Tailored Bregman Ball Trees for Effective Nearest Neighbors

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Outline

Nearest Neighbor (NN) search

Applications: computer vision, machine learning, data mining, etc.

Nearest neighbor $\mathrm{NN}(q)$

Given:

- a set $\mathcal{S} = \{p_1, ..., p_n\}$ of n d-dimensional points
- a *query* point q
- a dissimilarity measure D

then

$$\mathrm{NN}(q) = \arg\min_i D(q, p_i) \tag{1}$$

For asymmetric D (like Bregman divergences):

$$\mathrm{NN}_F^l(q) = \arg\min_i D(q, p_i) \quad \text{(left-sided)}$$

$$\mathrm{NN}_F^r(q) = \arg\min_i D(p_i, q) \quad \text{(right-sided)}$$

$$\mathrm{NN}_F(q) = \arg\min_i (D(p_i || q) + D(q || p_i))/2 \quad \text{(symmetrized)}$$

Bregman divergences D_F

$F(x) : \mathcal{X} \subset \mathbb{R}^d \mapsto \mathbb{R}$ strictly *convex* and *differentiable* generator

$$D_F(p||q) = F(p) - F(q) - (p-q)^T \nabla F(q) \tag{2}$$

Bregman sided NN queries are related by Legendre conjugates:
$D_{F^*}(\nabla F(q)||\nabla F(p)) = D_F(p||q)$ (dual divergence)

Widely used as distortion measures between image features:

- Mahalanobis squared distances (symmetric)
  $F(x) = \Sigma^{-1} x$ ($\Sigma \succ 0$ is the covariance matrix)
- Kullback-Leibler (KL) divergence (asymmetric)

$$F(x) = \sum_{j=1}^{d} x_j \log x_j$$

Naïve search methods

Brute-force linear search:

- exhaustive brute-force $O(dn)$
- randomized sampling $O(\alpha dn)$, $\alpha \in (0, 1)$

Randomized sampling

- keep a point with probability α
- mean size of the sample: αn
- speed-up: $\frac{1}{\alpha}$
- mean rank of the approximated NN: $\frac{1}{\alpha}$

Data structures for improved NN search

Two main sets of methods:

- mapping techniques (*e.g.* locality-sensitive hashing, random projections)
- tree-like space partitions with branch-and-bound queries (*e.g.* kD-trees, metric ball and vantage point trees)
  - faster than brute-force (pruning sub-trees)
  - approximate NN search

Extensions from the Euclidean distance to:

- arbitrary metrics: vp-trees *[Yianilos, SODA 1993]*
- Bregman divergences: k-means *[Banerjee et al., JMLR 2005]*

We focus on Bregman Ball trees *[Cayton, ICML 2008]*

Outline of BB-trees (I)

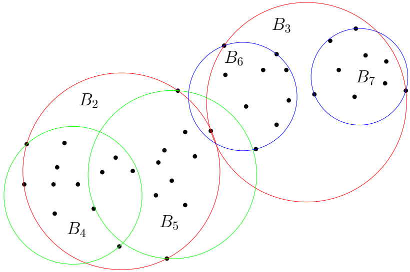
BB-tree construction

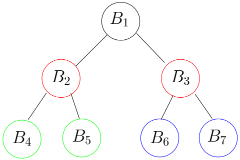
Recursive partitioning scheme

1. *2-means* clustering (keep the two centroids c_l, c_r)
2. Bregman Balls $B(c_l, R_l)$ and $B(c_r, R_r)$ (possibly overlapping)
3. continue recursively until matching a stop criterion

Termination criteria:

- maximum number of points l_0 stored at a leaf
- maximum leaf radius r_0





Outline of BB-trees (II)

Branch-and-bound search

1. Descend the tree from the root to the leaves
   - At internal nodes, choose child whose ball is "closer" to q (the sibling is temporarily ignored)
   - At leaves, search for the NN candidate p' (brute force)
2. Traverse back up the tree (check ignored nodes)
   - project q onto the ball $B(c, R)$ (bisection search):

$$q_B = \arg\min_{x \in B} D_F(x||q)$$

   - if $D_F(q_B||q) > D_F(p'||q)$ the node can be *pruned out*

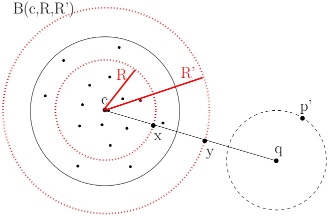
Outline of BB-trees (III)

Bregman annuli

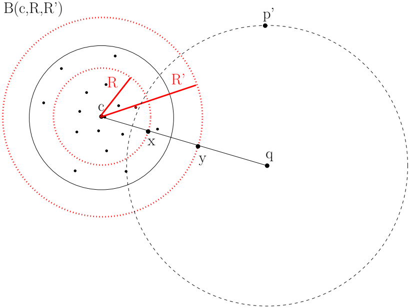
Lower/upper bounds to speed-up geodesic bisection search:

$$B(c, R, R') = \{x | R \leq D_F(x||c) \leq R'\}$$

$D_F(p'||q) < D_F(y||q)$ (prune out)



$D_F(p'||q) > D_F(x||q)$ (explore)



Our main contributions

From BB-tree to `BB-tree++`:

- Speed up construction time (`Bregman 2-means++`)
- Learn the tree branching factor (G-means)
- Explore nearest nodes first (*priority queue*)
- Handle symmetrized/mixed Bregman divergences

We mainly focus on *approximate* NN queries (stop the search once a few leaves have been explored)

Speed up construction time

We replace Bregman 2-means by a careful light *initialization* of the two cluster centers *[Arthur et al., SODA 2007]*

Bregman 2-means++

1. pick the first seed c_l uniformly at random
2. for each $p_i \in \mathcal{S}$ compute $D_F(p_i || c_l)$
3. pick the second seed c_r according to the distribution:

$$\pi_i = \frac{D_F(p_i || c_l)}{\sum_{p_j \in \mathcal{S}} D_F(p_j || c_l)} \tag{3}$$

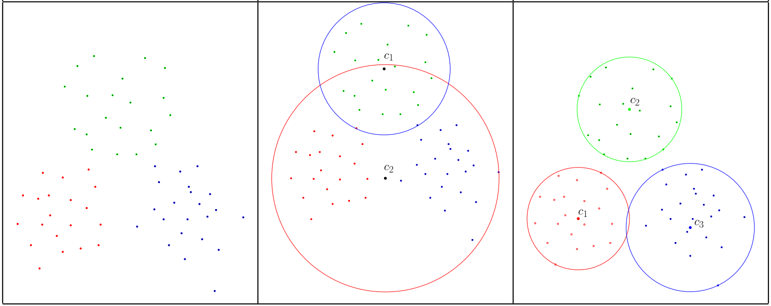
- Good approximation guaranties *[Nock et al., ECML 2008]*.
- Fast tree construction, nice splitting

Learning the tree branching factor (I)

Goal Get as many as possible *non-overlapping* Bregman balls

Example Three separated Gaussian samples.

dataset	$2-$*means*	$3-$*means*



Method

adapt the branching factor bf_i of each internal node

Learning the tree branching factor (II)

G-means

- assume Gaussian distribution of each group of points
- use Bregman 2-means++ inizialization to split a set
- apply the Anderson-Darling normality test to the two clusters
- if the test returns `true`, we keep the center, otherwise we split it into two
- repeat for each new cluster

Ongoing work: generalization to *goodness-of-fit* tests for exponential family distributions (e.g. Stephens test).

Handling symmetrized Bregman divergences

Why?

- required by content-based information retrieval (CBIR) systems
- technically are not Bregman divergences

Example: SKL & $\mathrm{JS}(p;q) = \frac{1}{2}\mathrm{KL}(p||\frac{p+q}{2}) + \frac{1}{2}\mathrm{KL}(q||\frac{p+q}{2})$

Proposed solutions:

- symmetrized Bregman centroid of $B(c,R)$: *geodesic-walk* algorithm of *[Nielsen et al., SODA 2007].*
- mixed BB-trees: store two centers for each ball $B(l,r,R)$ mixed Bregman divergence *[Nock et al., ECML 2008]*

$$D_{F,\alpha}(l||x||r) = (1-\alpha)D_F(l||x) + \alpha D_F(x||r),\ \alpha \in [0,1] \quad (4)$$

(for $\alpha = \frac{1}{2}$, $l = r$ we find the symmetrized Bregman div.)

Nearest neighbors for Image Retrieval

Task find similar images to a query

- $\mathcal{S}$ dataset of feature vectors (*descriptors*)
- q descriptor of a query image
- retrieve the most similar descriptor (image) $\mathrm{NN}(q)$

Example SIFT descriptors: *[Lowe, IJCV 2005].*

Dataset

10,000 images from PASCAL Visual Object Classes Challenge 2007

- 10,000 database points (for building the tree)
- 2,360 query points (for on-line search)
- dimension $d = 1111$

Performance evaluation

Approximate search

Find a "good" NN, i.e. a point close enough to the true NN

- explore a given amount of leaves
- from *near-exact* search to visiting one *single* leaf

speed-up: number of divergence computations (ratio of brute-force over BB-tree++)

R_{avg}: average approximated NN rank

NC: number of points closer to the approximated NN ($NC = R_{avg} - 1$)

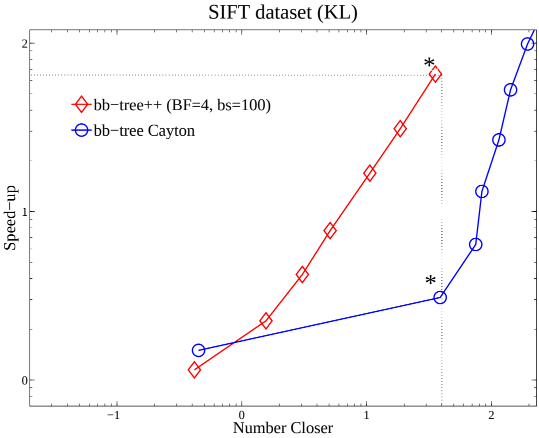
BB-tree construction performances

iter	number of k-means iterations
bs	maximum number of points in a leaf
depth	maximum tree depth
$depth_{avg}$	average tree depth
nLeaves	number of leaf nodes

Bb-tree construction ($bs = 50$)					
method	*iter*	*depth*	$depth_{avg}$	*nLeaves*	*speed-up*
2-means	10	53	28.57	594	1
2-means++	10	58.33	31.18	647	1.03
2-means++	**0**	**20**	**10.76**	**362**	**19.71**

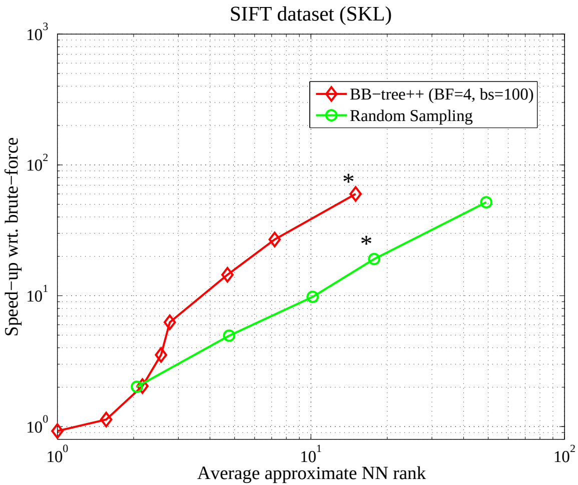
Asymmetric NN queries

BB-tree vs `BB-tree++`



Symmetrized NN queries

BB-tree++ vs Randomized Sampling



Conclusion

`BB-tree++`:

- adapted to the inner geometric characteristics of data
- speed up construction (k-means careful initialization)
- speed up search (priority queue)
- handle symmetrized Bregman divergences
- promising results for image retrieval (SIFT histograms)

Ongoing work:

- design the most appropriate divergence to a class of data
- extensive application to feature sets arising from image retrieval/classification