Hashing with Binary Autoencoders



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Large Scale Image Retrieval

Searching a large database for images that match a query. Query is an image that you already have.

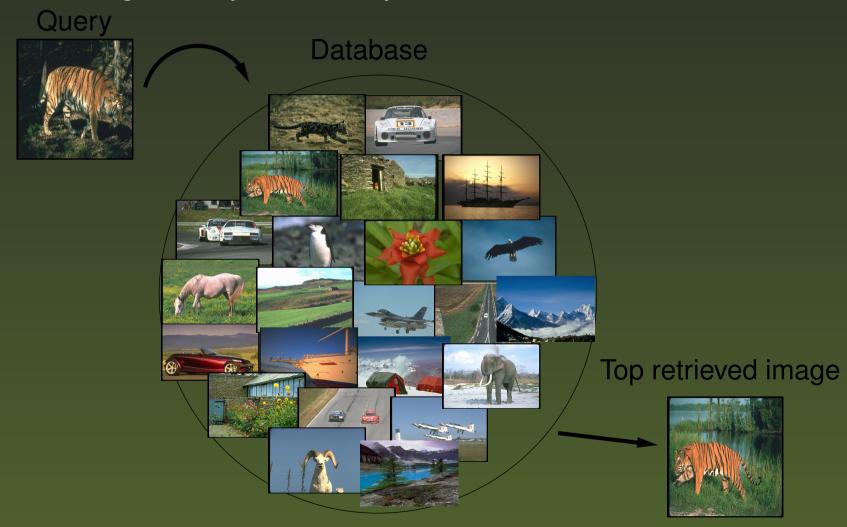
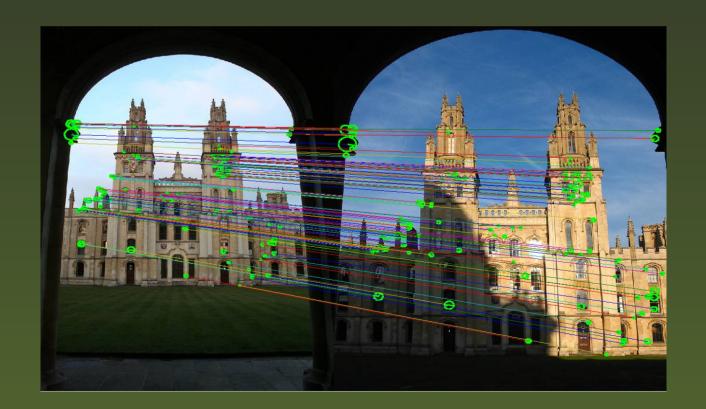


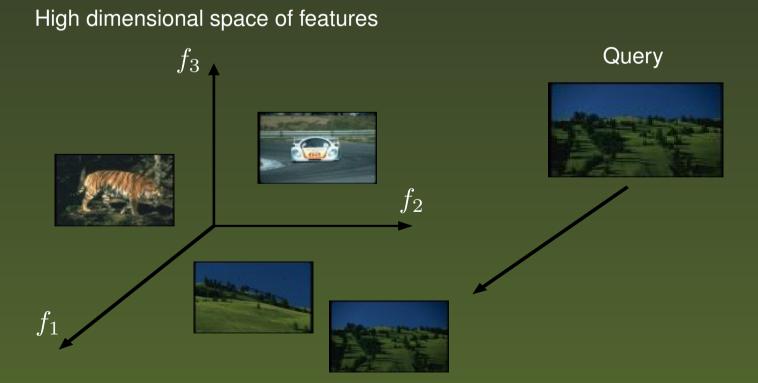
Image Representations

- We Compare images by comparing their feature vectors.
 - Extract features from images and represent each image by the feature vector.
- Common features in image retrieval problem are SIFT, GIST, wavelet.



K Nearest Neighbors Problem

- We have N training points in D dimensional space (usually D > 100) $\mathbf{x}_i \in \mathbb{R}^D, i = 1, \dots, N$.
- Find the K nearest neighbors of a query point $x_q \in \mathbb{R}^D$.
 - Two applications are image retrieval and classification.
 - Neighbors of a point are determined by the Euclidean distance.

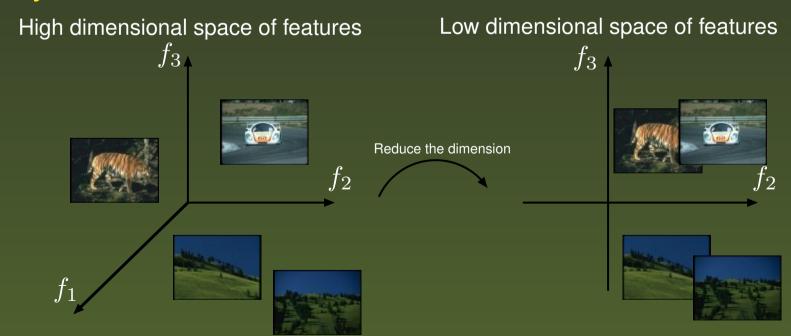


Exact vs Approximate Nearest Neighbors

Exact search in the original space is $\mathcal{O}(ND)$ in both time and space.

This does not scale to large, high-dimensional datasets. Algorithms for approximate nearest neighbors:

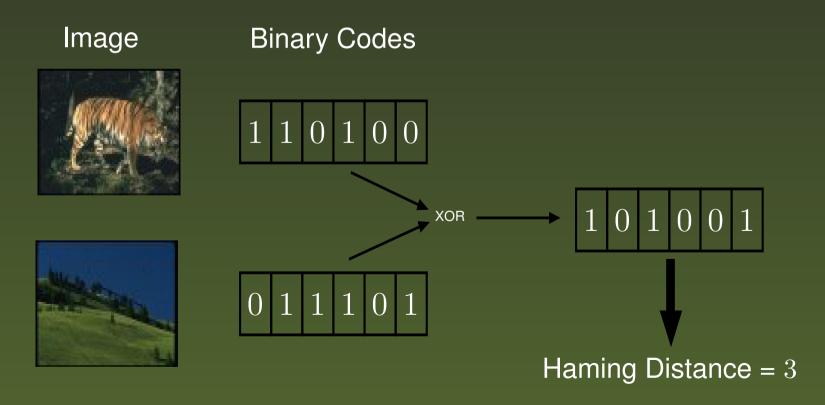
- Tree based methods
- Dimensionality reduction
- Binary hash functions



Binary Hash Functions

A binary hash function h takes as input a high-dimensional vector $\mathbf{x} \in \mathbb{R}^D$ and maps it to an L-bit vector $\mathbf{z} = \mathbf{h}(\mathbf{x}) \in \{0, 1\}^L$.

- Main goal: preserve neighbors, i.e., assign (dis)similar codes to (dis)similar patterns.
- Hamming distance computed using XOR and then counting.



Binary Hash Function in Large Scale Image Retrieval

Scalability: we have millions or billions of high-dimensional images.

- \diamond Time complexity: $\mathcal{O}(NL)$ instead of $\mathcal{O}(ND)$ with small constants.
 - Bit operations to compute Hamming distance instead of floating point operations to compute Euclidean distance.
- Space complexity: $\mathcal{O}(NL)$ instead of $\mathcal{O}(ND)$ with small constants. We can fit the binary codes of the entire dataset in memory, further speeding up the search.

Ex: N = 1000000 points, D = 300 and L = 32:

	Space	Time
Original space	1.2 GB	20 ms
Hamming space	4 MB	$30~\mu s$

Previous Works on Binary Hashing

Binary hash functions have attained a lot of attention in recent years:

- Locality-Sensitive Hashing (Indyk and Motwani 2008)
- Spectral Hashing (Weiss et al. 2008)
- Kernelized Locality-Sensitive Hashing (Kulis and Grauman 2009)
- Semantic Hashing (Salakhutdinov and Hinton 2009)
- Iterative Quantization (Gong and Lazebnik 2011)
- Semi-supervised hashing for scalable image retrieval (Wang et al. 2012)
- Hashing With Graphs (Liu et al. 2011)
- Spherical Hashing (Heo et al. 2012)

Categories of hash functions:

- Data-independent methods (e.g. LSH: threshold a random projection).
- Data-dependent methods: learn hash function from a training set.
 - Unsupervised: no labels
 - ♦ Semi-supervised: some labels
 - Supervised: all labels

Objective Functions in Dimensionality Reduction

Learning hash functions is often done with dimensionality reduction:

- We can optimize an objective over the hash h function directly, e.g.:
 - ♦ Autoencoder: encoder (h) and decoder (f) can be linear, neural nets, etc.

$$\min_{\mathbf{h}, \mathbf{f}} \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{f}(\mathbf{h}(\mathbf{x}_n))\|^2$$

- Or, we can optimize an objective over the projections Z and then use these to learn the hash function h, e.g.:
 - → Laplacian Eigenmaps (spectral problem):

$$\min_{\mathbf{Z}} \sum_{i,j=1}^N \mathbf{W}_{ij} \left\| \mathbf{z}_i - \mathbf{z}_j
ight\|^2 \quad ext{s.t.} \quad \sum_{i=1}^N \mathbf{z}_i = 0, \quad \mathbf{Z}^T \mathbf{Z} = \mathbf{I}$$

♦ Elastic Embedding (nonlinear optimization):

$$\min_{\mathbf{Z},\lambda} \sum_{i,j=1}^{N} \mathbf{W}_{ij}^{+} \|\mathbf{z}_{i} - \mathbf{z}_{j}\|^{2} + \lambda \sum_{i,j=1}^{N} \mathbf{W}_{ij}^{-} \exp(-\|\mathbf{z}_{i} - \mathbf{z}_{j}\|^{2})$$

Learning Binary Codes

These objective functions are difficult to optimize because the codes are binary. Most existing algorithms approximate this as follows:

- 1. Relax the binary constraints and solve a continuous problem to obtain continuous codes.
- 2. Binarize these codes. Several approaches:
 - Truncate the real values using threshold zero
 - Find the best threshold for truncation
 - Rotate the real vectors to minimize the quantization loss:

$$E(\mathbf{B}, \mathbf{R}) = \|\mathbf{B} - \mathbf{V}\mathbf{R}\|_F^2$$
 s.t. $\mathbf{R}^T \mathbf{R} = \mathbf{I}, \ \mathbf{B} \in \{0, 1\}^{NL}$

- 3. Fit a mapping to (patterns, codes) to obtain the hash function \mathbf{h} . Usually a classifier.
- This is a suboptimal, "filter" approach: find approximate binary codes first, then find the hash function. We seek an optimal, "wrapper" approach: optimize over the binary codes and hash function jointly.

Our Hashing Models: Continuous Autoencoder

Consider first a well-known model for continuous dimensionality reduction, the continuous autoencoder:

- The encoder $h: \mathbf{x} \to \mathbf{z}$ maps a real vector $\mathbf{x} \in \mathbb{R}^D$ onto a low-dimensional real vector $\mathbf{z} \in \mathbb{R}^L$ (with L < D).
- lacktriangle The decoder $\mathbf{f}: \mathbf{z} \to \mathbf{x}$ maps \mathbf{z} back to \mathbb{R}^D in an effort to reconstruct \mathbf{x} .

The objective function of an autoencoder is the reconstruction error:

$$E(\mathbf{h}, \mathbf{f}) = \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{f}(\mathbf{h}(\mathbf{x}_n))\|^2$$

We can also define the following two-step objective function:

first
$$\min E(\mathbf{f}, \mathbf{Z}) = \sum_{n=1}^N \|\mathbf{x}_n - \mathbf{f}(\mathbf{z}_n)\|^2$$
 then $\min E(\mathbf{h}) = \sum_{n=1}^N \|\mathbf{z}_n - \mathbf{h}(\mathbf{x}_n)\|^2$

In both cases, if f and h are linear then the optimal solution is PCA.

Our Hashing Models: Binary Autoencoder

We consider binary autoencoders as our hashing model:

- * The encoder $\mathbf{h}: \mathbf{x} \to \mathbf{z}$ maps a real vector $\mathbf{x} \in \mathbb{R}^D$ onto a low-dimensional binary vector $\mathbf{z} \in \{0,1\}^L$ (with L < D). This will be our hash function. We consider a thresholded linear encoder (hash function) $\mathbf{h}(\mathbf{x}) = \sigma(\mathbf{W}\mathbf{x})$ where $\sigma(t)$ is a step function elementwise.
- The $\frac{\operatorname{decoder} \mathbf{f} : \mathbf{z} \to \mathbf{x}}{\mathbf{x}}$ maps \mathbf{z} back to \mathbb{R}^D in an effort to reconstruct \mathbf{x} . We consider a linear decoder in our method.

Binary autoencoder: optimize jointly over h and f the reconstruction error:

$$E_{\mathsf{BA}}(\mathbf{h}, \mathbf{f}) = \sum_{n=1}^{\infty} \|\mathbf{x}_n - \mathbf{f}(\mathbf{h}(\mathbf{x}_n))\|^2$$
 s.t. $\mathbf{h}(\mathbf{x}_n) \in \{0, 1\}^L$

Binary factor analysis: first optimize over f and Z:

$$E_{\mathsf{BFA}}(\mathbf{Z},\mathbf{f}) = \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{f}(\mathbf{z}_n)\|^2$$
 s.t. $\mathbf{z}_n \in \{0,1\}^L, \ n = 1,\ldots,N$

then fit the hash function h to (X, Z).

Optimization of Binary Autoencoders: "filter" approach

A simple but suboptimal approach:

1. Minimize the following objective function over linear functions f, g:

$$E(\mathbf{g}, \mathbf{f}) = \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{f}(\mathbf{g}(\mathbf{x}_n))\|^2$$

which is equivalent to doing PCA on the input data.

2. Binarize the codes Z = g(X) by an optimal rotation:

$$E(\mathbf{B}, \mathbf{R}) = \|\mathbf{B} - \mathbf{R}\mathbf{Z}\|_{\mathsf{F}}^2$$
 s.t. $\mathbf{R}^T \mathbf{R} = \mathbf{I}, \ \mathbf{B} \in \{0, 1\}^{LN}$

The resulting hash function is $h(x) = \sigma(Rg(x))$.

This is what the Iterative Quantization algorithm (ITQ, Gong et al. 2011), a leading binary hashing method, does.

Can we obtain better hash functions by doing a better optimization, i.e., respecting the binary constraints on the codes?

Optimization of Binary Autoencoders using MAC

Minimize the autoencoder objective function to find the hash function:

$$E_{\mathsf{BA}}(\mathbf{h},\mathbf{f}) = \sum_{n=1}^N \|\mathbf{x}_n - \mathbf{f}(\mathbf{h}(\mathbf{x}_n))\|^2$$
 s.t. $\mathbf{h}(\mathbf{x}_n) \in \{0,1\}^L$

We use the method of auxiliary coordinates (MAC) (Carreira-Perpiñán & Wang 2012, 2014). The idea is to break nested functional relationships judiciously by introducing variables as equality constraints, apply a penalty method and use alternating optimization.

We introduce as auxiliary coordinates the outputs of h, i.e., the codes for each of the N input patterns and obtain a constrained problem:

$$\min_{\mathbf{h}, \mathbf{f}, \mathbf{Z}} \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{f}(\mathbf{z}_n)\|^2 \quad \text{s.t.} \quad \mathbf{z}_n = \mathbf{h}(\mathbf{x}_n), \ \mathbf{z}_n \in \{0, 1\}^L, \ n = 1, \dots, N.$$

Optimization of Binary Autoencoders (cont.)

We now apply the quadratic-penalty method (we could also apply the augmented Lagrangian):

$$E_Q(\mathbf{h}, \mathbf{f}, \mathbf{Z}; \mu) = \sum_{n=1}^{N} \left(\|\mathbf{x}_n - \mathbf{f}(\mathbf{z}_n)\|^2 + \mu \|\mathbf{z}_n - \mathbf{h}(\mathbf{x}_n)\|^2 \right) \text{ s.t. } \left\{ \begin{array}{l} \mathbf{z}_n \in \{0, 1\}^L \\ n = 1, \dots, N. \end{array} \right.$$

Effects of the new parameter μ on the objective function:

- During the iterations, we allow the encoder and decoder to be mismatched.
- \bullet When μ is small, there will be a lot of mismatch. As μ increases, the mismatch is reduced.
- $As \mu \to \infty$ there will be no mismatch and E_Q becomes like E_{BA} .
- \bullet In fact, this occurs for a finite value of μ .

Optimization of Binary Autoencoders using MAC (cont.)

In order to minimize:

$$E_Q(\mathbf{h}, \mathbf{f}, \mathbf{Z}; \mu) = \sum_{n=1}^{N} \left(\|\mathbf{x}_n - \mathbf{f}(\mathbf{z}_n)\|^2 + \mu \|\mathbf{z}_n - \mathbf{h}(\mathbf{x}_n)\|^2 \right)$$
s.t. $\mathbf{z}_n \in \{0, 1\}^L, \ n = 1, \dots, N.$

we apply alternating optimization. The algorithm learns the hash function h and the decoder f given the current codes, and learns the patterns' codes given h and f:

- Over (h, f) for fixed \mathbb{Z} , we obtain L + 1 independent problems for each of the L single-bit hash functions, and for f.
- Over Z for fixed (\mathbf{h}, \mathbf{f}) , the problem separates for each of the N codes. The optimal code vector for pattern \mathbf{x}_n tries to be close to the prediction $\mathbf{h}(\mathbf{x}_n)$ while reconstructing \mathbf{x}_n well.

We have to solve each of these steps.

Optimization over f for fixed Z (decoder given codes)

We have to minimize the following over the linear decoder \mathbf{f} (where $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$):

$$E_Q(\mathbf{h}, \mathbf{f}, \mathbf{Z}; \mu) = \sum_{n=1}^{N} \left(\|\mathbf{x}_n - \mathbf{f}(\mathbf{z}_n)\|^2 + \mu \|\mathbf{z}_n - \mathbf{h}(\mathbf{x}_n)\|^2 \right) \text{ s.t. } \left\{ \begin{array}{l} \mathbf{z}_n \in \{0, 1\}^L \\ n = 1, \dots, N. \end{array} \right.$$

A simple linear regression with data (\mathbf{Z}, \mathbf{X}) :

$$\min_{\mathbf{f}} \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{f}(\mathbf{z}_n)\|^2 = \min_{\mathbf{A}, \mathbf{b}} \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{A}\mathbf{z}_n - \mathbf{b}\|^2$$

The solution is (ignoring the bias for simplicity) $\mathbf{A} = \mathbf{X}\mathbf{Z}^T(\mathbf{Z}\mathbf{Z}^T)^{-1}$ and can be computed in $\mathcal{O}(NDL)$.

The constant factor in the \mathcal{O} -notation is small because \mathbf{Z} is binary, e.g. $\mathbf{X}\mathbf{Z}^T$ involves only sums, not multiplications.

Optimization over h for fixed Z (encoder given codes)

We have to minimize the following over the linear hash function h (where $h(x) = \sigma(Wx)$):

$$E_Q(\mathbf{h}, \mathbf{f}, \mathbf{Z}; \mu) = \sum_{n=1}^{N} \left(\|\mathbf{x}_n - \mathbf{f}(\mathbf{z}_n)\|^2 + \mu \|\mathbf{z}_n - \mathbf{h}(\mathbf{x}_n)\|^2 \right) \text{ s.t. } \left\{ \begin{array}{l} \mathbf{z}_n \in \{0, 1\}^L \\ n = 1, \dots, N. \end{array} \right.$$

The hash function has the following form:

$$\min_{\mathbf{h}} \sum_{n=1}^{N} \|\mathbf{z}_n - \mathbf{h}(\mathbf{x}_n)\|^2 = \min_{\mathbf{W}} \sum_{n=1}^{N} \|\mathbf{z}_n - \sigma(\mathbf{W}\mathbf{x}_n)\|^2$$
$$= \sum_{l=1}^{L} \min_{\mathbf{W}_l} \sum_{r=1}^{N} (\mathbf{z}_{nl} - \sigma(\mathbf{w}_l^T \mathbf{x}_n))^2$$

so it separates for each bit $l = 1 \dots L$.

The subproblem for each bit is a binary classification problem with data $(\mathbf{X}, \mathbf{Z}_{\cdot l})$ using the number of misclassified patterns as loss function. We approximately solve it with a linear SVM.

Optimization over ${f Z}$ for fixed (h,f) (adjust codes given encoder/decoder)

This is a binary optimization on NL variables, but it separates into N independent optimizations each on only L variables:

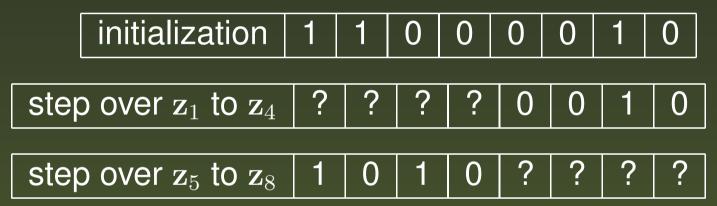
$$\min_{\mathbf{z}} e(\mathbf{z}) = \|\mathbf{x} - \mathbf{f}(\mathbf{z})\|^2 + \mu \|\mathbf{z} - \mathbf{h}(\mathbf{x})\|^2 \quad \text{s.t.} \quad \mathbf{z} \in \{0, 1\}^L$$

- This is a quadratic objective function on binary variables, which is NP-complete in general, but L is small.
- With $L \lesssim 16$ we can afford an exhaustive search over the 2^L codes. Besides, we don't need to evaluate every code vector, or every bit of every code vectors:
 - Intuitively, the optimum will not be far from h(x), at least if μ is large.
 - * We don't need to test vectors beyond a Hamming distance $\|\mathbf{x} \mathbf{f}(\mathbf{h}(\mathbf{x}))\|^2 / \mu$ (they cannot be optima).

Z Step for Large L: Approximate Solution

For larger L, we use alternating optimization over groups of g bits.

- The optimization over a g-bit group is done by enumeration using the accelerations described earlier.
- \diamond Consider an example where L=8 and g=4:



How to initialize z? We have used the following two approaches:

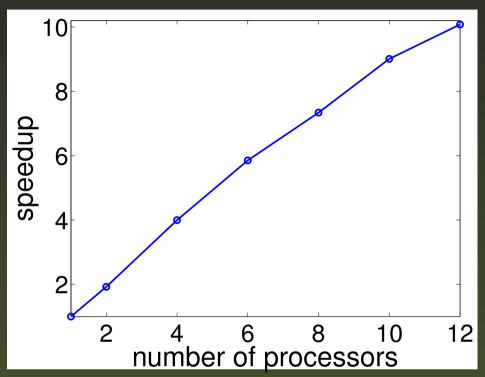
- Warm start: Initialize z to the code found in the previous iteration's Z step. Convenient in later iterations, when the codes change slowly.
- Solve the relaxed problem on $\mathbf{z} \in [0,1]^L$ and then truncate it. We use an ADMM algorithm, caching one matrix factorization for all $n=1,\ldots,N$. Convenient in early iterations, when the codes change fast.

Summary of the Binary Autoencoder MAC Algorithm

```
input \mathbf{X}_{D\times N}=(\mathbf{x}_1,\ldots,\mathbf{x}_N),\,L\in\mathbb{N}
Initialize \mathbf{Z}_{L \times N} = (\mathbf{z}_1, \dots, \mathbf{z}_N) \in \{0, 1\}^{LN}
for \mu = 0 < \mu_1 < \dots < \mu_{\infty}
    for l = 1, ..., L
                                                                                                                                                   h step
        h_l \leftarrow \mathsf{fit} \; \mathsf{SVM} \; \mathsf{to} \; (\mathbf{X}, \mathbf{Z}_{\cdot l})
    f \leftarrow least-squares fit to (Z, X)
    for n = 1, ..., N
                                                                                                                                                   Z step
         \mathbf{z}_n \leftarrow \operatorname{arg\,min}_{\mathbf{z}_n \in \{0,1\}^L} \|\mathbf{y}_n - \mathbf{f}(\mathbf{z}_n)\|^2 + \mu \|\mathbf{z}_n - \mathbf{h}(\mathbf{x}_n)\|^2
    \underline{\mathbf{if}} \ \mathbf{Z} = \mathbf{h}(\mathbf{X}) \ \underline{\mathbf{then}} \ \mathsf{stop}
return h, Z = h(X)
```

Repeatedly solve: classification (h), regression (f), binarization (Z).

Optimization of Binary Autoencoders using MAC (cont.)



The steps can be parallelized:

- * Z step: N independent problems, one per binary code vector \mathbf{z}_n .
- f and h steps are independent. h step: L independent problems, one per binary SVM.

Schedule for the penalty parameter μ :

- With exact steps, the algorithm terminates at a finite μ . This occurs when the solution of the **Z** step equals the output of the hash function, and gives a practical termination criterion.
- lacktriangle We start with a small μ and increase it slowly until termination.

Experimental Setup: Precision and Recall

The performance of binary hash functions is usually reported using precision and recall.

Retrieved set for a qery point can be defined in two ways:

- The K nearest neighbors in the Hamming space.
- \leftarrow The points in the Hamming radius of r.

Ground-truth for a query point contains the first K nearest neighbors of the point in the original (D-dimensional) space.

```
\frac{|\{\text{retrieved points}\} \cap \{\text{groundtruth}\}|}{|\{\text{groundtruth}\}|} \frac{|\{\text{retrieved points}\} \cap \{\text{groundtruth}\}|}{|\{\text{retrieved points}\}|}
```

Experiment: Datasets

CIFAR-10 dataset: $60\,000\,32\times32$ color images in 10 classes; training/test $50\,000/10\,000$, 320 GIST features.

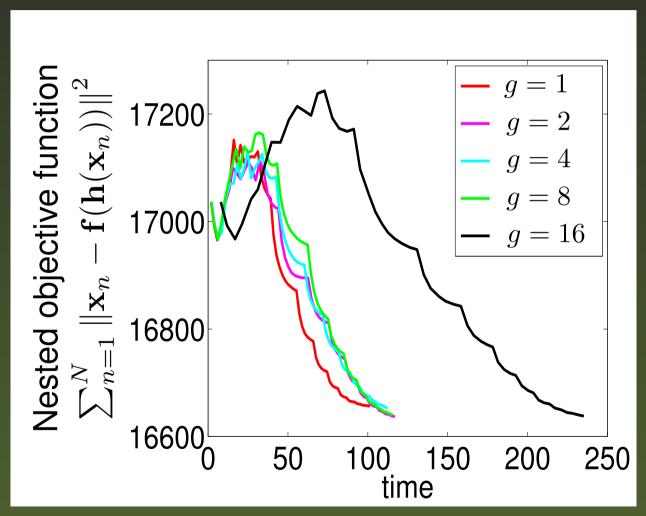
airplane automobile bird ship truck NUS-WIDE dataset: 269 648 high resolution color images in 81 concepts; training/test 161 789/107 859, 128 Wavelet features.

SIFT-1M dataset: 1 010 000 high resolution color images; training/test 1 000 000/10 000, 128 SIFT features.



Experiment: Exact vs. Inexact Optimization

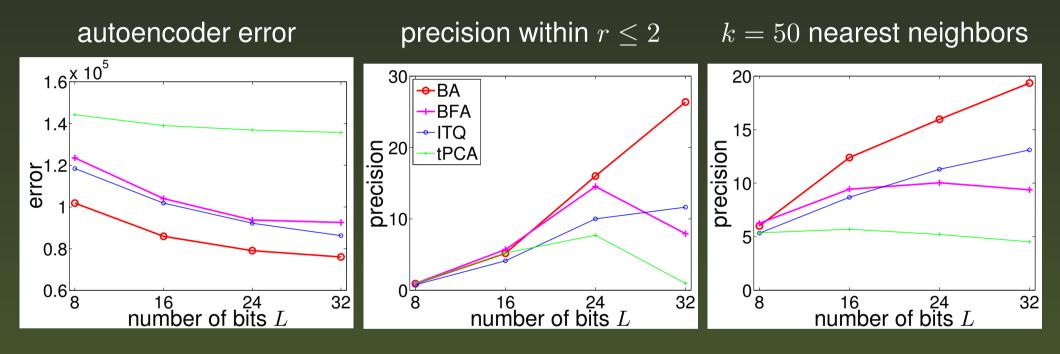
Inexact $\overline{\mathbf{Z}}$ steps achieve solutions of similar quality than exact steps but much faster. Best results occur for $g \approx 1$ in alternating optimization.



 $N=50\,000$ images of CIFAR dataset, L=16 bits, relaxed initial **Z**.

Optimizing Binary Autoencoders Improves Precision

NUS-WIDE-LITE dataset, $N=27\,807$ training/ $27\,808$ test images, D=128 wavelet features.



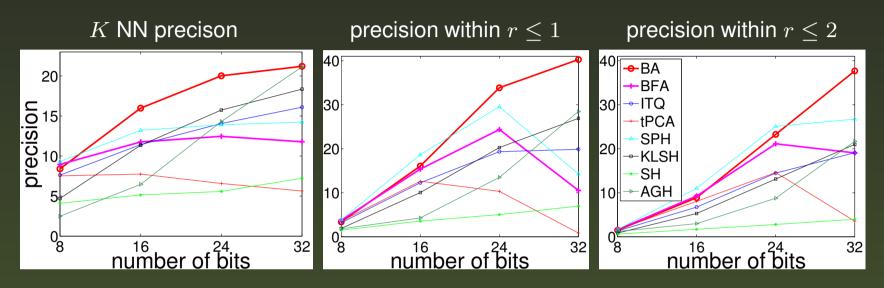
ITQ and tPCA use a filter approach (suboptimal): They solve the continuous problem and truncate the solution.

BA uses a wrapper approach (optimal): It optimizes the objective function respecting the binary nature of the codes.

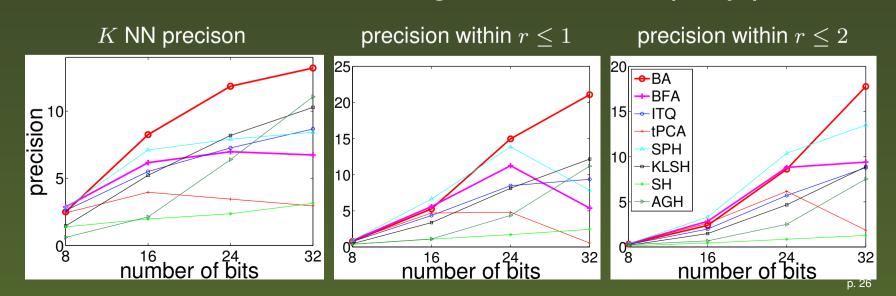
BA achieves lower reconstruction error and also better precision/recall.

Experimental Results on NUS-WIDE Dataset (cont.)

Ground truth: K = 500 nearest neighbors of each query point:

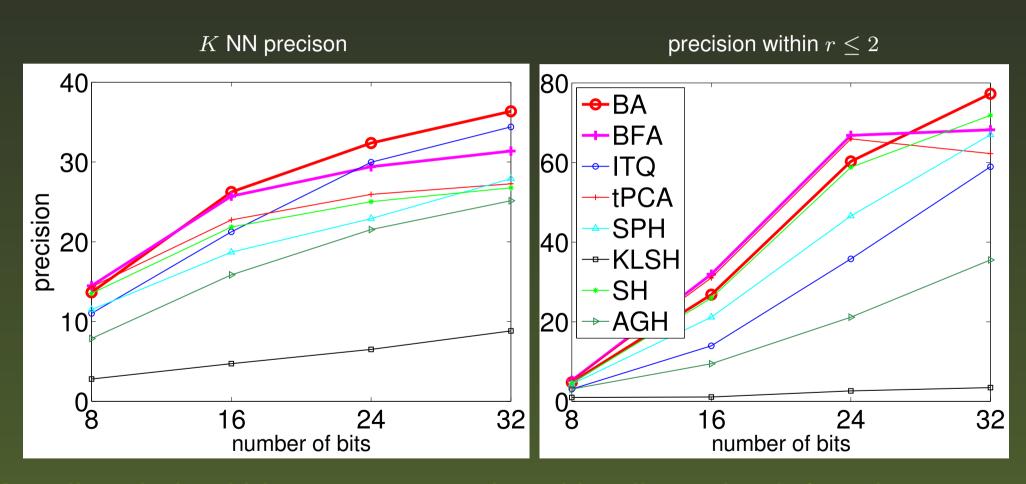


Ground truth: K = 100 nearest neighbors of each query point:



Experimental Results On ANNSIFT-1m

Ground truth: K = 10000 nearest neighbors of each query point:



A well-optimized binary autoencoder with a linear hash function consistently beats state-of-the-art methods.

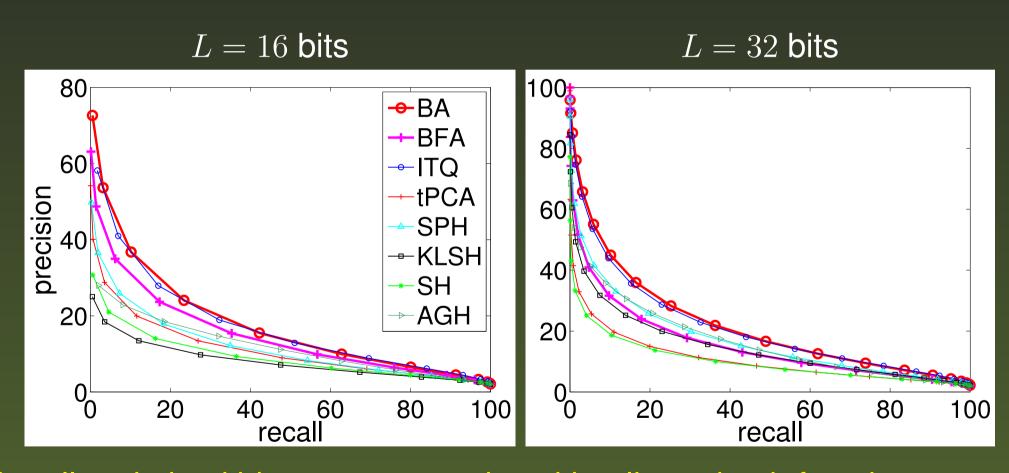
Conclusion

- A fundamental difficulty in learning hash functions is binary optimization.
 - Most existing methods relax the problem and find its continuous solution. Then, they threshold the result to obtain binary codes, which is sub-optimal.
 - Using the method of auxiliary coordinates, we can do the optimization correctly and efficiently for binary autoencoders.
 - ★ Encoder (hash function): train one SVM per bit.
 - ★ Decoder: solve a linear regression problem.
 - ★ Highly parallel.
- Remarkably, with proper optimization, a simple model (autoencoder with linear encoder and decoder) beats state-of-the-art methods using nonlinear hash functions and/or better objective functions.

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Experimental Results on CIFAR Dataset

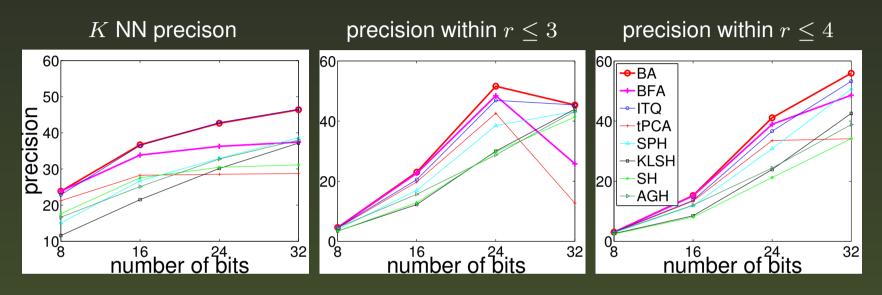
Ground truth: K = 1000 nearest neighbors of each query point.



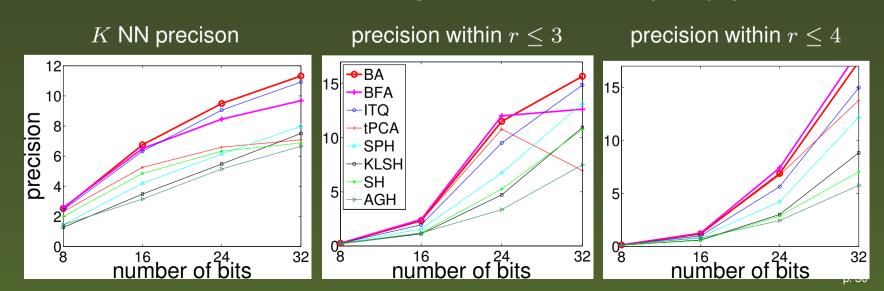
A well-optimized binary autoencoder with a linear hash function consistently beats state-of-the-art methods.

Experimental Results on CIFAR Dataset (cont.)

Ground truth: K = 1000 nearest neighbors of each query point:



Ground truth: K = 50 nearest neighbors of each query point:

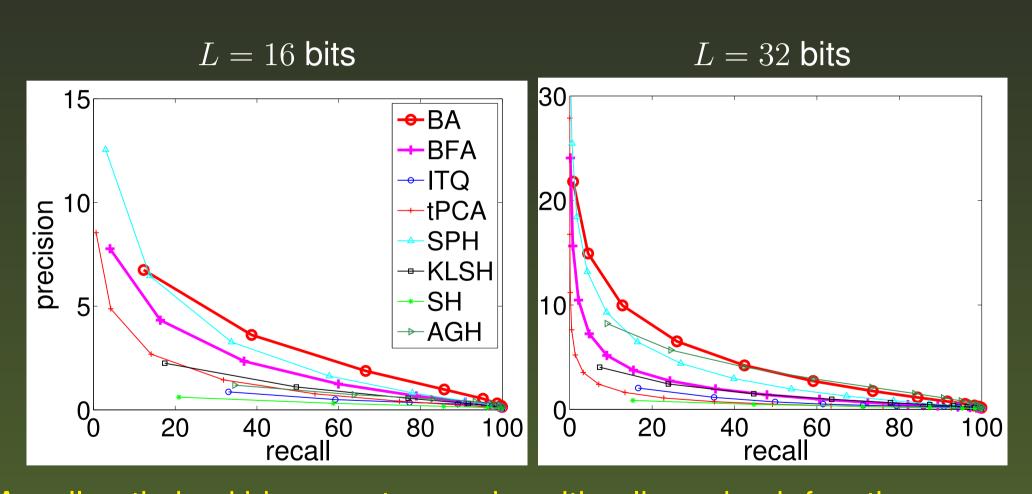


Top retrieved images from CIFAR Dataset

input

Experimental Results on NUS-WIDE Dataset

Ground truth: K=100 nearest neighbors of each query point:



A well-optimized binary autoencoder with a linear hash function consistently beats state-of-the-art methods using more sophisticated objectives and (nonlinear) hash functions.

Comparison Algorithms

Algorithm with Kernel hash functions:

KLSH(Kulis et al. 2009): Generalizes locality-sensitive hashing to accommodate arbitrary kernel functions.

Algorithms with embedding objective function(laplacian eigenmap):

- SH(Weiss et al. 2008): Finds the relaxed solution of laplacian eigenmap and truncates it.
- \diamond AGH(Liu et al. 2011): Approximates eigenfunctions using K points and finds thresholds to make the codes binary.

Algorithms that maximize the variance:

- ITQ(Gong et al.) and tPCA: First compute PCA on the input patterns and then truncate the continous solution.
- SPH(Heo et al. 2012): Iteratively refines the thresholds and pivots to maximize the variance of binary codes.