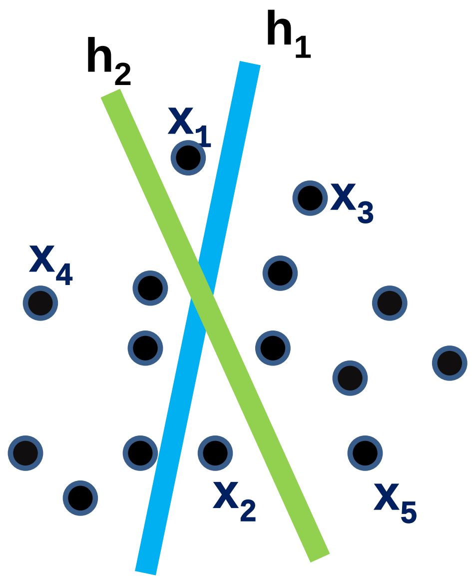
- Recursively partition the data: Divide and Conquer
- Expected query time: O(log n) (with constants exponential in dimension)
- Performance degrades with high-dimensional data
- Large storage needs
- Original data is required at run-time

Hashing approaches

- Each item in database represented as a code
- Significant reduction in storage
  - For 64 bit codes, just 8GB storage instead of 40TB
- Expected query time: O(1) or sublinear in n
  - Search in 64-bit hamming space: ~13 sec instead of ~15 hrs/query
- Compact codes preferred

Example: Binary Codes

Linear projection (hyperplane) based partitioning



X	x_1	x_2	x_3	x_4	x_5
y_1	0	1	1	0	1
y_2	1	0	1	0	1
…	…	…	…	…	…
y_m	…	…	…	…	…
	010…	100…	111…	001…	110…

No recursive partitioning unlike trees!

Hashing: Main Steps

1. Training
   - Define a model to convert an input item in a code
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Example: Binary codes using linear projections

$$h_k(x) = \mathrm{sgn}(w_k^T x + b_k) \qquad h_k(x) \in \{-1, 1\}$$

equivalent to $y_k(x) = (1 + h_k(x))/2$ $y_k(x) \in \{0, 1\}$

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Training goal: To learn parameters for m hash functions

$$\{w_k, b_k\}_{k=1,\ldots,m}$$

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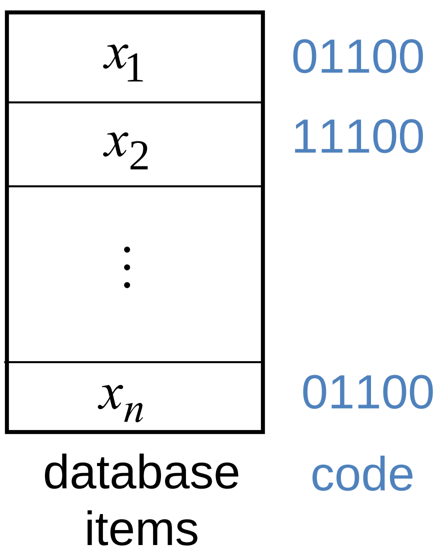

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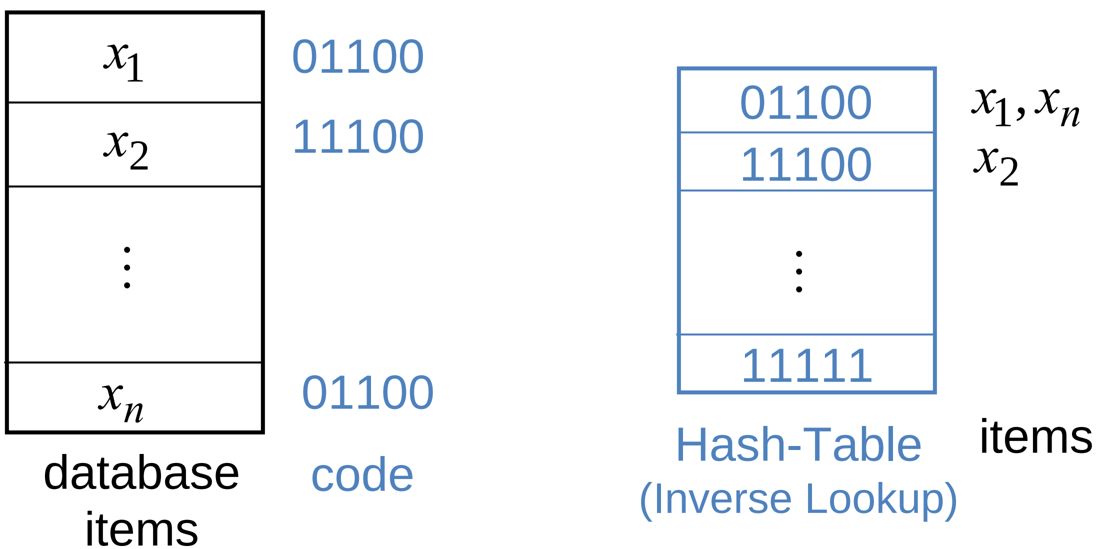

Hashing: Main Steps

3. Querying
   - Convert the query to code
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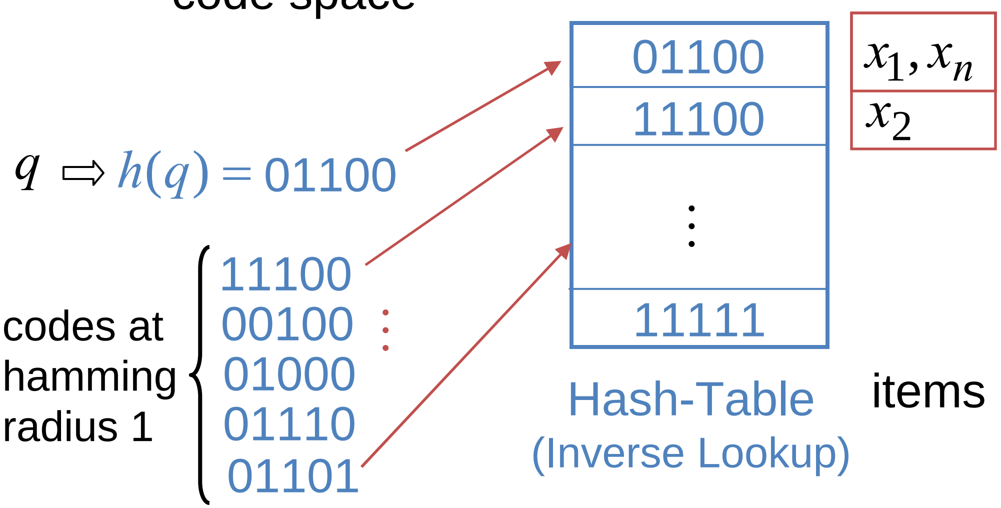

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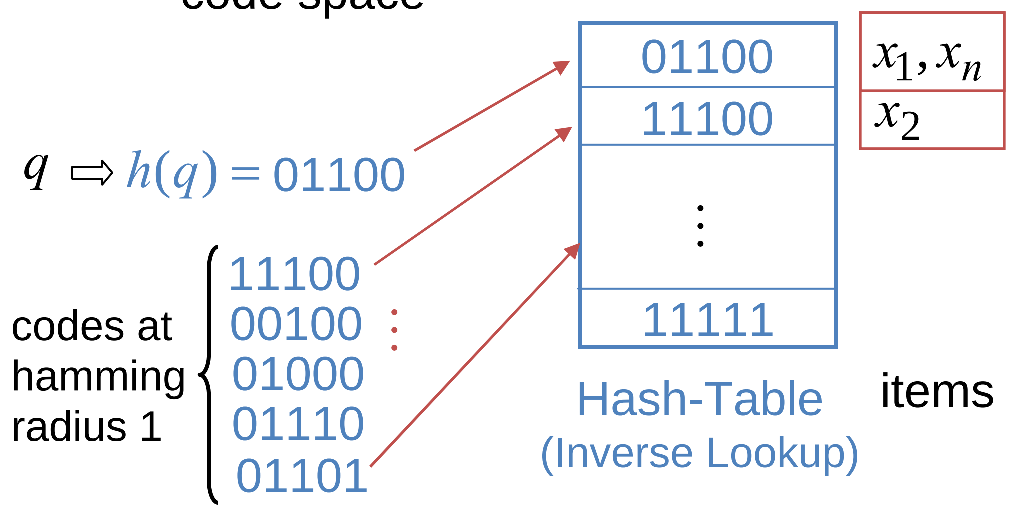

$O(nm)$ space

$O(1)$ time

Number of codes to search at radius r : $O(m^r)$

Buckets for many codes may be empty: with high probability for large m !

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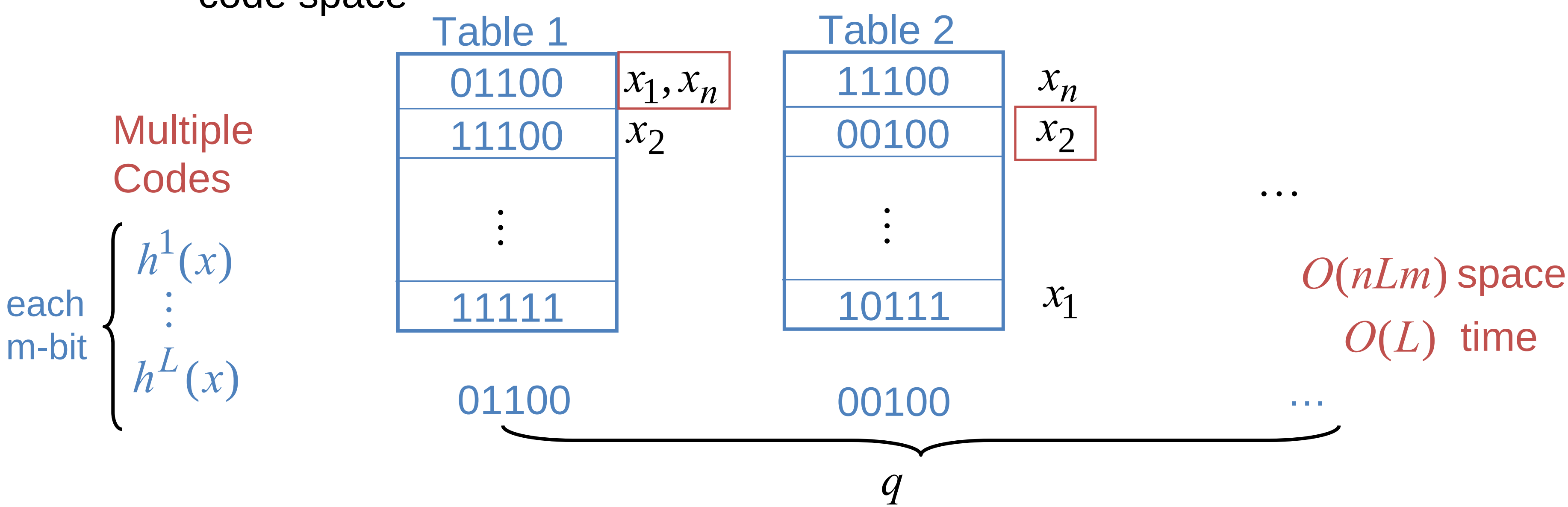

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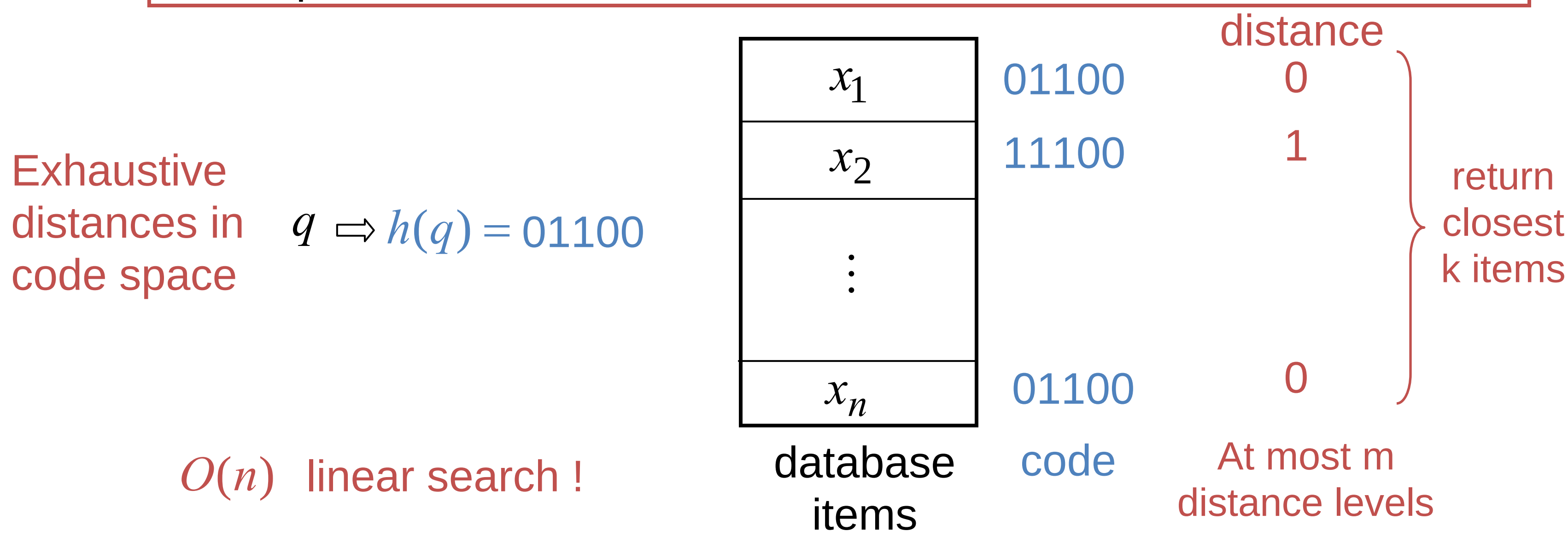

Hashing Techniques

1. Unsupervised – use unlabeled data to learn hash functions
   - Locality Sensitive Hashing (LSH), PCA Hashing, Spectral Hashing, Min-Hashing, Kernel-LSH, …
2. Supervised – use labeled pairs to learn hash functions
   - Boosted Hashing, Binary Reconstructive Embedding,…
3. Semi-Supervised – use labeled pairs and unlabeled data both
   - Sequential Learning,…
4. Type of Hash Function
   - Linear/Quasi-linear: LSH, Min-Hash, SH, PCA-Hash, …
   - Nonlinear: KLSH, RBM, BRE,…

Locality Sensitive Hashing (LSH)

A family of hash functions $H = \{h : X \rightarrow Z\}$ is called (r_1, r_2, p_1, p_2)- sensitive if for any $x_1, x_2 \in X$

$$\text{if } d(x_1, x_2) \le r_1 \text{ then } \Pr[h(x_1) = h(x_2)] \ge p_1,$$

$$\text{if } d(x_1, x_2) > r_2 \text{ then } \Pr[h(x_1) = h(x_2)] \le p_2.$$

where $r_1 < r_2$ and $p_1 > p_2$

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A simple LSH family

$$h_k(x) = \left\lfloor (w_k^T x + b_k)/t \right\rfloor \quad w_k \sim P_s(w) \quad b_k \sim U[0, t]$$

s-stable distribution

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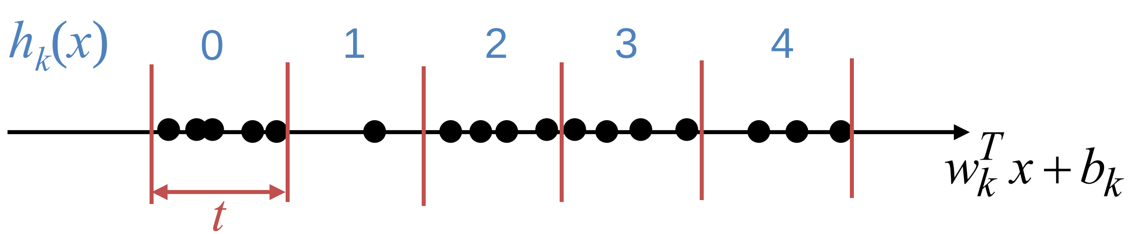
Special case:
binary hashing



s-Stable Distributions

A distribution $P_s(r)$ is called s-stable if there exists an $s \geq 0$ such that for any $x \in \Re^d$, and any w with $i.i.d.\ w^i \sim P_s$, then

$$x^T w \sim \|x\|_s w^i$$

$$\Rightarrow (x_1 - x_2)^T w \sim \|(x_1 - x_2)\|_s w^i$$

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Special Case: s = 2 (Euclidean distance)

$$w^i \sim P_s = N(0,1) \Rightarrow w \sim N(0, I)$$

$$E[x^T w] = 0$$

$$Var[x^T w] = E[x^T w w^T x] = x^T E[w w^T] x = \|x\|_2^2$$

$$x^T w \sim \|x\|_2 w^i$$

Gaussian distribution is 2-stable !

Which distribution is 1-stable? Cauchy !

One can find s-stable distribution for all s $\in$(0, 2]

Collision Probability

Suppose $u = \|(x_1 - x_2)\|_s$ and $f_s(a)$ is pdf of absolute of s-stable random variable, i.e., $a = |w^i|$, then probability of collision,

$$p(u) = \Pr[h(x_1) = h(x_2)] = \int_0^t (1/u) f_s(a/u)(1 - a/t)da$$

$p(u)$ increases as u decreases !

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$$\hat{t} = \arg\min_t \rho = \arg\min_t [\log(1/p_1)/\log(1/p_2)]$$

Can be computed analytically for s = 1, 2

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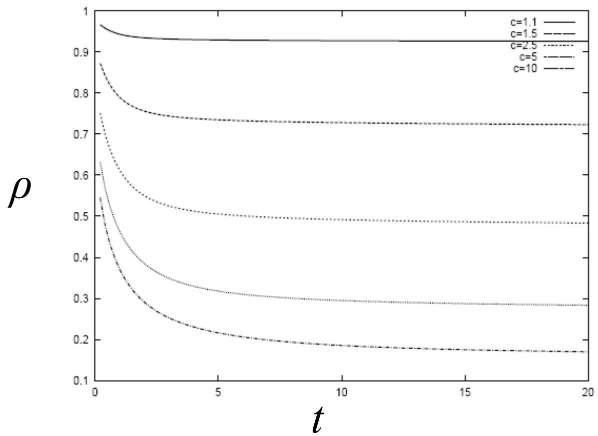

ρ not too sensitive to t if sufficiently away from 0 !

Datar et al.[5]

Parameter selection in LSH

How many tables (L) and how many bits per table (m)?

Given a query q and its near-neighbor x', suppose each hash function satisfies

$$\Pr[h_k(q) = h_k(x')] \geq p_1$$

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Probability of collision falls exponentially with m !

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Probability of collision falls exponentially with m !

Probability that q and x' will fail to collide for all L tables

$$\leq (1 - p_1^m)^L$$

Bound the probability that q and x' will collide for at least one of L tables

$$1 - (1 - p_1^m)^L \leq 1 - \delta$$

$$\boxed{L \geq -\log(1/\delta) / \log(1 - p_1^m)}$$

Precision-Recall Tradeoff

- For high precision, longer codes (i.e. large m) preferred
- Large m reduces the probability of collision exponentially → low recall
- Many tables (large L) necessary to get good recall → Large storage

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Design L and m such that run-time is minimized for a given application:

$$T_{total} = T_h + T_r$$

T_h: To compute L m-bit hash functions and retrieve points from tables via lookups

T_r: To compute exact distance with retrieved points and return top k (sublinear in n)

- Larger m increases T_h but decreases T_r
- Empirically estimate total time averaged over many queries
- In some cases, T_r is simply vote over how many tables returned an item

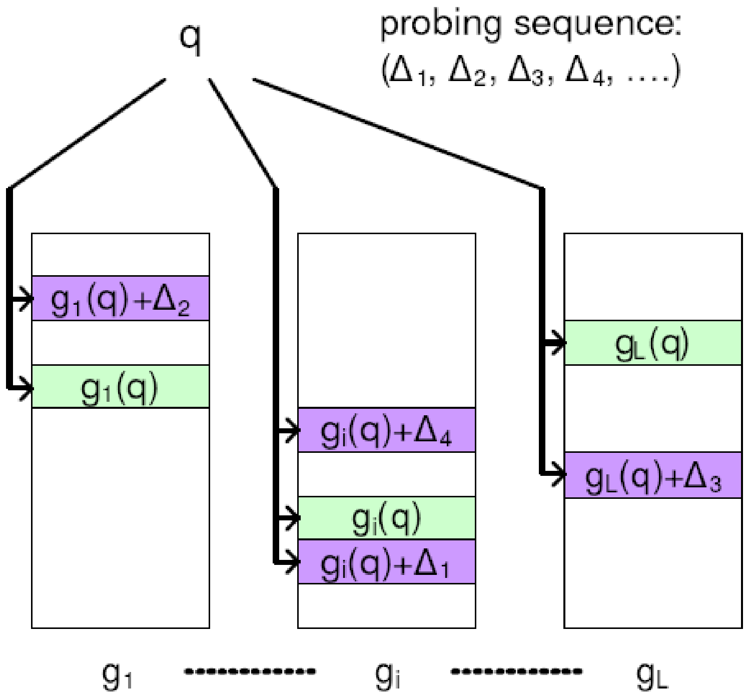
How to avoid large number of tables?

Multi-Probe LSH

Strategy to increase recall without using large number of tables

Basic idea

- If two neighbors do not fall in the same bucket, they should fall in a nearby one, e.g., within a hamming distance of 1



Lv et al.[7]

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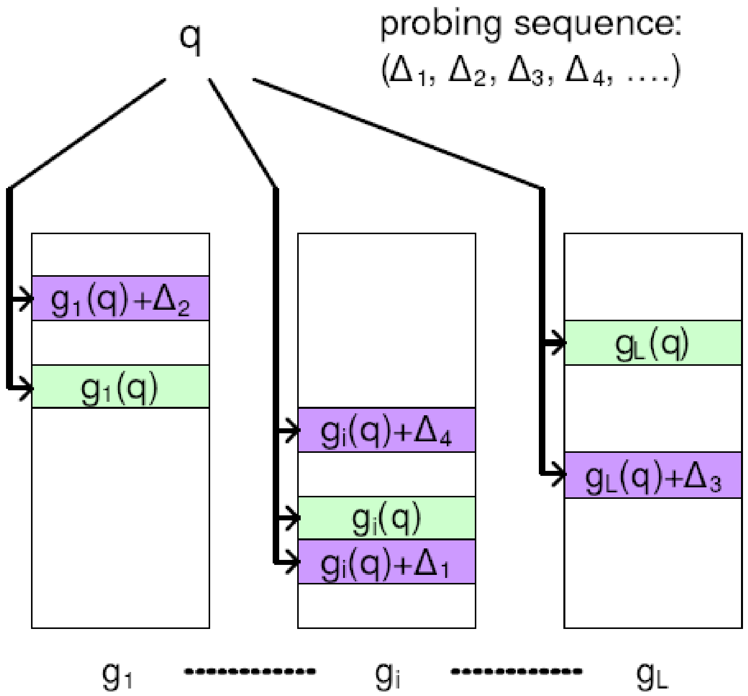
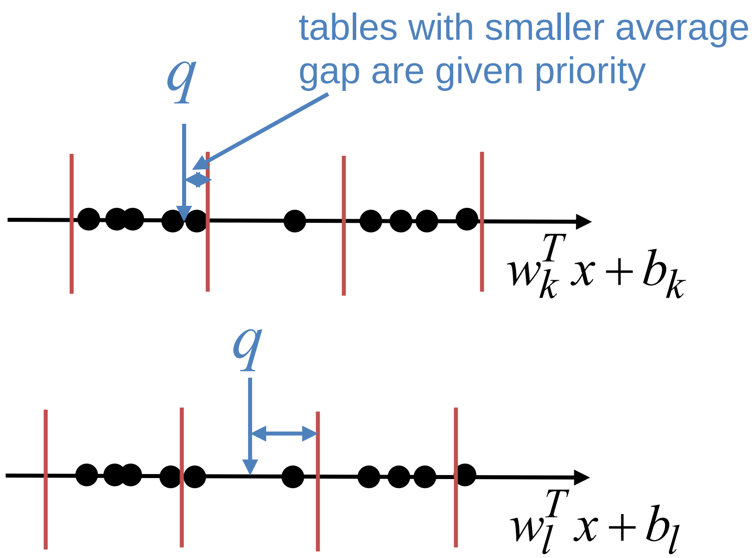


How to choose the sequence?



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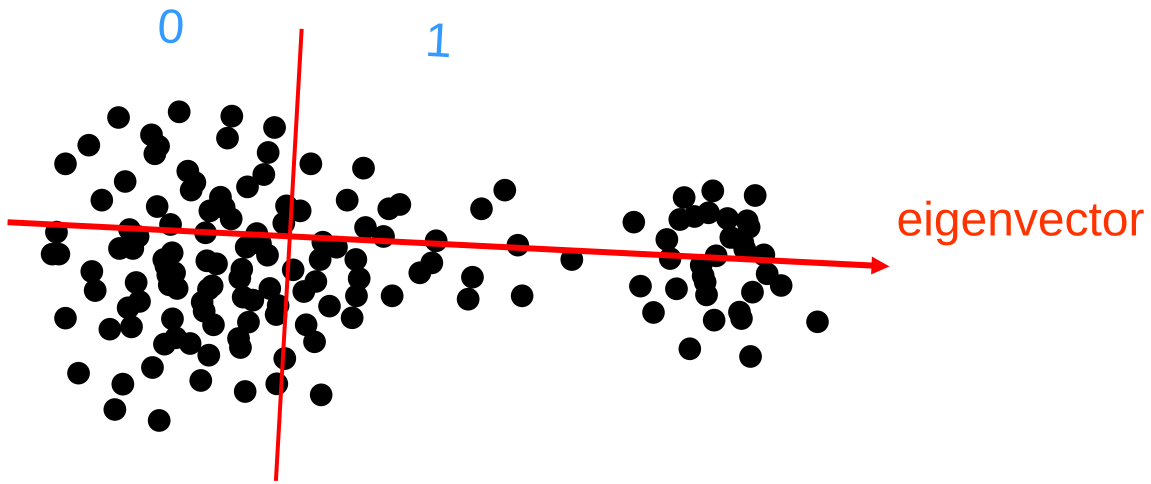
Data-Dependent Projections

– PCA-Hash: Let's focus on binary codes



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Projection on max variance directions followed by median threshold

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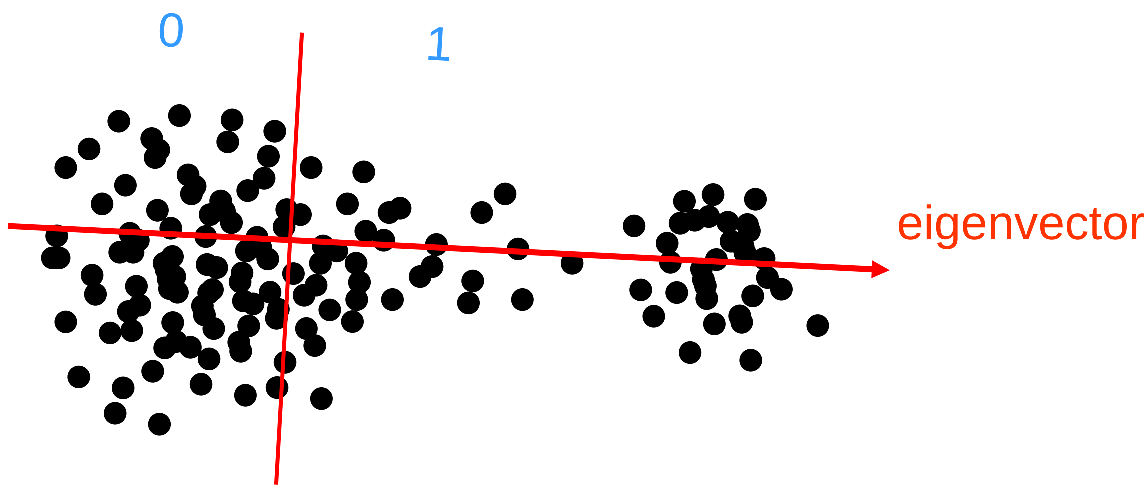

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Performance degrades with larger number of bits

- Variance decreases rapidly for most real-world data
- Can one reuse the high variance directions?

Spectral Hash

Data-dependent learning of binary codes $h(x)$ such that

similarity between x_i, x_j

$$\min \sum_{i,j} W_{ij} \left\| h(x_i) - h(x_j) \right\|^2$$

subject to

$$\sum_i h_k(x_i) = 0 \quad \forall\, k$$

balanced partitioning $h_k(x) \in \{-1, 1\}$

$$\sum_i h_k(x_i) h_l(x_i) = 0 \quad \forall\, k \neq l$$

uncorrelated

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Graph Laplacian → O(n²)

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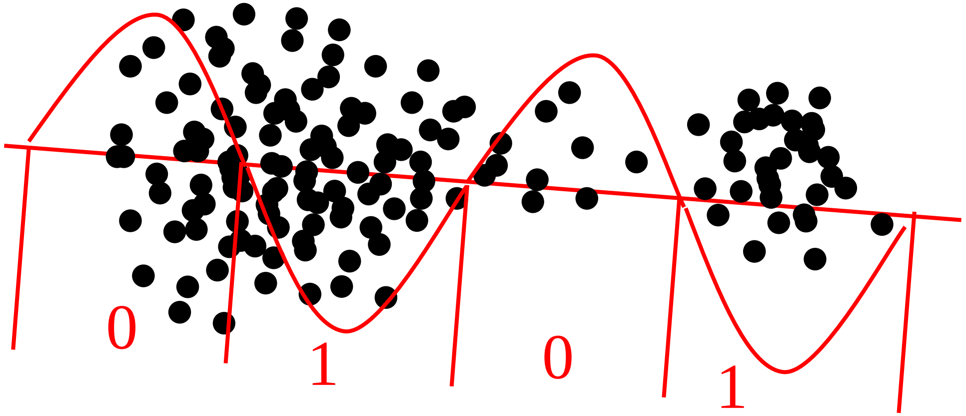
Issues

- Computationally extremely expensive (needs complete NN search)
- Balanced graph partitioning problem even with single bit → NP hard

Approximation

- Assumes uniform data distribution and solves 1D Laplacian eigenfunctions analytically

Spectral Hash



Three main steps

- Extract max-variance directions using PCA
- Select which direction to pick next based on modes of 1D-Laplacian
  - High variance PCA directions may be picked again
- Create bits by thresholding sinusoidal eigenfunctions at zero
  - slower than simple thresholding

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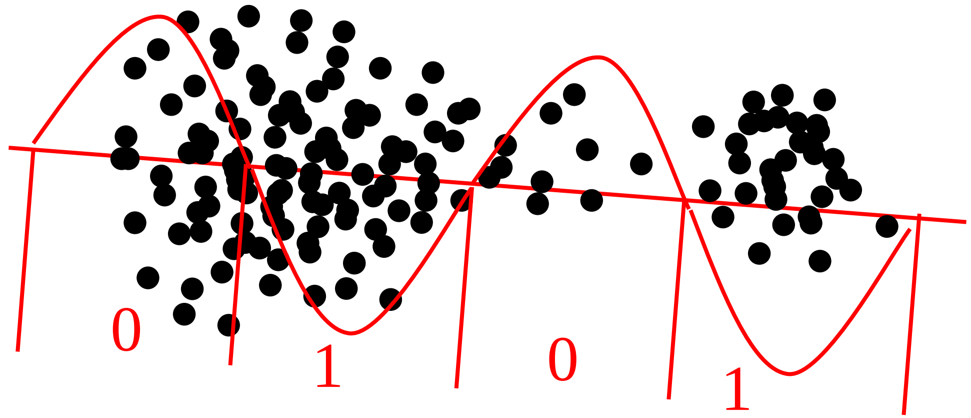

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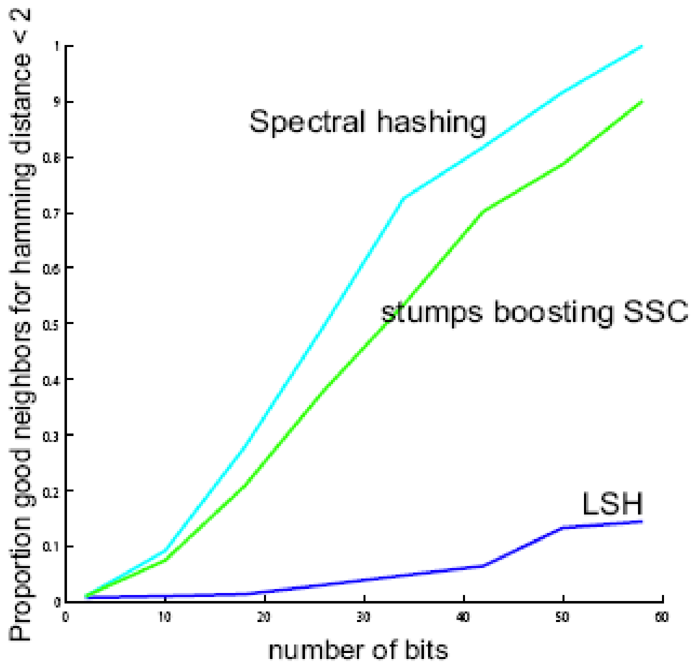
In practice, PCA-hash with median threshold may do better but both suffer from low-variance directions

Spectral Hash Experiment



- Testing using Hamming radius around the query
- Dense 384-dim vector → PCA-Hash gives similar or better performance
- For Hamming-radius testing, better to use LSH with median threshold

Weiss et al.[9]

Shift-Invariant Kernel Embedding

Use random projections along with sinusoidal thresholding

Key idea

- Suppose similarity between a pair of points is given by a shift-invariant kernel, i.e.,

$$s(x,y) = K(x,y) = K(x-y) \le 1 \qquad K(x-x) = K(0) = 1$$

Examples $s(x,y) = \exp(-\gamma \|x-y\|^2 / 2)$ L_2 distance

$s(x,y) = \exp(-\gamma \|x-y\|_1)$ L_1 distance

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Examples $s(x,y) = \exp(-\gamma \|x-y\|^2 / 2)$ L_2 distance

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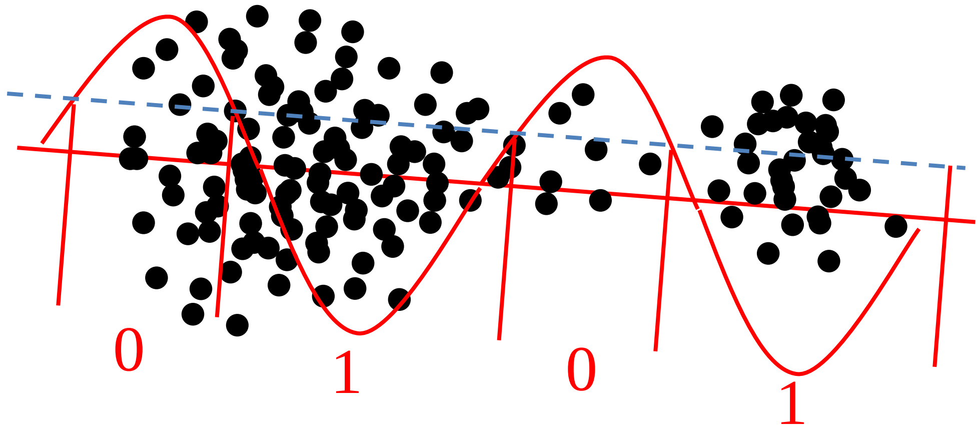
Want to learn m-bit code $h(x)$ such that

$$f_1(K(x-y)) \le \underbrace{(1/m) d_H(h(x), h(y))}_{\text{normalized Hamming distance}} \le f_2(K(x-y))$$

decreasing functions → small for similar points

$$f_1(1) = f_2(1) = 0, \; f_1(0) = f_2(0) = c > 0$$

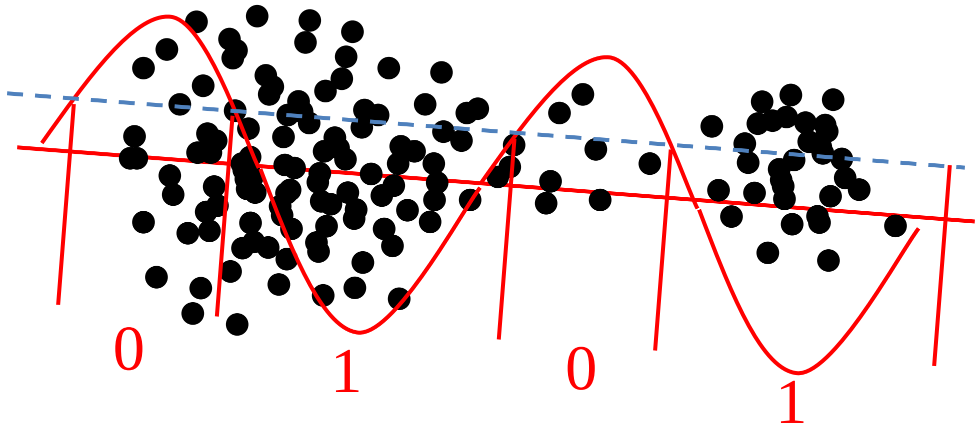
Shift-Invariant Kernel Embedding



Main steps

- Approximate shift-invariant kernels as dot products of random fourier features
- Pick directions from distribution induced by kernel → similar to s-stable directions
- Create bits by thresholding sinusoidal eigenfunctions

Shift-Invariant Kernel Embedding



standard conversion into 0/1

$$h_k(x) = \mathrm{sgn}(\cos(w_k^T x + b_k) + t_k) \qquad w_k \sim N(0, \gamma I) \;\; b_k \sim U[0, 2\pi] \;\; t_k \sim U[-1, 1]$$

critical for performance

Main steps

- Approximate shift-invariant kernels as dot products of random fourier features
- Pick directions from distribution induced by kernel → similar to s-stable directions
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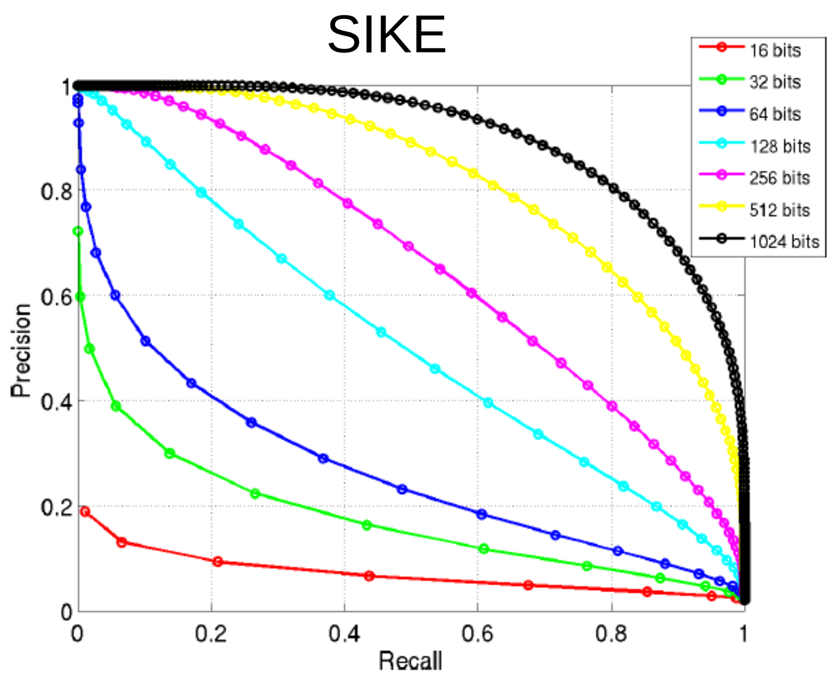
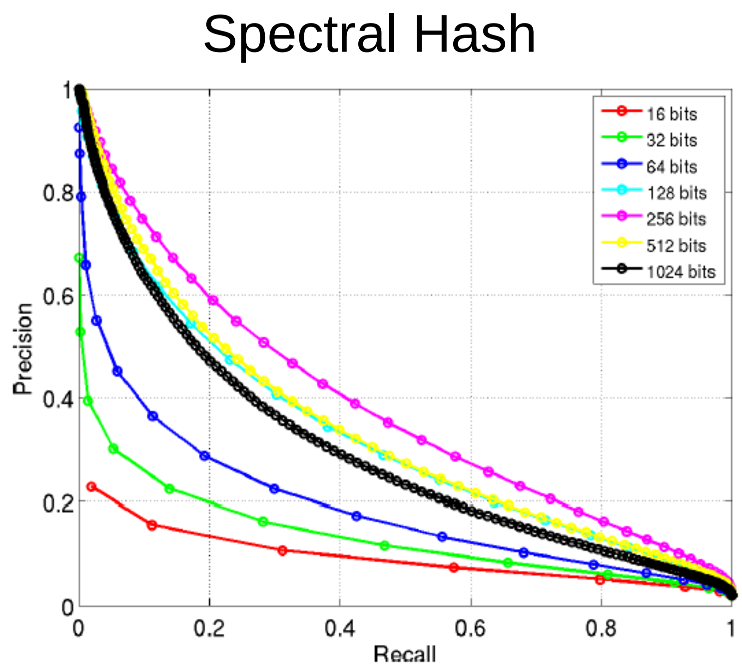
Performance (with hamming ranking) better if large number of bits are used !

Shift-Invariant Kernel Embedding





- Test using exhaustive hamming ranking with all database items
- Dense 384-dim vectors
- After 256 bits, performance of Spectral Hash falls
- Even regular LSH quite powerful if large number of bits are used

Raginsky et al.[11]

Min-Hash

A method to estimate Jaccard similarity between sets (or vectors)

- Jaccard similarity between two sets (A, B) or two vectors (x, y)

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|} \qquad J(x,y) = \frac{\sum_i \min(x^i, y^i)}{\sum_i \max(x^i, y^i)} \quad \forall\, x^i, y^i \geq 0$$

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relation with L_1 ?

- The above two definitions equivalent → represent each set as a binary vector of length $|A \cup B|$

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relation with L_1 ?

- The above two definitions equivalent → represent each set as a binary vector of length $|A \cup B|$
- Suppose $h_k(.)$ is a random function that maps each item to a real number

$$h_k(x^i) \neq h_k(x^j) \quad \text{and} \quad \Pr[h_k(x^i) < h_k(x^j)] = 0.5$$

simple choice $h_k(x^i) = U[0,1]$

Min-Hash

A method to estimate Jaccard similarity between sets (or vectors)

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min-hash $m(A, h_k) = \arg\min_{x^i \in A} h_k(x^i)$

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

Min-Hash

min-hash $m(A, h_k) = \arg\min_{x^i \in A} h_k(x^i)$

suppose $m(A \bigcup B, h_k) = x^u$

if $x^u \in A \bigcap B \Rightarrow x^u = m(A, h_k) \;\&\; x^u = m(B, h_k)$

Thus $\Pr[m(A, h_k) = m(B, h_k)] = \frac{|A \bigcap B|}{|A \bigcup B|}$

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Sketches

- For retrieval efficiency, min-hashes are grouped in s-tuples. For s random functions $(h_1, \ldots, h_s)$,

$$sketch\,(A) = (m(A, h_1), \ldots, m(A, h_s))$$

$$\Pr[sketch\,(A) = sketch\,(B)] = J(A, B)^s$$

- In practice, many sketches are created and sets (i.e. vectors) that have at least k sketches in common are retrieved for further testing.
- Generalizations to non-binary vectors, continuous valued vectors possible
- Good performance for high-dim (but mostly sparse) vectors

Kernel Locality Sensitive Hashing (KLSH)

Learn LSH-type codes but when only kernel similarity, $k(x,y)$, is known

- Data may not be given in explicit vector space

A different view of LSH

$$\Pr[h(x) = h(y)] = sim\,(x, y)$$

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query-time to find (1+ε)-neighbor $O(n^{1/(1+\varepsilon)})$

Example

$$sim(x, y) = x^T y \qquad h_k(x) = \begin{cases} 1, & \text{if } r^T x > 0 \\ 0 & \text{otherwise} \end{cases} \quad r \sim N(0, I)$$

$$\Pr[\text{sgn}(r^T x) = \text{sgn}(r^T y)] = 1 - \frac{1}{\pi}\cos^{-1}\left(\frac{x^T y}{\|x\|\|y\|}\right)$$

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Suppose we are given only similarity

implicit (unknown) feature vector

$$sim(x, y) = k(x, y) = \Phi(x)^T \Phi(y)$$

How to compute the hash function when vector is not known ?

Kernel Locality Sensitive Hashing (KLSH)

Goal: To find appropriate random projection in implicit feature space $r^T \Phi(x)$

From RKHS argument

$$r = \sum_{i=1}^{n} w_i \Phi(x_i) \approx \sum_{i=1}^{p} w_i \Phi(x_i)$$

$$= \Phi w$$

randomly chosen $p << n$

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Find w such that $E[r] = 0,\ E[rr^T] = I$

$$w = K^{-1/2} e_s$$

$K = \Phi^T \Phi,\ \ e_s = \underbrace{[0,0,1,0,1\ldots]^T}$

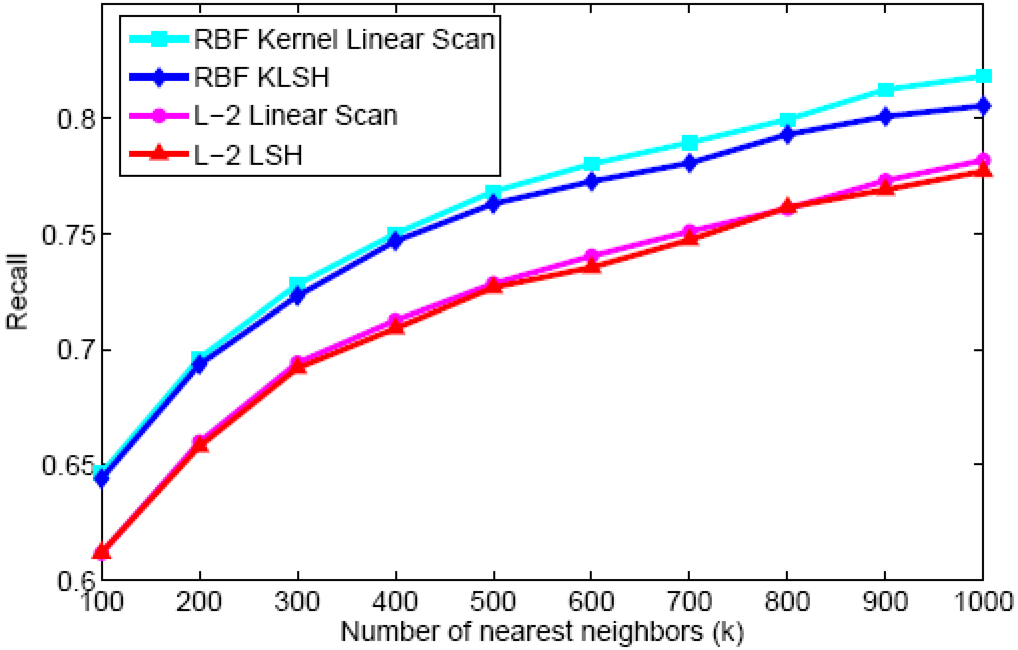
\# of 1's is a parameter

$$h(\Phi(x)) = \text{sgn}(r^T \Phi(x) = \text{sgn} \sum_{i=1}^{p} w_i k(x, x_i)$$

non-linear hashing

usually slower run-time !

KLSH vs LSH



n = 100K image patches

Kulis et al.[12]

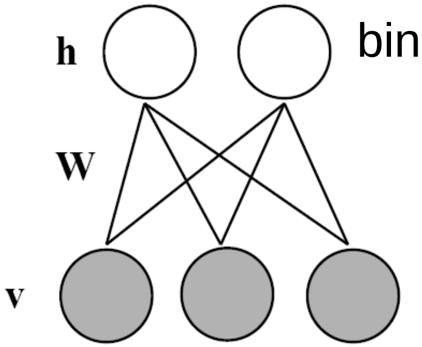
Semantic Hashing (RBM)

Nonlinear method to create binary codes using Restricted Boltzmann Machines (RBMs)

– Special type of Markov Random Fields

$$p(v,h) = \exp\{-E(v,h)\} / Z$$

$$p(v) = \sum_h p(v,h)$$



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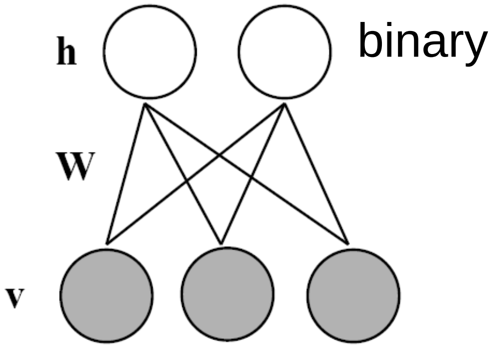


$$p(v,h) = \exp\{-E(v,h)\}/Z$$

$$p(v) = \sum_h p(v,h)$$

$$p(h_j = 1 | v) = \sigma(b_j + \sum_i w_{ij} v_i) \qquad \sigma(x) = 1/(1+e^{-x})$$

$$p(v_i | h) = N(f(h), \tau I)$$

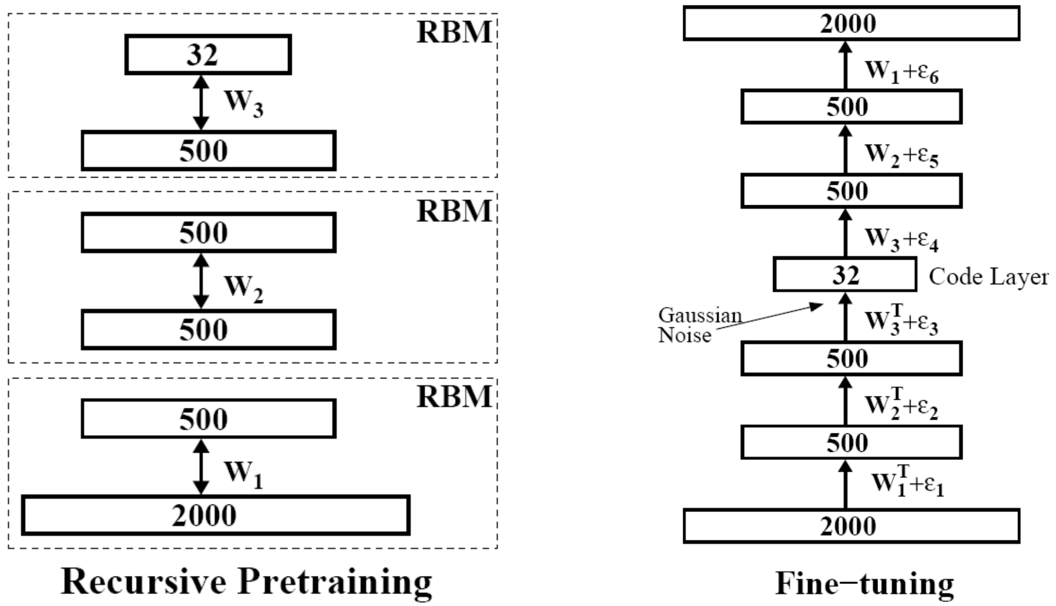
Learn parameters (W and b) using (approx) max-likelihood $p(v)$

How to learn codes ? → Stack multiple RBMs (Deep Belief Networks)

Semantic Hashing (RBM)

Deep Belief Networks

– Similar functionality as multi-layer Neural Nets



Output of each stage used as input to next

Back-propagation (coordinate descent) with Auto-encoding objective

Many parameters, architecture choices, usually slow to train and to apply !

Salakhutdinov et al.[8]

Binary Reconstructive Embedding

Construct binary codes by minimizing difference between original (metric) distance and hamming distance

$$h_k(x) = \text{sgn}(w_k^T v(x)) \quad \text{where} \quad v(x) = [1, K(x_{k_1}, x), \ldots, K(x_{k_s}, x)]^T$$

kernel

chosen randomly or learned

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$$\hat{W} = \arg\min_{W} \sum_{(x_i, x_j) \in T} [d_M(x_i, x_j) - d_H(x_i, x_j)]^2$$

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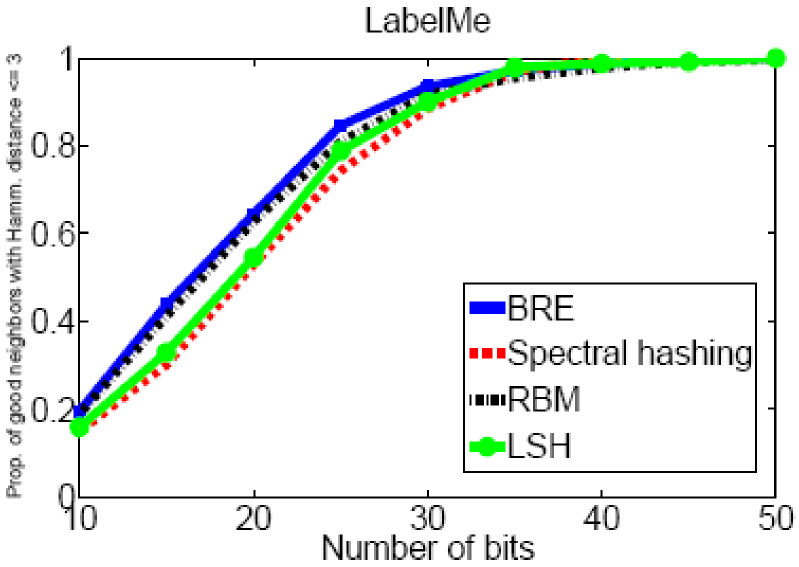
$(1/2)\|x_i - x_j\|^2$

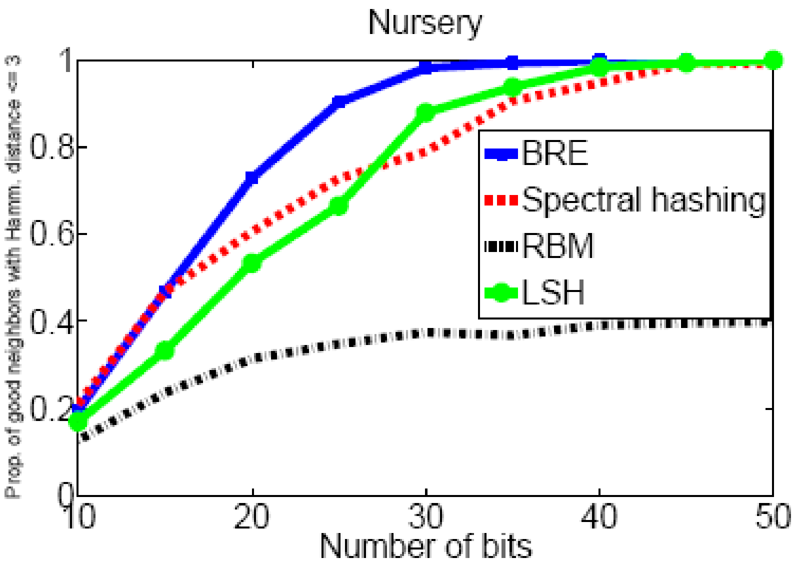
$(1/4m)\sum_{k=1}^{m}[h_k(x_i) - h_k(x_j)]^2$

- Data scaled to unit norm to remove the effect of scale (but this changes the distance between points), uniform scaling better
- Coordinate Descent for optimization, deals with discontinuities
- Expensive to compute codes, learning appropriate anchors for kernel representations hard

Binary Reconstructive Embedding

Testing based on points retrieved within hamming radius 3



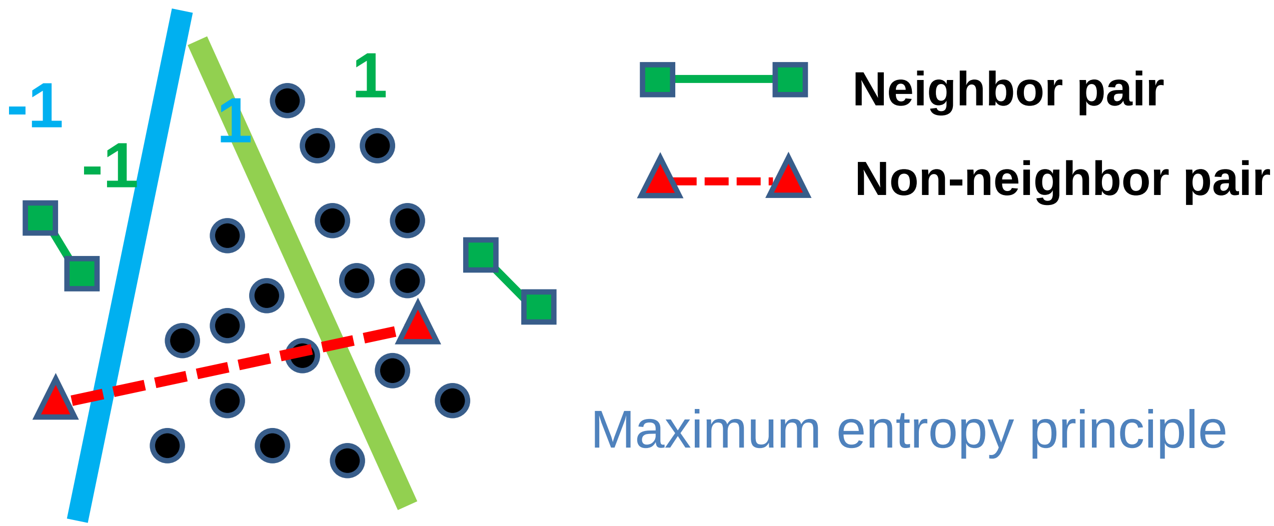


LSH is quite close even for moderate number of bits !

Kulis et al.[13]

Semi-supervised Hashing

Suppose a few neighbor pairs and a few non-neighbor pairs are given



Maximum entropy principle

Semi-supervised Formulation

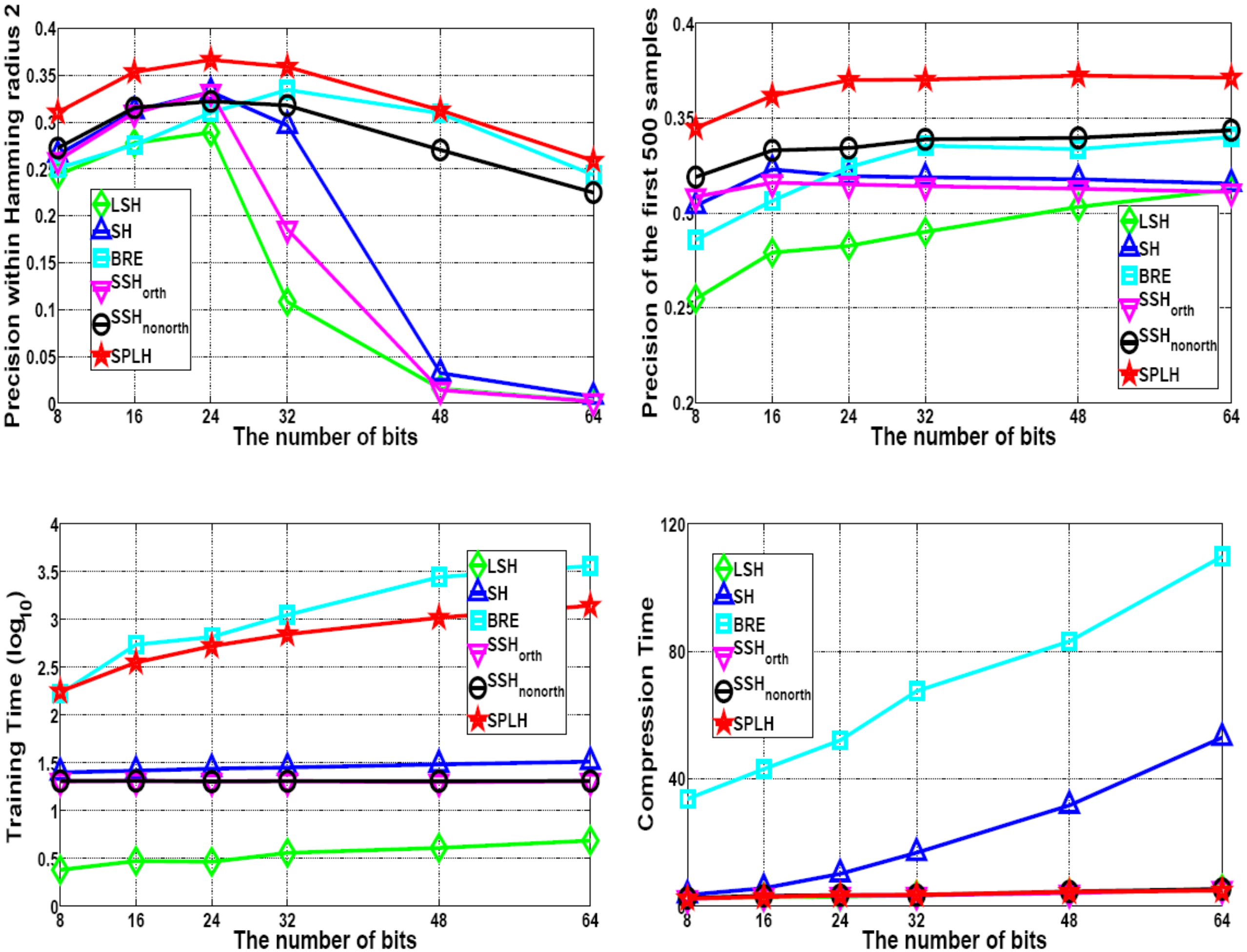
$$\max_{h_k} \{ J(h_k(\mathbf{X}_l)) + \eta \cdot Entropy(h_k(\mathbf{X})) \}$$

Empirical fitness (labeled data)

Regularizer (all data)

Wang et al.[14]

Flickr-270K



Wang et al.[15]

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