# On the Lipschitz Continuity of Set Aggregation Functions and Neural Networks for Sets

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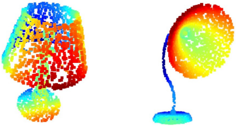
# Introduction

Complex datasets often decomposed into sets (or multisets) of simpler objects

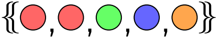


**Point clouds**

$\{\!\{$the, quick, brown, fox, jumps, over, lazy, dog $\}\!\}$

**Textual documents**

WL colors



**Graphs**

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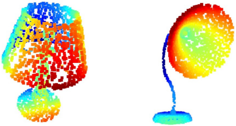

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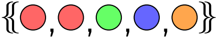

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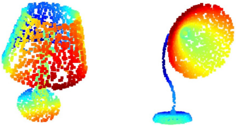

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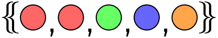

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**Question**: Are these functions and architectures that employ these functions stable (from a Lipschitz perspective)?

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- **Earth Mover's Distance (EMD)**: A measure of dissimilarity between two distributions:

$$d_{\mathrm{EMD}}(X, Y) = \min_{\mathbf{F} \geq 0} \sum_{i=1}^{m} \sum_{j=1}^{n} [\mathbf{F}]_{ij} \, \|\mathbf{v}_i - \mathbf{u}_j\|_2, \quad \text{s.t.} \ \sum_{j=1}^{n} [\mathbf{F}]_{ij} = \frac{1}{m}, \ \sum_{i=1}^{m} [\mathbf{F}]_{ij} = \frac{1}{n}$$

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- **Hausdorff Distance**: Defined as follows:

$$d_H(X, Y) = \max\big(h(X, Y), h(Y, X)\big) \quad \text{where } h(X, Y) = \max_{i \in [m]} \min_{j \in [n]} ||\mathbf{v}_i - \mathbf{u}_j||_2$$

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- **Matching Distance**: Assigns elements of one multiset to elements of the other. The assignments are determined by a permutation of the elements of the larger multiset ($m \geq n$):

$$d_M(X, Y) = \min_{\pi \in \mathfrak{S}_m} \left[ \sum_{i=1}^{n} ||\mathbf{v}_{\pi(i)} - \mathbf{u}_i||_2 + \sum_{i=n+1}^{m} ||\mathbf{v}_{\pi(i)}||_2 \right]$$

  $\mathfrak{S}_m$ denotes the set of all permutations of a multiset with $m$ elements.

Functions considered are metrics for sets and pseudometrics for multisets

# Lipschitz Continuity of Aggregation Functions

**Main result #1**:

- There is some correspondence between the three aggregation functions and the three metrics for unordered multisets.
  - Mean $\leftrightsquigarrow$ EMD
  - Sum $\leftrightsquigarrow$ Matching Dist.
  - Max $\leftrightsquigarrow$ Hausdorff Dist.
- If the multisets have fixed size (denoted by $^\dagger$ in the Table), the aggregation functions are Lipschitz continuous also with respect to other metrics.

| | Sum | Mean | Max |
|---|---|---|---|
| EMD | $^\dagger L = M$ | $L = 1$ | $^\dagger L = M$ |
| Hausdorff Dist. | – | – | $L = \sqrt{d}$ |
| Matching Dist. | $L = 1$ | $^\dagger L = 1/M$ | $^\dagger L = 1$ |

# Upper Bounds of Lipschitz Constants of Neural Networks for Sets

Neural network that operates on multisets:

$$\mathrm{NN}_g(X) = f_2\Big(g\big(\{\!\{ f_1(\mathbf{v}_1), \ldots, f_1(\mathbf{v}_m) \}\!\}\big)\Big)$$

where $\{\!\{\mathbf{v}_1, \ldots, \mathbf{v}_m\}\!\}$ is the input multiset, $g$ the employed aggregation function and $f_1, f_2$ neural network modules (e. g., MLPs)

**Main result #2**:

- The results for the aggregation functions transfer to neural networks that operate on multisets:
  - This does **not** hold for the Sum function!
  - **Lipschitz continuity**: only guaranteed if multisets have fixed size (denoted by $^\dagger$ in the Table).

| | Sum | Mean | Max |
|---|---|---|---|
| EMD | $^\dagger L \leq \mathrm{Lip}(f_1)\mathrm{Lip}(f_2)M$ | $L \leq \mathrm{Lip}(f_1)\mathrm{Lip}(f_2)$ | $^\dagger L \leq \mathrm{Lip}(f_1)\mathrm{Lip}(f_2)M$ |
| Hausdorff Dist. | – | – | $L \leq \mathrm{Lip}(f_1)\mathrm{Lip}(f_2)\sqrt{d}$ |
| Matching Dist. | $^\dagger L \leq \mathrm{Lip}(f_1)\mathrm{Lip}(f_2)$ | $^\dagger L \leq \mathrm{Lip}(f_1)\mathrm{Lip}(f_2)(1/M)$ | $^\dagger L \leq \mathrm{Lip}(f_1)\mathrm{Lip}(f_2)$ |

# Conclusion

**Experiments reported in the paper**:

- Validation of theoretical results
- Stability under perturbations of input multisets
- Generalization under distribution shifts

**Main guideline**: choose an aggregation function that is Lipschitz continuous with respect to the distance function that best reflects similarity in the dataset (might require domain knowledge).

| Data Characteristic | Ideal Distance Metric | Aggregator |
|---|---|---|
| Shape and Boundary Outliers (e. g., 3D scans) | Hausdorff | MAX |
| Overall Distribution (e. g., documents represented as sets of word vectors) | EMD | MEAN |
| Direct 1-to-1 Element Correspondence (e. g., images represented as sets of keypoints) | Matching | SUM |

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