Fast nearest neighbor retrieval for bregman divergences

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Nearest neighbor search

query: \( q = \) find best match in \( X = \)

- NN methods ubiquitous, but expensive
- Many NN data structures designed to reduce the complexity, mostly for metrics
- In learning, vision, text, use many non-metric measures; a prominent example is the KL-divergence.

This work: a data structure designed for bregman divergences.
Bregman divergence def

For strictly convex $f : \mathbb{R}^d \to \mathbb{R}$,

$$d_f(x, y) \equiv f(x) - f(y) - \langle \nabla f(y), x - y \rangle$$
Bregman divergence examples

\( \ell^2_2 \)

\[ d_f(x, y) = \frac{1}{2} \| x - y \|_2^2 \]

KL-divergence

\[ d_f(x, y) = \sum x_i \log \frac{x_i}{y_i} \]

Mahalanobis (\( Q \succ 0 \))

\[ d_f(x, y) = \frac{1}{2} (x - y)^\top Q (x - y) \]

Itakura-Saito

\[ d_f(x, y) = \sum \left( \frac{x_i}{y_i} - \log \frac{x_i}{y_i} - 1 \right) \]
Bregman divergences VS metrics

**Metrics:**

- **non-negativity**
  \[ d(x, y) \geq 0 \]

- **symmetry**
  \[ d(x, y) = d(y, x) \]

- **triangle inequality**
  \[ d(x, y) + d(y, z) \geq d(x, z) \]
Bregman divergences VS metrics

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Bregman divergences:

- non-negativity: $d_f(x, y) \geq 0$
- symmetry: $d_f(x, y) = d_f(y, x)$
- triangle inequality: $d_f(x, y) + d_f(y, z) \geq d_f(x, z)$
Review: tree-based NN retrieval
e.g. kd-trees, metric trees, many many variants

Hierarchical space decomposition

Search via branch and bound exploration
Bregman ball trees

• Fundamental geometric unit: bregman ball.
  \[ B(\mu, R) \equiv \{ x \ : \ d_f(x, \mu) \leq R \} \]

• Need a reasonable build heuristic.

• Can’t use the triangle inequality for bounds.

• Need to handle asymmetry of divergence.
  (Not covered here -- see paper)
Intuition: at each level, want balls that are well separated & compact.

Can prune left node

VS

Have to search both
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**Build method:** Deploy $k$-means hierarchically (top-down).

($k$-means was generalized to bregman divergences in Banerjee et al. 2005)
bbtree -- search

Want to find the left NN:

$$\text{argmin}_{x \in X} d_f(x, q)$$

Branch & bound search:

1. Descend tree, choosing child whose mean is closest to $q$. Ignore the sibling.

2. At leaf, compute distances to all points; call the nearest the candidate NN $x_c$.

3. Traverse back up tree; check the ignored nodes. If

$$d_f(x_c, q) > \min_{x \in B(\mu, R)} d_f(x, q)$$

need to explore it.
Computing the bound

Need to check if

\[ d_f(x_c, q) > \min_{x \in B(\mu, R)} d_f(x, q) \]
Computing the bound

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The Bregman projection onto a Bregman ball

Convex, but need to compute it in time comparable to evaluating an analytic expression
The $\ell_2^2$ case

$$\min_x \frac{1}{2} \|x - q\|^2$$
subject to: $$\frac{1}{2} \|x - \mu\|^2 \leq R$$

Can compute projection analytically:

$$x_p = \theta \mu + (1 - \theta)q$$

where $$\theta = \frac{\sqrt{2R}}{\|q - \mu\|}$$

Easy because $x_p$ is on line between $\mu$ and $q$
The general case

\[
\min_x d_f(x, q)
\]

subject to: \( d_f(x, \mu) \leq R \)

Something similar holds..
The general case

\[
\begin{aligned}
\min_{x} & \quad d_f(x, q) \\
\text{subject to:} & \quad d_f(x, \mu) \leq R
\end{aligned}
\]

Something similar holds..

Claim 1: \( \nabla f(x_p) = \theta \nabla f(\mu) + (1 - \theta) \nabla f(q). \)

The \( l_2^2 \) relationship is a special case since \( \nabla f(x) = x. \)

Nearly as useful....
Since $f$ strictly convex, 

$$\nabla f$$ is one-to-one.

Moreover, its inverse is given by the gradient of 

$$f^*(y) \equiv \sup_x \{ \langle x, y \rangle - f(x) \}.$$

Thus can recover $x_p$ from $\nabla f(x_p)$.
Notation:

\[ \begin{align*}
\mu' & \equiv \nabla f(\mu) \\
q' & \equiv \nabla f(q) \\
x_{\theta}' & \equiv \theta \mu' + (1 - \theta)q' 
\end{align*} \]

Solution lies on this curve.

\[ \nabla f^*(x_{\theta}'), \quad \theta \in [0, 1] \]
Algorithm

Bisection search on $\theta$ for $x$ satisfying $d_f(x, \mu) = R$.

1. $\theta_1 = \frac{1}{2}$
2. $\theta_2 = \frac{1}{4}$
3. $\theta_3 = \frac{3}{8}$
4. $\theta_4 = \frac{5}{16}$
Algorithm

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- Can compute a solution to accuracy $\epsilon$ in $\log \frac{1}{\epsilon}$ steps.
- Each step requires 1 gradient evaluation and 1 divergence evaluation.

Very fast.
But: Don’t actually need an exact solution.

Only need to determine if:

\[ d_f(x_c, q) > \min_{x \in B(\mu, R)} d_f(x, q) \]

\(x_c\) is the current candidate NN)}
**But:** Don’t actually need an *exact* solution.

Only need to determine if: \[ d_f(x_c, q) > \min_{x \in B(\mu, R)} d_f(x, q) \]

\((x_c\text{ is the current candidate NN})\)

**i.e.** upper and lower bounds suffice

**Lower bound:** weak duality

\[
\mathcal{L}(\theta) \equiv d_f(x_\theta, q) + \frac{\theta}{1 - \theta} \left( d_f(x_\theta, \mu) - R \right) \\
\leq \min_{x \in B(\mu, R)} d_f(x, q)
\]

**Upper bound:** primal

\[
d_f(x_\theta, q) \geq \min_{x \in B(\mu, R)} d_f(x, q)\text{ for feasible } x_\theta
\]

Evaluate bounds at each step of bisection to stop early.
Experiments: KL-divergence

Why KL divergence?

- Used extensively to compare histograms (e.g. text, vision).
- No (correct) NN schemes out there for it.
- Mahalanobis, $\ell_2^2$ can be handled by metric methods.
Data sets

- **rcv-$D$**: 500k documents from the RCV corpus represented as a $D$-dimensional distribution over topic (generated using LDA).
- **Corel histograms**: 60k color histograms, 64-dimensional.
- **Semantic space**: 371-dimensional representation of 5000 images (from CBIR literature)
- **SIFT signatures**: 1111-dimensional quantized histogram representation of 10k images from PASCAL 2007 dataset
Approx search experiments

Stop search early (after examining only a few leaves)
-- standard practice with metric, kd-trees, etc.

Evaluation

Speedup over brute-force search in execution time.

VS

NC for number closer: how many closer points are there? e.g. if NC=3, the bbtree returned the fourth NN.
Approximate search

![Graph showing speedup (exponent) vs. num closer (exponent) for rcv-128 dataset. The graph plots a series of points that increase with num closer, indicating a positive correlation between speedup and num closer.](image)
rcv data
corel, semantic space, SIFT
## Exact search

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