Overlapping Spaces for Compact Graph Representations

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NeurIPS 2021

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Summary

- We introduce Overlapping Spaces (OS) for embedding structured data
- Main idea: subsets of coordinates can be shared between spaces of different types (Euclidean, hyperbolic, spherical, etc.)
- OS automatically learns optimal combination of spaces
- Due to complex geometry, OS allows for more compact representations

Embeddings

- Vector representations of objects are needed for many applications
- Distance between vector representations should preserve 'distance' between objects

Embeddings

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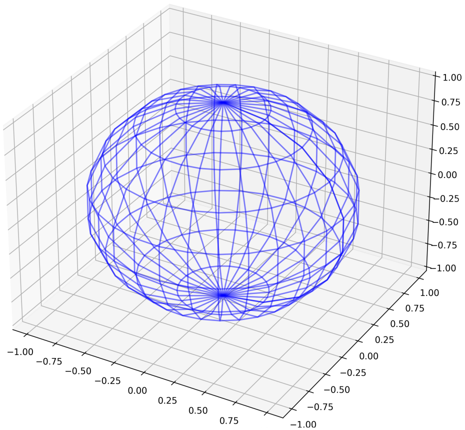
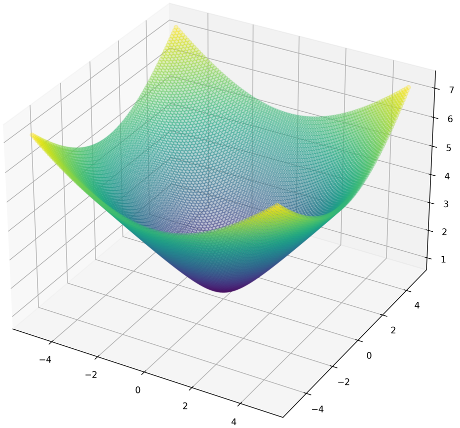
- Besides Euclidean space, what other options do we have?

Spherical space



$$S = \{x \in R^n | \, \|x\| = 1\}$$
$$d_S(x, y) = \arccos(x^T y)$$

Hyperbolic space: Lorentz Model



$$\langle x, y \rangle_H = x_1 y_1 - \sum_{i=2}^{n+1} x_i y_i$$

$$\mathrm{H} = \{x \in \mathrm{R}^{n+1} | \, \langle x, y \rangle_H = 1, x_1 \geq 0\}, \; d_H(x, y) = \mathrm{arccosh}(\langle x, y \rangle_H)$$

Product space

Definition

Given metric spaces $(M_1, d_{M_1}), \ldots, (M_n, d_{M_n})$, product space is defined as $M_1 \times \ldots \times M_n$ equipped with distance function $d_{l1} = \sum_{i=1}^{n} d_{M_i}$ or $d_{l2}^2 = \sum_{i=1}^{n} d_{M_i}^2$.

Examples: $\mathrm{S}_5 \times \mathrm{S}_5$, $\mathrm{S}_5 \times \mathrm{H}_5$, $\mathrm{S}_2 \times \mathrm{S}_2 \times \mathrm{H}_2 \times \mathrm{H}_2 \times \mathrm{E}_2$, ...

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Problem: the best combination of spaces depends on the dataset.

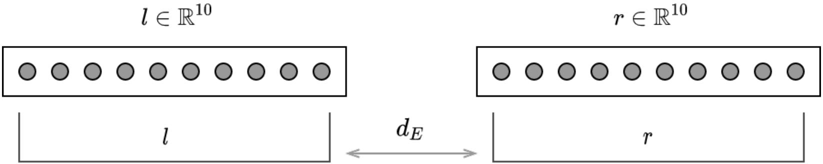
Gu, Sala, Gunel, Ré, "Learning mixed-curvature representations in product spaces", ICLR 2018.

Our approach

Overlapping spaces generalize product spaces

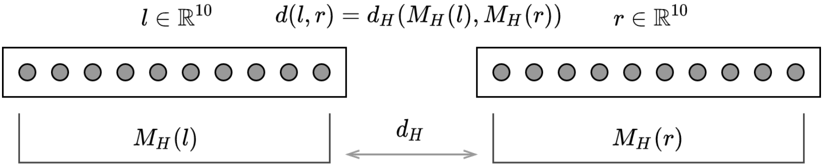
Importantly, they do not require signature brute-forcing

For two vectors we can compute the Euclidean distance (E^{10}):



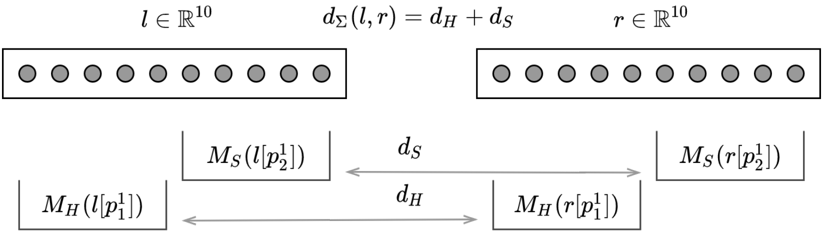
$$d_E^2(l, r) = \sum_{i=1}^{10} (l_i - r_i)^2$$

For spherical and hyperbolic spaces, we can use differentiable mappings $M_S(x) : \mathrm{R}^{10} \rightarrow \mathrm{S}^{10}$ and $M_H(x) : \mathrm{R}^{10} \rightarrow \mathrm{H}^{10}$:



With such parameterization, we can use any conventional optimizer

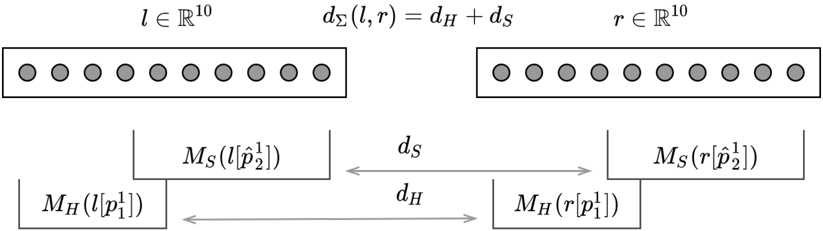
In a similar way, we may construct a product space, e.g., $\mathsf{H}_5 \times \mathsf{S}_5$:



Here $p_1^1 = [1..5]$, $p_2^1 = [6..10]$

From single to overlapping space

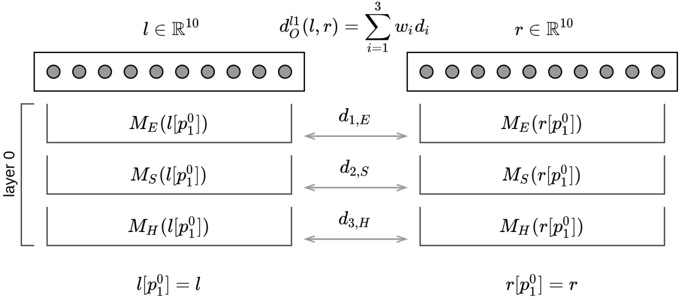
Let us allow the mappings **overlap**:



We constructed a subspace of product space $H_5 \times S_6$ with only 10 parameters per item

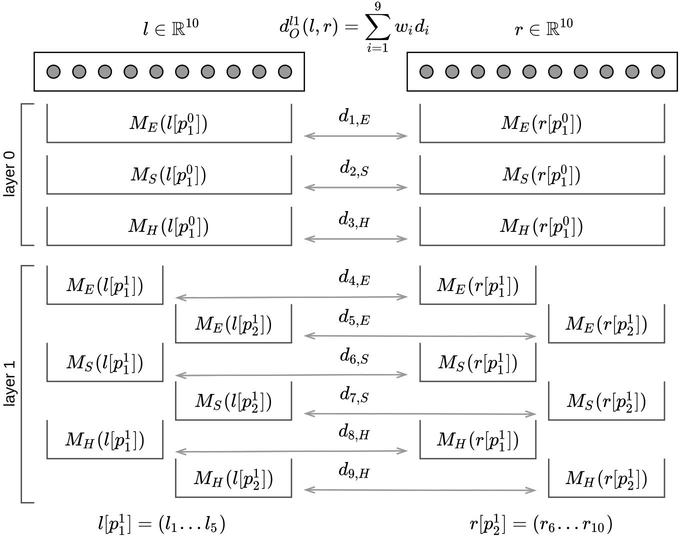
From single to overlapping space

Proposed implementation, layer 0:



From single to overlapping space

Layer 1:



OS-Mixed

Statement

Overlapping space is a metric space.

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Extension: add shifted weighted inner product (WIPS) to OS

Shifted WIPS: $d_{WIPS}(x, y) = c - \sum w_i x_i y_i$

$d_{OS\ \ Mixed} = d_{OS} + d_{WIPS}$

Experiments

Time for some experiments!

Graph reconstruction

Table: Graph reconstruction

	UCSA312	CS PhDs	Power	Facebook	WLA6	EuCore
Nodes	312	1025	4941	4039	3227	986
Edges	48516 (weighted)	1043	6594	88234	3604	16687

Graph reconstruction

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Quality measures: distortion D_{avg} and mean average precision (mAP)

$$D_{avg} = \frac{2}{|V|(|V|-1)} \sum_{(v,u) \in V^2, v \neq u} \frac{|d_U(e(v), e(u)) - d_G(v,u)|}{d_G(v,u)}$$

Here d_G — original distance, d_U — distance between vector representations

Graph reconstruction (distortion)

Table: Distortion graph reconstruction, top results are highlighted, top metric results are underlined.

Signature	UCSA312	CS PhDs	Power	Facebook	WLA6	EuCore
E_{10}	0.00318	0.0475	0.0408	0.0487	0.0530	0.1242
H_{10}	0.01104	0.0443	0.0348	0.0483	0.0279	0.1144
S_{10}	0.01065	0.0519	0.0453	0.0561	0.0608	0.1260
$H_5^2 \equiv H_5 \times H_5$	0.00573	0.0345	0.0255	0.0372	0.0279	0.1106
$S_5 \times S_5 \equiv S_5^2$	0.00700	0.0501	0.0438	0.0552	0.0584	0.1251
$H_5 \times S_5$	0.00541	0.0341	0.0254	0.0346	0.0310	0.1195
H_2^5	0.00592	0.0344	0.0273	0.0439	0.0356	0.1163
S_2^5	0.00604	0.0464	0.0416	0.0512	0.0543	0.1244
$H_2^2 \times E_2 \times S_2^2$	0.00537	0.0344	0.0302	0.0406	0.0437	0.1193
$O_{l1}, t = 0$	0.00324	0.0368	0.0281	0.0458	0.0286	0.1141
$O_{l1}, t = 1$	0.00325	0.0300	0.0231	0.0371	0.0272	0.1117
$O_{l2}, t = 1$	0.00530	0.0328	0.0246	0.0324	0.0278	0.1127
$c-$ dot	0.04005	0.0412	0.0461	0.0236	0.0296	0.1085
$c-$ wips	0.06468	0.0358	0.0442	0.0161	0.0238	0.1016
$ce^{-\text{dot}}$	0.08142	0.0424	0.0505	0.0192	0.0270	0.1048
$O_{mix-l1}, t = 1$	0.00277	0.0243	0.0235	0.0172	0.0187	0.1026
$O_{mix-l2}, t = 1$	0.00464	0.0220	0.0258	0.0163	0.0198	0.1028

Graph reconstruction (mAP)

Table: mAP graph reconstruction, top results are highlighted, top metric results are underlined.

Signature	UCSA312	CS PhDs	Power	Facebook	WLA6	EuCore
E_{10}	0.9290	0.9487	0.9380	0.7876	0.7199	0.6108
H_{10}	0.9173	0.9399	0.9385	0.7997	0.9617	0.6670
S_{10}	0.9183	0.9519	0.9445	0.7768	0.7289	0.6037
H_5^2	0.9247	0.9481	0.9415	0.8084	0.9682	0.6783
S_5^2	0.9316	0.9600	0.9482	0.7790	0.7307	0.6116
$H_5 \times S_5$	0.9397	0.9538	0.9505	0.7947	0.9751	0.6847
H_2^5	0.9364	0.9671	0.9508	0.7979	0.8597	0.6611
S_2^5	0.9439	0.9656	0.9511	0.7800	0.7358	0.6169
$H_2^2 \times E_2 \times S_2^2$	0.9519	0.9638	0.9507	0.7873	0.7794	0.6492
$O_{l1}, t = 0$	0.9538	0.9879	0.9728	0.8093	0.6759	0.6580
$O_{l1}, t = 1$	0.9522	0.9904	0.9762	0.8185	0.9598	0.6691
$O_{l2}, t = 1$	0.9522	0.9938	0.9907	0.8326	0.9694	0.7078
c − dot	1	1	0.9983	0.8745	0.9990	0.7409
c − wips	1	1	1	0.8704	1	0.7742
$O_{mix-l1}, t = 1$	1	1	0.9994	0.8806	0.9997	0.7860
$O_{mix-l2}, t = 1$	1	1	1	0.9021	1	0.8405

Weight analysis

For many datasets, more than half of the weights are near-zero, so unnecessary components can be removed.

For Power dataset:

$$d_{O_{l1},t=1}(l,r) \propto 0.1 d_E(l_1^0, r_1^0) + 0.5 d_R(l_1^0, r_1^0) + 0.4 d_H(l_1^1, r_1^1),$$

$$\text{where } l_1^0 = l[0..5], l_1^1 = l[6..10]$$

We trained classical DSSM with different distance functions on Wikipedia search dataset:

Table: Search query examples

Query	Web site
Kris Wallace	en.wikipedia.org/wiki/Chris_Wallace
1980: Mitsubishi produces one million cars...	en.wikipedia.org/wiki/Mitsubishi_Motors
code napoleon	en.wikipedia.org/wiki/Napoleonic_Code

Information Retrieval with DSSM

Table: DSSM results, dimension 10, top three results are highlighted

Signature	Test mAP
E_{10}	0.4459
H_{10}	0.4047
S_{10}	0.4364
H_5^2	0.4492
S_5^2	0.4573
$H_5 \times S_5$	0.3295
H_2^5	0.3681
S_2^5	0.4616
$H_2^2 \times E_2 \times S_2^2$	0.3526
$c-\mathbf{dot}$	0.4194
$O_{l1}, t=0$	0.4562
$O_{l1}, t=1$	0.4498
$O_{l2}, t=1$	0.4456
$O_{mix-l1}, t=1$	0.4447
$O_{mix-l2}, t=1$	0.4483

To sum up

1. We propose overlapping spaces that allow for parameter sharing between different sub-spaces
2. OS automatically learns optimal combination of combined spaces
3. OS allows for compact representations in various setups
4. The proposed method can be combined with non-metric similarities leading to even more flexibility