

On Low Distortion Embeddings of Statistical Distance Measures into Low Dimensional Spaces



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January 10, 2010

Introduction



Why “embed” distances anywhere at all

- Applications dealing with huge amounts of high dimensional data



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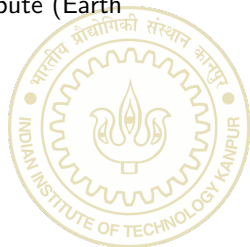
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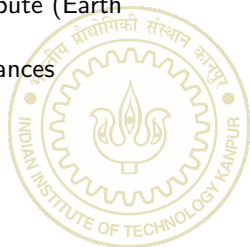
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 - Certain distance measures inherently difficult to compute (Earth Mover’s distance)
 - Absence of good index structures for non-metric distances



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- Obtain easily estimable upper/lower-bounds on the distance measures (EMD/Edit distance)



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- Find embeddings which allow specific proximity queries
- Embed into a metric space for which efficient algorithms for answering proximity queries exist



Statistical Distance Measures

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 - Many other applications ...
- However these are seldom metrics



Our contributions

- We examine 3 statistical distance measures with the goal of obtaining low-dimensional, low distortion embeddings



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- Applying them we get non-embeddability results (into metric spaces) for the Bhattacharyya and Kullback Leibler measures
- We also present dimensionality reduction schemes for the Bhattacharyya and the Mahalanobis distance measure



Preliminaries



Low distortion embeddings

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- Preserve the geometry of the original space almost exactly



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- Presence of several index structures for metric spaces motivates embeddings into metric spaces



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- Ensure that notions of distance are almost preserved
- Preserve the geometry of the original space almost exactly
- Give performance guarantees in terms of accuracy for all proximity queries
- Presence of several index structures for metric spaces motivates embeddings into metric spaces
- In case the embedding is into ℓ_2 , added benefit of dimensionality reduction



Some Preliminary definitions

Definition (Metric Space)

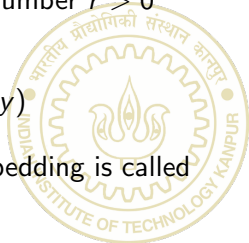
A pair $M = (X, \rho)$ where X is a set and $\rho : X \times X \rightarrow \mathbb{R}^+ \cup \{0\}$ is called a metric space provided the distance measure ρ satisfies the properties of identity, symmetry and triangular inequality.

Definition (D -embedding and Distortion)

Given two metric spaces (X, ρ) and (Y, σ) , a mapping $f : X \rightarrow Y$ is called a D -embedding where $D \geq 1$, if there exists a number $r > 0$ such that for all $x, y \in X$,

$$r \cdot \rho(x, y) \leq \sigma(f(x), f(y)) \leq D \cdot r \cdot \rho(x, y)$$

The infimum of all numbers D such that f is a D -embedding is called the *distortion* of f .



The JL Lemma

- A classic result in the field of metric embeddings



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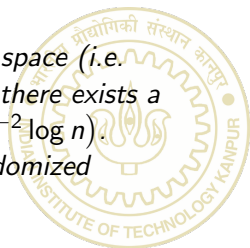


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Theorem (Johnson-Lindenstrauss Lemma)

Let X be an n -point set in a d -dimensional Euclidean space (i.e. $(X, \ell_2) \subset (\mathbb{R}^d, \ell_2)$), and let $\epsilon \in (0, 1]$ be given. Then there exists a $(1 + \epsilon)$ -embedding of X into (\mathbb{R}^k, ℓ_2) where $k = O(\epsilon^{-2} \log n)$. Furthermore, this embedding can be found out in randomized polynomial time.



The JL Lemma

- The lemma ensures that even inner products are preserved to an arbitrarily low additive error



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- Will be useful for dimensionality reduction with the Bhattacharyya distance measure

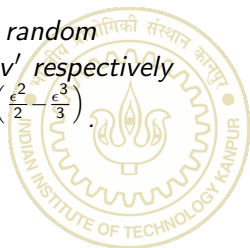


The JL Lemma

- The lemma ensures that even inner products are preserved to an arbitrarily low additive error
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Corollary

Let u, v be unit vectors in \mathbb{R}^d . Then, for any $\epsilon > 0$, a random projection of these vectors to yield the vectors u' and v' respectively satisfies $\Pr[u \cdot v - \epsilon \leq u' \cdot v' \leq u \cdot v + \epsilon] \geq 1 - 4e^{-\frac{k}{2} \left(\frac{\epsilon^2}{2} - \frac{\epsilon^3}{3} \right)}$.



Some definitions ...

Definition (Representative vector)

Given a d -dimensional histogram $P = (p_1, \dots, p_d)$, let \sqrt{P} denote the unit vector $(\sqrt{p_1}, \dots, \sqrt{p_d})$. We shall call this the *representative vector* of P .



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Definition (α -constrained histogram)

A histogram $P = (p_1, p_2, \dots, p_d)$ is said to be α -constrained if $p_i \geq \frac{\alpha}{d}$ for $i = 1, 2, \dots, d$.



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Given two α -constrained histograms P and Q , the inner product between the representative vectors is at least α , i.e., $\langle \sqrt{P}, \sqrt{Q} \rangle \geq \alpha$.



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We will denote $\frac{\alpha}{d}$ by β



The Distance Measures



The Bhattacharyya Distance Measures

Definition (Bhattacharyya Coefficient)

For two histograms $P = (p_1, p_2, \dots, p_d)$ and $Q = (q_1, q_2, \dots, q_d)$ with $\sum_{i=1}^d p_i = \sum_{i=1}^d q_i = 1$ and each $p_i, q_i \geq 0$, the *Bhattacharyya coefficient* is described as $BC(P, Q) = \sum_{i=1}^d \sqrt{p_i q_i}$.

We define two distance measures using this coefficient :



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$$H(P, Q) = 1 - BC(P, Q) = \frac{1}{2} \left(\left\| \sqrt{P} - \sqrt{Q} \right\| \right)^2.$$



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Definition (Bhattacharyya Distance)

$$BD(P, Q) = -\ln BC(P, Q).$$



Kullback Leibler Divergence

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Given two histograms $P = \{p_1, p_2, \dots, p_d\}$ and $Q = \{q_1, q_2, \dots, q_d\}$, the Kullback-Leibler divergence between the two distributions is

defined as $KL(P, Q) = \sum_{i=1}^d p_i \ln \frac{p_i}{q_i}$.



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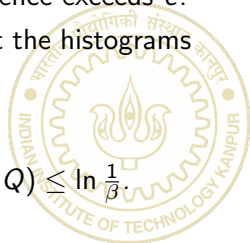
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Lemma

Given two β -constrained histograms P, Q , $0 \leq KL(P, Q) \leq \ln \frac{1}{\beta}$.



The Class of Quadratic Form Distance Measures

Definition (Quadratic Form Distance Measure)

A $d \times d$ positive definite matrix A defines a Quadratic Form Distance measure over \mathbb{R}^d given by $Q_A(x, y) = \sqrt{(x - y)^T A (x - y)}$.



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- Can be defined for any matrix but the resulting distance measure is a metric if and only if the matrix is positive definite
- The Mahalanobis distance is a special case of QFD where the underlying distance measure is the covariance matrix of some distribution



Results on Dimensionality Reduction



Hellinger Distance

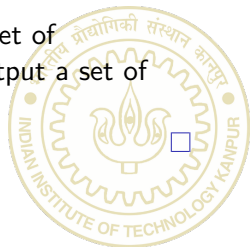
The fact that $H(P, Q)$ is the Euclidean distance between the points \sqrt{P} and \sqrt{Q} allows us to state the following theorem.

Theorem

The Hellinger distance admits a low distortion dimensionality reduction.

Proof. (Sketch).

Given a set of histograms, subject the corresponding set of representative vectors to a JL-type embedding and output a set of vectors for which the embedded set of vectors are the representatives. \square



Bhattacharyya Distance

- The Bhattacharyya distance is unbounded even on the probability simplex - precisely when α is small



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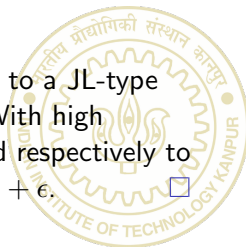
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Proof. (Sketch).

Given a set of α -constrained histograms, subject them to a JL-type embedding with the error parameter set to $\epsilon' = \frac{\epsilon \cdot \alpha}{2}$. With high probability the following occurs : if P, Q are embedded respectively to P', Q' , then $BD(P, Q) - \epsilon \leq BD(P', Q') \leq BD(P, Q) + \epsilon$. \square



Quadratic Form Distance Measures

Theorem

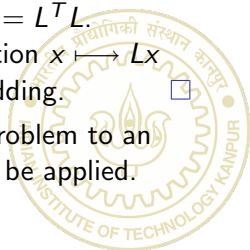
The family of metric quadratic form distance measures admit a low distortion JL-type embedding into a Euclidean spaces.

Proof.

Every quadratic form distance measure forming a metric is characterized by a positive definite matrix A . Such matrices can be subjected to a Cholesky Decomposition of the form $A = L^T L$.

Given a set of vectors subject them to the transformation $x \mapsto Lx$ and subject there resulting vectors to a JL-type embedding. \square

The proposed transformation essentially reduces the problem to an undistorted Euclidean space where the JL Lemma can be applied.



How to prove Non-embeddability results into metric spaces



The Asymmetry Technique

Definition (γ -Relaxed Symmetry)

A set X equipped with a distance function $d : X \times X \rightarrow \mathbb{R}^+ \cup \{0\}$, is said to satisfy γ -relaxed symmetry if there exists $\gamma \geq 0$ such that for all point pairs $p, q \in X$, the following holds $|d(p, q) - d(q, p)| \leq \gamma$.



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Metrics satisfy the γ -relaxed triangle inequality for $\gamma = 0$



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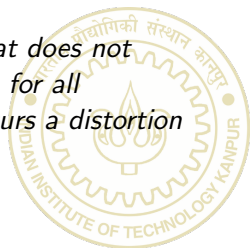
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Lemma

Given a set X equipped with a distance function d that does not satisfy the γ -relaxed symmetry such that $d(x, y) \leq M$ for all $x, y \in X$, any embedding of X into a metric space incurs a distortion of at least $1 + \frac{\gamma}{M}$.



The Relaxed Triangle Inequality Technique

Definition (λ -Relaxed Triangle Inequality)

A set X equipped with a distance function $d : X \times X \rightarrow \mathbb{R}^+ \cup \{0\}$, is said to satisfy the λ -relaxed triangle inequality if there exists some constant $\lambda \leq 1$ such that for all triplets $p, q, r \in X$, the following holds $d(p, r) + d(r, q) \geq \lambda \cdot d(p, q)$.



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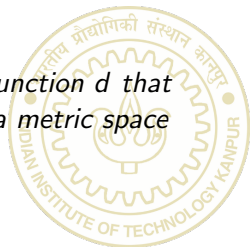
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Metrics satisfy the λ -relaxed triangle inequality for $\lambda = 1$

Lemma

Any embedding of a set X equipped with a distance function d that does not satisfy the λ -relaxed triangle inequality into a metric space incurs a distortion of at least $\frac{1}{\lambda}$.



Non-“metric-embeddability” Results



Metric Embeddings for Bhattacharyya Distance

Theorem

There exist d -dimensional β -constrained distributions such that any embedding of these distributions under the Bhattacharyya distance measure into a metric space must incur a distortion of

$$D = \begin{cases} \Omega\left(\frac{\ln \frac{1}{d\beta}}{\ln d}\right) & \text{when } \beta > \frac{4}{d^2} \\ \Omega\left(\frac{\ln \frac{1}{\beta}}{\ln d}\right) & \text{when } \beta \leq \frac{4}{d^2} \end{cases}$$



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Proof. (Sketch).

Choose three distributions that violate the relaxed triangle inequality with appropriate λ . □



Metric Embeddings for Bhattacharyya Distance

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For any two d -dimensional β -constrained distributions P and Q with $\beta < \frac{1}{2d}$, we have $H(P, Q) \leq BD(P, Q) \leq \frac{d}{1-2\beta d} \ln \frac{1}{(d-1)\beta} H(P, Q)$.

- Since the Hellinger distance forms a metric in the positive orthant, this constitutes a metric embedding



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- Additionally this embedding allows for dimensionality reduction as well



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For sufficiently large d and small β , there exists a set S of d -dimensional β -constrained histograms and a constant $c > 0$ such that any embedding of S into a metric space incurs a distortion of at least $1 + c$.



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- However the situation is much worse ...



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Metric Embeddings for Kullback-Leibler Divergence

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Theorem

For sufficiently large d , there exist d -dimensional β -constrained distributions such that embedding these under the Kullback-Leibler divergence into a metric space must incur a distortion of

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For sufficiently large d , there exist d -dimensional β -constrained distributions such that embedding these under the Kullback-Leibler divergence into a metric space must incur a distortion of

$$\Omega \left(\frac{\ln \frac{1}{d\beta}}{\ln \left(d \ln \frac{1}{\beta} \right)} \right).$$

- The lower bound diverges for small β



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- Thus, by choosing point sets appropriately, we can force the embedding distortion to be arbitrarily large !



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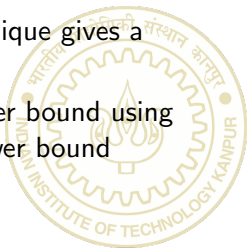
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- For smaller β (say $\beta = o\left(\frac{1}{d^4}\right)$) we get a better lower bound using the Relaxed Triangle Inequality Technique - this lower bound diverges



A Useful Embedding for Kullback-Leibler Divergence

Theorem

For any two d -dimensional β -constrained distributions P and Q ,

$$\frac{\ell_2^2(P, Q)}{2} \leq KL(P, Q) \leq \left(\frac{1}{2\beta} + \frac{1}{3\beta^5} \right) \ell_2^2(P, Q).$$



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- The ℓ_2^2 measure is not a metric - however very close to one
- It also admits dimensionality reduction via the JL Lemma
- Hence despite the poor bound on distortion, can be useful



Future Directions



Open Questions

- A low multiplicative distortion dimensionality reduction scheme for the Bhattacharyya distance measure



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- A low multiplicative distortion dimensionality reduction scheme for the Bhattacharyya distance measure
- A low distortion dimensionality reduction scheme for the Kullback-Leibler distance measure
- Tightening of the bounds for the Bhattacharyya distance measure shown in this paper
- In short - a theory of Non-Metric Embeddings

