Magnitude Distance: A Geometric Measure of Dataset Similarity

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Background and Motivation

Distance between Finite Datasets

The problem of measuring the similarity or distance between two finite datasets plays an important role in generative modelling:

- Evaluating the generative models performance by the similarity of generated samples with the reference dataset.
  - Such as Inception Score or the Maximum Mean Discrepancy (MMD).
- Providing a learning signal during the optimization of model parameters.
  - Such as Wasserstein Generative Adversarial Networks (WGANs).

Goal

Introduce a distance, measuring the dissimilarity between finite sets $X, Y \subset \mathbb{R}^D$, which is **outlier robust** and **captures geometric properties of the data**.

Magnitude of Metric Space

For a finite metric space, (X, d), we define the **similarity matrix** as $\zeta_X(x_i, x_j) := \exp(-d(x_i, x_j))$, for every $x_i, x_j \in X$.

A weighting of (X, d) is a function $w_X : X \to \mathbb{R}$ satisfying

$$\sum_{j \in X} \zeta_X(x_i, x_j)\, w_X(x_j) = 1$$

for every $x_i \in X$, where $w_X(x_i)$ is called the **magnitude weight**.

The **magnitude** of (X, d) is defined as $Mag(X, d) = \sum_{x_i \in X} w_X(x_i)$.

When X is a finite subset of $\mathbb{R}^D$, then ζ_X is invertible and magnitude is the sum of all the entries of the similarity matrix's inverse.

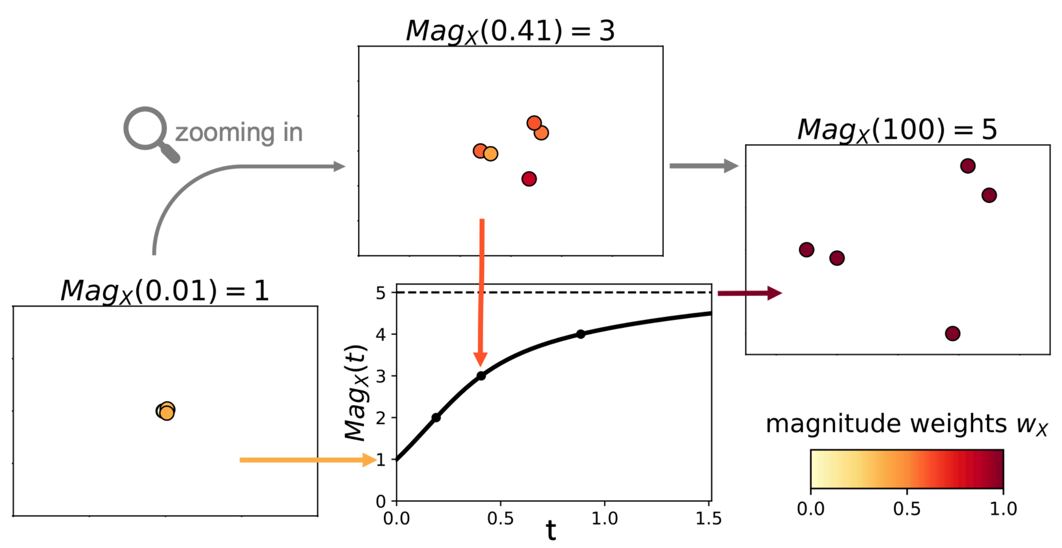


Image Credit: Limbeck, Katharina, et al.(2023).

Magnitude Function

For scaling parameter $t \in \mathbb{R}_+$, the **scaled metric space** (tX, d_t) is the metric with the same points as X and metric $d_t(x, y) = t \cdot d(x, y)$.

The **magnitude function** assigns each finite metric space X to a family of scaled metric spaces $\{tX\}_{t>0}$ by $Mag_X(t) = Mag(tX)$.

Magnitude Distance

Magnitude Distance

In the literature, a metric space is understood to be a **set** of distinct points, i.e., without duplicates. By extending the notion of magnitude to finite **collections** of points that may contain duplicates, we define the magnitude distance for every two finite two collection of point in $\mathbb{R}^D$.

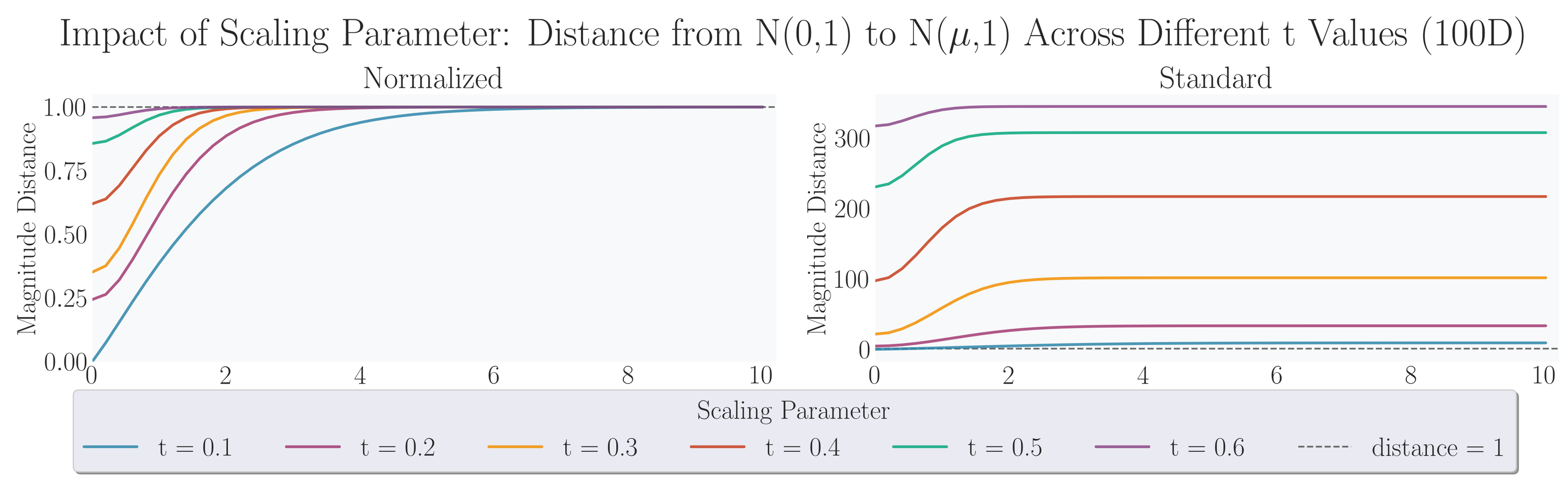
Definition

For two finite sets $X, Y \subset \mathbb{R}^D$, the magnitude distance with scale parameter $t \in \mathbb{R}_+$ is defined as

$$d^t_{Mag}(X, Y) = 2Mag_{X \cup Y}(t) - Mag_X(t) - Mag_Y(t),$$

and the normalized magnitude distance is defined as

$$\tilde{d}^t_{Mag}(X, Y) = \frac{d^t_{Mag}(X, Y)}{Mag_{X \cup Y}(t)}.$$



Scaling Parameter t

We show that the magnitude distance inherits similar properties of the magnitude function stated in [Proposition 2.2.6, Leinster *et al.*, 2013].

Theorem

For every finite metric sets X and Y, the magnitude distance $d^t_{Mag}(X)$:

- Converges to 0 as $t \to 0$.
- Converges to the cardinality of $X \Delta Y$ as $t \to \infty$.
- For $t \gg 0$, the magnitude distance $d^t_{Mag}(X)$ is increasing with respect to t.

The lower semicontinuity with respect to the Gromov-Hausdorff distance of the magnitude function on finite subsets of Euclidean space ensures that the magnitude distance is also lower semicontinuous.

➡ For every two finite sets $X, Y \in \mathbb{R}^D$, there exists a sufficiently small value of t for which the magnitude distance is meaningful.

Result

$d^t_{Mag}(X)$ remains discriminative even in high-dimensional settings.

In contrast, classical distances are known to suffer from the **curse of dimensionality.**

Properties

Metric Axioms

Theorem

Magnitude distance satisfies the following properties for $X, Y \subset \mathbb{R}^D$ and $t > 0$:

- **Symmetry:** $d^t_{\text{Mag}}(X, Y) = d^t_{\text{Mag}}(Y, X)$ by definition.
- **Non-negativity:** For any $t > 0$, we have $d^t_{\text{Mag}}(X, Y) \geq 0$.
- **Identity of indiscernibles:** $d^t_{Mag}(X, Y) = 0 \iff X \underset{Mag(t)}{=} Y$.
- **Triangle inequality:** $d^t_{\text{Mag}}(X, Y)$ does not satisfy the triangle inequality in $\mathbb{R}^D$ for $D > 1$.

Outlier Robustness

Theorem

Let $X, Y \subset \mathbb{R}^D$ be finite sets with nonnegative weighting vectors of X, Y, and $X \cup Y$. Then, we have:

$$0 \leq d^t_{Mag}(X, Y) \leq 2(|X \cup Y|).$$

where $|X|$ and $|Y|$ denote the number of points in X and Y respectively.

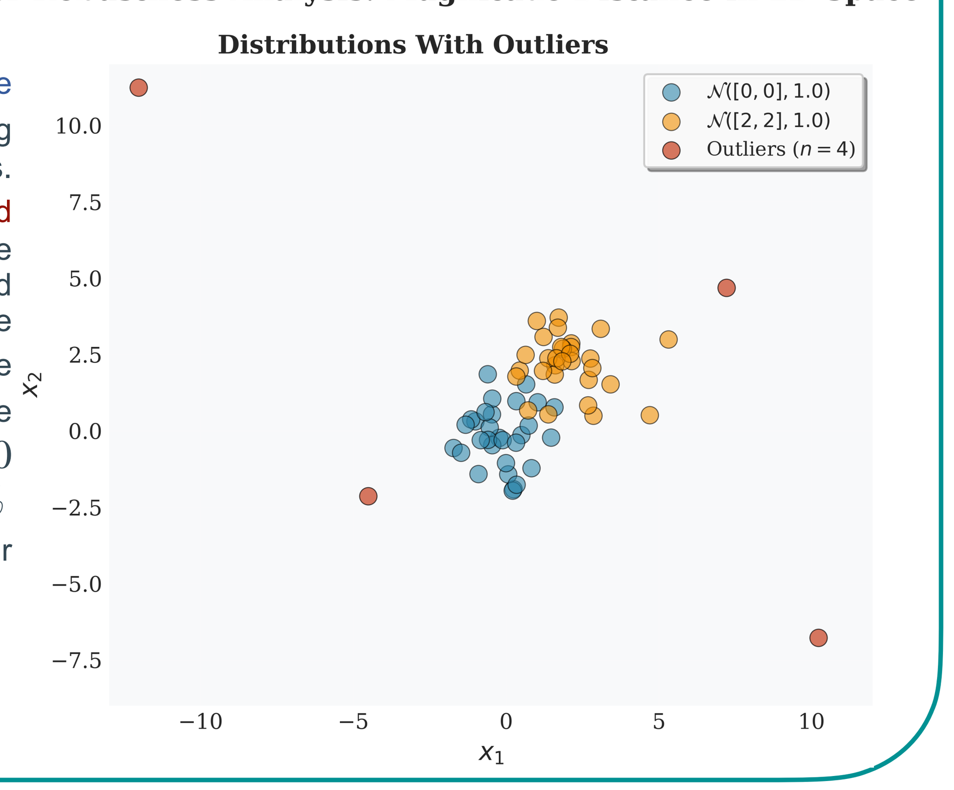
Nonnegative weighting vectors are guaranteed in all subsets of metric spaces when scaled up sufficiently, i.e., $t \gg 0$, and also $\mathbb{R}$ which this bound exists for any scaling parameter.

Result

$d^t_{Mag}(X)$'s sensitivity to adding or adjusting samples is also bounded.

Outlier Robustness Analysis: Magnitude Distance in 2D Space

Caption: We generate two datasets, B (blue points) and Y (yellow points), by sampling from normal distributions with different means. We also generate a third set of points, Y' (red points), with much higher dispersion. We consider the magnitude distance and Wasserstein distance for two cases: the distance between B and Y, and the distance between B and $Y^* = Y \cup Y'$. The relative change in magnitude distance with $t = 20$ and $t = 5$ are $6.85\,\%$ and $10.29\,\%$ respectively, compared to $17.61\,\%$ for Wasserstein distance.



References

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