A Trainable Optimal Transport Embedding for Feature Aggregation

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INVENTEURS DU MONDE NUMÉRIQUE

NEURAL INFORMATION PROCESSING SYSTEMS

Motivation: biological sequences

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- Long sequences (1000+ base pairs).
- Few labeled data (e.g, 20 labels per class for SCOP1.75).

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We need a **trainable** embedding for sets with **lower memory/sample requirements**.

Idea: attention with optimal transport and kernel methods

We provide an embedding with an inductive bias akin to that of self-attention. Two steps:

Figure 2: The input point cloud x is transported onto the reference $\mathrm{z} = (\mathrm{z}_1, \dots, \mathrm{z}_p)$ (left), yielding the optimal transport plan $\mathrm{P}_\kappa(\mathrm{x}, \mathrm{z})$ used to aggregate the embedded features and form $\Phi_\mathrm{z}(\mathrm{x})$ (right).

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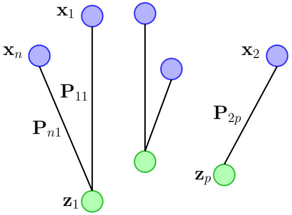
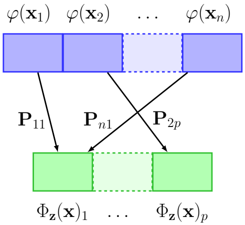
1. Non-linear layer: we use a parametrized kernel embedding in the fashion of [Chen et al., 2019a].
2. Pooling: similar elements are **pooled** together. The measure of similarity is the optimal **transport plan** between the input set $x \in \mathbb{R}^{n \times d}$ and a **learned reference** $z \in \mathbb{R}^{p \times d}$.





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Results

The resulting (non-standard) kernel formulation provides a rich representation for sequences with **relatively few parameters** that can be trained end-to-end or without supervision.

Table 1: Classification accuracy (top 1/5/10) on test set for SCOP 1.75 for different unsupervised and supervised baselines, averaged from 10 different runs. (q references $\times$ p supports).

Method	Unsupervised	Supervised
DeepSF [Hou et al., 2019]	Not available.	73.0/90.3/94.5
CKN [Chen et al., 2019a]	81.8±0.8/92.8±0.2/95.0±0.2	84.1±0.1/94.3±0.2/96.4±0.1
RKN [Chen et al., 2019b]	Not available.	85.3±0.3/95.0±0.2/96.5±0.1
Set Transformer [Lee et al., 2019]	Not available.	79.2±4.6/91.5±1.4/94.3±0.6
Approximate Rep the Set [Skianis et al., 2020]	Not available.	84.5±0.6/94.0±0.4/95.7±0.4
Ours (dot-product instead of OT)	78.2±1.9/93.1±0.7/96.0±0.4	87.5±0.3/95.5±0.2/96.9±0.1
Ours (Unsup.: 1×100 / Sup.: 5×10)	**85.8±0.2/95.3±0.1/96.8±0.1**	**88.7±0.3/95.9±0.2/97.3±0.1**

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Thank you!

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