GDA HW 3

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1 Metric Tree Curvature

Want to show that a metric tree space has negative curvate, where a metric tree space (M, d) is a metric space such that:

 $\forall x, y \in M, \exists a \text{ unique path } x \leadsto y \text{ that is homeomorphic to } [0, 1]$

Proof. We will show that a metric tree space (M, d) has negative curvature by showing that for all $x, y, z \in M$:

$$d(x,y) + d(y,z) - d(x,z) \ge 0$$

We will prove this by cases. First, consider the case where x,y,z are all on the same path. Then, d(x,y)+d(y,z)=d(x,z), so d(x,y)+d(y,z)-d(x,z)=0. Thus, the inequality holds.

Now, consider the case where x,y,z are not all on the same path. Then, there are two cases: either x and y are on the same path, or y and z are on the same path. Without loss of generality, assume that x and y are on the same path. Then, d(x,y) = d(x,z) - d(y,z). Thus, d(x,y) + d(y,z) - d(x,z) = d(x,z) - d(y,z) + d(y,z) - d(x,z) = 0. Thus, the inequality holds.

2 Hausdorff and Gromov-Hausdorff Metrics

Want to show that Hausdorff and Gromov-Hausdorff metrics are indeed metrics. Recall that a metric space is defined as (M, d) for set M and metric (distance) function d such that for all $x, y, z \in M$:

$$\begin{aligned} d_M(x,y) &= 0 \iff x = y \\ d_M(x,y) &> 0 \text{ for } x \neq y \\ d_M(x,y) &= d_M(y,x) \end{aligned} & \text{(positivity)} \\ d_M(x,z) &\leq d_M(x,y) + d_M(y,z) \end{aligned} & \text{(triangle inequality)}$$

2.1 Hausdorff Metric

The Hausdorff distance is defined on two non-empty subsets X, Y of a metric space (M, d_M) as:

$$d_H(X,Y) = \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x,y), \sup_{y \in Y} \inf_{x \in X} d_M(x,y) \right\}$$

Want to show that the Hausdorff distance d_H is a metric that satisfies the four properties above.

 ${\it Proof.}$ We will prove all four properties of a metric in a metric space for the Hausdorff distance.

1. **Equality:** To show the property of equality we prove both directions. If X = Y then:

$$\begin{aligned} d_H(X,Y) &= d_H(X,X) \\ &= \max \left\{ \sup_{x \in X} \inf_{x' \in X} d_M(x,x'), \sup_{x \in X} \inf_{x' \in X} d_M(x,x') \right\} \\ &= \max \left\{ 0,0 \right\} \qquad \text{by } d_M(x,x') = 0 \text{ for } x = x' \\ &= 0 \end{aligned}$$

If $d_H(X,Y) = 0$ then:

$$\begin{split} d_H(X,Y) &= 0 \\ &= \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x,y), \sup_{y \in Y} \inf_{x \in X} d_M(x,y) \right\} \end{split}$$

By the max operation, one or both arguments must be equal to zero. However, since metric-distances are non-negative, both arguments must be zero:

$$\sup_{x \in X} \inf_{y \in Y} d_M(x, y) = \sup_{y \in Y} \inf_{x \in X} d_M(x, y) = 0$$

By the definition of the sup and inf operators, this implies that for all $x \in X$ and $y \in Y$, $d_M(x,y) = 0$. Since d_M is a metric, this implies that x = y for all $x \in X$ and $y \in Y$. Thus, X = Y.

Therefore d_H satisfies the property of equality.

2. **Positivity:** To show the property of positivity we prove the following: if $X \neq Y$ then $d_H(X,Y) > 0$. We will prove this by contradiction. Suppose $d_H(X,Y) = 0$ for $X \neq Y$. Then:

$$\begin{split} d_H(X,Y) &= 0 \\ &= \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x,y), \sup_{y \in Y} \inf_{x \in X} d_M(x,y) \right\} \end{split}$$

By the max operation, one or both arguments must be equal to zero. However, since metric-distances are non-negative, both arguments must be zero:

$$\sup_{x \in X} \inf_{y \in Y} d_M(x, y) = \sup_{y \in Y} \inf_{x \in X} d_M(x, y) = 0$$

By the definition of the sup and inf operators, this implies that for all $x \in X$ and $y \in Y$, $d_M(x, y) = 0$. Since d_M is a metric, this implies that x = y for all $x \in X$ and $y \in Y$. Thus, X = Y.

This contradicts the assumption that $X \neq Y$. Therefore d_H satisfies the property of positivity since d_M is always non-negative.

3. **Symmetry:** To show the property of symmetry, prove that $d_H(X,Y) = d_H(Y,X)$. If X = Y, this proof is trivial because $d_H(X,Y) = 0$ and $d_H(Y,X) = 0$. If $X \neq Y$, then:

$$d_H(X,Y) = \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x,y), \sup_{y \in Y} \inf_{x \in X} d_M(x,y) \right\}$$
$$= \max \left\{ \sup_{y \in Y} \inf_{x \in X} d_M(x,y), \sup_{x \in X} \inf_{y \in Y} d_M(x,y) \right\}$$
$$= d_H(Y,X)$$

4. **Triangle Inequality:** To show the property of triangle inequality, prove that $d_H(X,Z) \leq d_H(X,Y) + d_H(Y,Z)$. If X = Y or Y = Z, this proof is trivial because $d_H(X,Y) = 0$ or $d_H(Y,Z) = 0$ and $d_H(X,Z) = 0$. If $X \neq Y$ and $Y \neq Z$, then:

$$d_H(X,Z) = \max \left\{ \sup_{x \in X} \inf_{z \in Z} d_M(x,z), \sup_{z \in Z} \inf_{x \in X} d_M(x,z) \right\}$$

Because d_M is a metric, it satisfies the triangle inequality for x, y, z for all choices of x, y, z. In particular, any choice of y holds, letting us pick $y' := \inf_{y \in Y} d_M(x, y)$ and $y'' := \inf_{y \in Y} d_M(y, z)$:

$$\begin{split} d_H(X,Z) &= \max \left\{ \sup_{x \in X} \inf_{z \in Z} d_M(x,z), \sup_{z \in Z} \inf_{x \in X} d_M(x,z) \right\} \\ &\leq \max \left\{ \sup_{x \in X} \inf_{z \in Z} \left(d_M(x,y') + d_M(y',z) \right), \sup_{z \in Z} \inf_{x \in X} \left(d_M(x,y'') + d_M(y'',z) \right) \right\} \\ &= \max \left\{ \sup_{x \in X} d_M(x,y') + \inf_{z \in Z} d_M(y',z), \sup_{z \in Z} d_M(y'',z) + \inf_{x \in X} d_M(x,y'') \right\} \\ &\leq \max \left\{ \sup_{x \in X} d_M(x,y'), \inf_{x \in X} d_M(x,y'') \right\} + \max \left\{ \inf_{z \in Z} d_M(y',z), \sup_{z \in Z} d_M(y'',z) \right\} \\ &\leq \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x,y), \inf_{x \in X} d_M(x,y'') \right\} + \max \left\{ \inf_{z \in Z} d_M(y',z), \sup_{z \in Z} \inf_{y \in Y} d_M(y,z) \right\} \\ &\leq \max \left\{ \sup_{x \in X} \inf_{y \in Y} d_M(x,y), \inf_{x \in X} \sup_{y \in Y} d_M(x,y) \right\} + \max \left\{ \inf_{z \in Z} \sup_{y \in Y} d_M(y,z), \sup_{z \in Z} \inf_{y \in Y} d_M(y,z) \right\} \\ &= d_H(X,Y) + d_H(Y,Z) \end{split}$$

Therefore, because the Hausdorff distance has all four properties of a metric, it is inded a metric. $\hfill\Box$

2.2 Gromov-Hausdorff Metric

The Gromov-Hausdorff distance is defined for two metric spaces (X, d_X) and (Y, d_Y) with two isometric functions $\phi: X \to A$ and $\psi: Y \to A$ as:

$$d_{GH}(X,Y) := \inf_{\phi,\psi} d_H(\phi(X),\psi(Y))$$

Want to show that the Gromov-Hausdorff distance d_{GH} is a metric that satisfies the four metric properties above.

Proof. We will prove all four proerties of a metric in a metric space for the Gromov-Hausdorff distance.

Equality: We will prove both directions of $d_{GH}(X,Y) = 0 \iff X = Y$

First, let $d_{GH}(X,Y) = 0$. Because $d_H \ge 0$, we know by the def of infimum that $d_H(\phi(X), \psi(Y)) = 0$. Because d_H is a metric, we know that $\phi(X) = \psi(Y)$ only when X = Y. Therefore, $d_{GH}(X,Y) = 0 \implies X = Y$.

Now let X = Y. By the metric property of the Hausdorff distance, we know $d_H(X,Y) = 0$ for X = Y. Therefore, no matter the isometric embeddings ϕ and ψ , there is always an isometric embedding $\phi = \psi$ such that $d_H(\phi(X), \psi(Y)) = 0$. Therefore, $d_{GH}(X,Y) = 0$.

- **2. Positivity:** We will prove that $d_{GH}(X,Y) > 0$ for all $X \neq Y$.
 - Because d_H is a metric, we know that $d_H(\phi(X), \psi(Y)) > 0$ is always true when $X \neq Y$. Therefore, no matter the isometric embedding, the infimum of $d_H(\phi(X), \psi(Y))$ is always positive. Thus $d_{GH}(X, Y) > 0$.
- 3. **Symmetry:** We will prove that $d_{GH}(X,Y) = d_{GH}(Y,X)$. This is trivially true by relabeling X and Y since the isometric embedding functions ϕ, ψ can be anything.
- 4. Triangle Inequality: We will prove that $d_{GH}(X,Z) \leq d_{GH}(X,Y) + d_{GH}(Y,Z)$ for all X,Y,Z.

By the metric property of the Hausdorff distance we know for spaces $\phi(X), \theta(Y), \psi(Z)$ that:

$$d_H(\phi(X), \psi(Z)) \le d_H(\phi(X), \theta(Y)) + d_H(\theta(Y), \psi(Z))$$

Taking the infimum of both sides, we get:

$$d_{GH}(X,Z) \le d_{GH}(X,Y) + d_{GH}(Y,Z)$$

Thus we have shown that the Gromov-Hausdorff distance is a metric. \Box

3 Bounding Gromov-Hausdorff Distance With Diameter

Want to bound the Gromov-Hausdorff distance d_GH in terms of the diameter of metric spaces X and Y:

$$\operatorname{diam}(X) := \max_{x,x' \in X} d_X(x,x') \qquad \operatorname{diam}(Y) := \max_{y,y' \in Y} d_X(y,y')$$

Proof. Let \tilde{R} be an arbitrary relation.

$$\begin{split} d_{GH}(X,Y) &= \inf_{\phi,\psi} d_H(\phi(X), \psi(Y)) \\ &= \frac{1}{2} \inf_{R} \sup_{\substack{(x,y) \in R \\ (x',y') \in R}} |d_X(x,x') - d_Y(y,y')| \\ &\leq \frac{1}{2} \sup_{\substack{(x,y) \in \tilde{R} \\ (x',y') \in \tilde{R}}} |d_X(x,x') - d_Y(y,y')| \\ &\leq \frac{1}{2} \sup_{\substack{(x,y) \in \tilde{R} \\ (x',y') \in \tilde{R}}} \{d_X(x,x'), d_Y(y,y')\} \\ &= \frac{1}{2} \max \{ \operatorname{diam}(X), \operatorname{diam}(Y) \} \end{split}$$

4 Bounding Gromov-Hausdorff Distance With $\epsilon\text{-Nets}$

Want to bound the Gromov Hausdorff distance $d_{GH}(X,Y)$ for metric spaces X and Y. Here, $Y \subset X$ is an ϵ -net such that:

$$\forall x \in X, \exists y \in Y \text{ such that } d(x,y) < \epsilon$$

Proof.

$$\begin{split} d_{GH}(X,Y) &= \inf_{\phi,\psi} d_H(\phi(X),\psi(Y)) \\ &= \inf_{\phi,\psi} \max \left\{ \sup_{x \in \phi(X)} \inf_{y \in \psi(Y)} d(x,y), \sup_{y \in \psi(Y)} \inf_{x \in \phi(X)} d(x,y) \right\} \\ &\leq \inf_{\phi,\psi} \max \left\{ \sup_{x \in \phi(X)} \inf_{y \in \psi(Y)} \epsilon, \sup_{y \in \psi(Y)} \inf_{x \in \phi(X)} \epsilon \right\} \\ &= \inf_{\phi,\psi} \max \left\{ \epsilon, \epsilon \right\} \\ &= \epsilon \end{split}$$

5 Intrinsic Dimensionality Estimation

I estimate the intrinsic dimensionality of a multidimensional Gaussian and hypercube from estimating the tangent plane. I do this by examining the nearest

neighbors of a point and computing its rank – this is an appoximation of the intrinsic dimension. I then take the average of the intrinsic dimension of all points in the dataset.

I use n = 5000 data points and an ambient dimension of D = 50. I use k = 2*ambient-dim nearest neighbors. I then use intrinsic dimensions of $d = \{2, 4, 8, 16, 32\}$ and estimate it with my method. The results are plotted below, with the figures demonstrating the accuracy of my method.

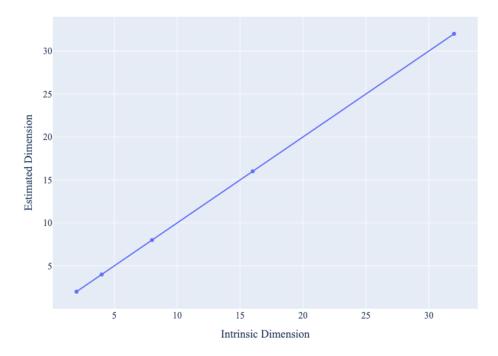


Figure 1: Intrinsic Dimension Estimation for Gaussian

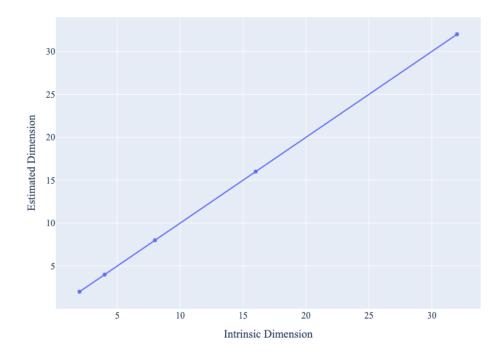


Figure 2: Intrinsic Dimension Estimation for Hypercube

6 Numerical Exploration of Johnson-Lindenstrauss Lemma

Recall the Johnson-Lindenstrauss Lemma:

Lemma: For $0 < \epsilon < 1$, set $X = \{x_1 \dots x_m\}$ with $x_i \in \mathbb{R}^N$, and $n > 8 \ln(m)/\epsilon^2$ there exists a linear map $f : \mathbb{R}^N \to \mathbb{R}^n$ such that:

$$(1 - \epsilon)||u - v||^2 \le ||f(u) - f(v)||^2 \le (1 + \epsilon)||u - v||^2$$

for all $u, v \in X$.

Furthermore, the linear map that satisfies this condition is given by $A \in \mathbb{R}^{n \times N}$ where $A_{ij} \sim \mathcal{N}(0, 1/n)$.

To test this out numerically, I simulated the original data X, a projection matrix A, and then actually projected the data to AX.

By the JL Lemma, we expect the distortion of distances to be bounded. Thus, for every pair of points $u, v \in X$, I computed the lower bound $(1-\epsilon)||u-v||^2$, the upper bound $(1+\epsilon)||u-v||^2$, and the true distortion $||Au-Av||^2$. I numerically confirmed that the true distortion is between the upper and lower bounds for all pairs of points $u, v \in X$ for multiple dimensions.

I then plotted these distortion values for a given dimension to visually demonstrate this result: on the vertical axis, the embedding distortion (in black) falls between the upper and lower distortion bounds (in blue).

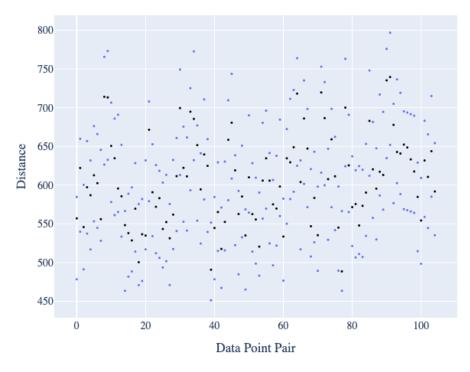


Figure 3: Distortion of Distances for JL Lemma

- Lower Distortion Bound
- · Upper Distortion Bound
- · Embedding Distortion

7 Centroid in Wasserstein Space

Code can be found in q7.py.

7.1 MNIST

Finding the centroid in Wasserstein space for each digit in the MNIST dataset.

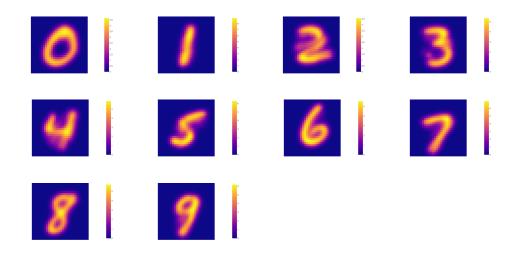


Figure 4: Centroids in Wasserstein Space for MNIST Digits

7.2 Gaussians

Finding the centroid in Wasserstein space for a few Gaussians.

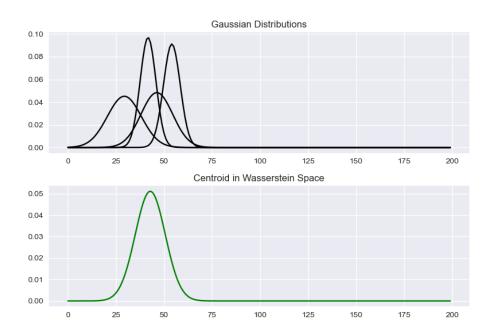


Figure 5: Centroid in Wasserstein Space for Gaussians