Hashing with Binary Autoencoders



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Large Scale Image Retrieval

Searching a large database for images that are closest to a query image.



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 Functions in Large Scale Image Retrieval

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

- 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: O(NL) instead of O(ND) with small constants.
 Ex: N = 1000000 points take
 ◆ 1.2 Gigabytes of memory if D = 300 floats
 - ◆ 4 Megabytes of memory if L = 32 bits

We can fit the binary codes of the entire dataset in memory, further speeding up the search.

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)
- Most of the methods find the binary codes in two steps:
 - 1. Relax the binary constraints and solve a continuous problem.
 - 2. Binarize these continuous codes to obtain binary codes.

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: Binary Autoencoder

We consider binary autoencoders as our hashing model:

★ The encoder h: x → z maps a real vector x ∈ \mathbb{R}^D onto a low-dimensional binary vector z ∈ {0,1}^L (with L < D). This will be our hash function.</p>

The decoder $f: z \to x$ maps z back to \mathbb{R}^D in order to reconstruct x. The optimal autoencoder will preserve neighborhoods to some extent.

We want to optimize the reconstruction error jointly over \mathbf{h} and \mathbf{f} :

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

We consider a linear decoder and a thresholded linear encoder (hash function) $h(x) = \sigma(Wx)$ where $\sigma(t)$ is a step function elementwise.

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 $\mathbf{Z} = \mathbf{g}(\mathbf{X})$ 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:

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

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.

1. 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 using MAC (cont.)

2. Apply the quadratic-penalty method (can also apply augmented Lagrangian):

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

We start with a small μ and increase it slowly towards infinity.

3. To minimize $E_Q(\mathbf{h}, \mathbf{f}, \mathbf{Z}; \mu)$, we apply alternating optimization. The algorithm learns the hash function \mathbf{h} and the decoder \mathbf{f} given the current codes, and learns the patterns' codes given \mathbf{h} and \mathbf{f} :

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

We have to solve each of these steps.

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

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

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

This is easily done by reusing existing algorithms for regression/classif.

Fit f to (\mathbf{Z}, \mathbf{X}) : a simple linear regression with data (\mathbf{Z}, \mathbf{X}) :

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

Fit h to (X, Z): L separate binary classifications with data (X, Z_{l}) :

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

We approximately solve each with a binary linear SVM.

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

Fit Z given (f, h): This is a binary optimization on NL variables, but it separates into N independent optimizations each on only L variables:

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

This is a quadratic objective function on binary variables, which is NP-complete in general, but L is small.

♦ With $L \leq 16$ we can afford an exhaustive search over the 2^L codes. Speedups: try $\mathbf{h}(\mathbf{x}_n)$ first; use bit operations, necessary/sufficient conditions, parallel processing...

For larger *L*, we use alternating optimization over groups of *g* bits. How to initialize z_n ? We have used the following two approaches:

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

Optimization of Binary Autoencoders using MAC (cont.)



The steps can be parallelized:

- Z step: N independent problems, one per binary code vector 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.
- We start with a small μ and increase it slowly until termination.

Summary of the Binary Autoencoder MAC Algorithm

$$\begin{array}{ll} \underbrace{\text{input}}_{\mathbf{I}} \mathbf{X}_{D \times N} = (\mathbf{x}_1, \dots, \mathbf{x}_N), L \in \mathbb{N} \\ \text{Initialize } \mathbf{Z}_{L \times N} = (\mathbf{z}_1, \dots, \mathbf{z}_N) \in \{0, 1\}^{LN} \\ \underbrace{\text{for } \mu = 0 < \mu_1 < \dots < \mu_{\infty}}_{\mathbf{for } l = 1, \dots, L} & \text{h step} \\ h_l \leftarrow \text{fit SVM to } (\mathbf{X}, \mathbf{Z}_{\cdot l}) & \text{f step} \\ \mathbf{f} \leftarrow \text{least-squares fit to } (\mathbf{Z}, \mathbf{X}) & \text{f step} \\ \underbrace{\text{for } n = 1, \dots, N}_{\mathbf{z}_n \leftarrow \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}_{\mathbf{if } \mathbf{Z} = \mathbf{h}(\mathbf{X})} & \underbrace{\text{fit } \mathbf{S} \mathbf{U} \mathbf{I} \mathbf{I} \mathbf{U}_{\mathbf{X}}}_{\mathbf{I} \mathbf{U}_{\mathbf{X}}} & \mathbf{I} \mathbf{U}_{\mathbf{X}} - \mathbf{I} \mathbf{U}_{\mathbf{X}} \\ \underbrace{\text{for } \mathbf{I} = \mathbf{I}_{\mathbf{X}}}_{\mathbf{I} \mathbf{U}_{\mathbf{X}}} & \mathbf{I} \mathbf{U}_{\mathbf{X}} - \mathbf{I} \mathbf{U}_{\mathbf{X}} \\ \mathbf{I} \mathbf{U}_{\mathbf{X}} - \mathbf{I} \mathbf{U}_{\mathbf{X}} \\ \mathbf{I} \mathbf{U}_{\mathbf{X}} + \mathbf{U}_{\mathbf{X}} - \mathbf{U}_{\mathbf{X}} \\ \mathbf{I} \mathbf{U}_{\mathbf{X}} + \mathbf{U}_{\mathbf{X}} \\ \mathbf{I} \mathbf{U}_{\mathbf{X}} + \mathbf{U}_{\mathbf{X}} \\ \mathbf{U}_{\mathbf{U}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{X}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}}} \\ \mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{\mathbf{U}_{$$

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

Experiment: Initialization of Z Step

If using alternating optimization in the Z step (in groups of g bits), we need an initial z_n . Initializing z_n using the truncated relaxed solution achieves better local optima than using warm starts. Also, using small $g (\approx 1)$ is fastest while giving good optima.



 $N = 50\,000$ images of CIFAR dataset, D = 320 GIST features, L = 16 bits.

Optimizing Binary Autoencoders Improves Precision

NUS-WIDE-LITE dataset, $N = 27\,807$ training/ 27808 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.

Comparison with other hashing algorithms

NUS-WIDE dataset: 269 648 high resolution color images in 81 concepts; training/test N = 161 789/107 859, D = 128 wavelet features. Ground truth: K = 500 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. Runtime with L = 32 bits: a few hours.

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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