ParaDime

A FRAMEWORK FOR PARAMETRIC DIMENSIONALITY REDUCTION

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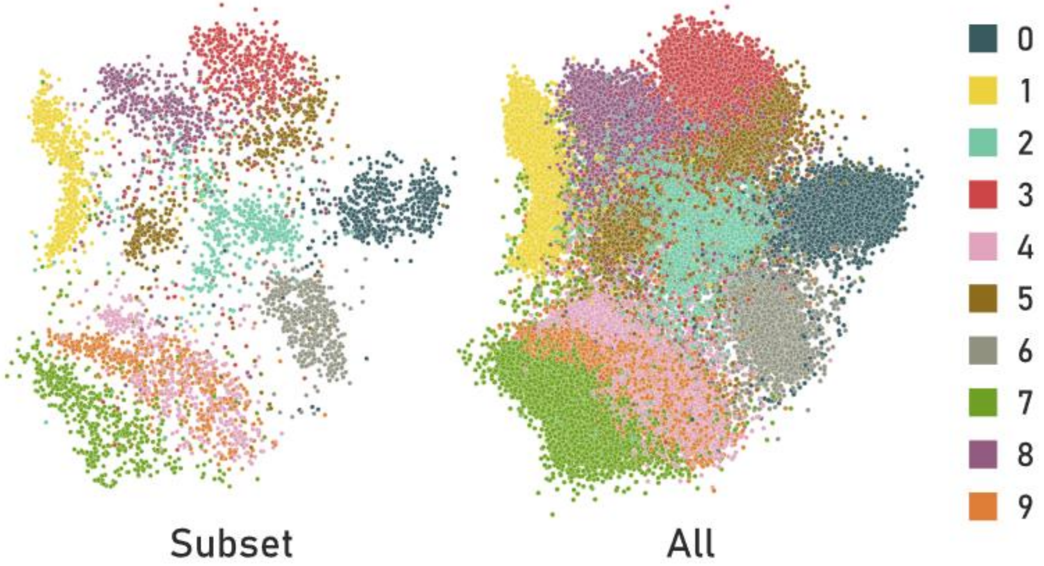
paraDime




```yaml
relations:
  - name: dists hd
    level: global
    type: pairwise
    options:
      metric: euclidean
  - name: dists ld
    level: batch
    type: pairwise
    options:
      metric: euclidean
```

```yaml
losses:
  - name: mds
    type: relation
    func: mse
    keys:
      rels:
        - dists hd
        - dists ld
training phases:
  - loss:
      components: mds
```

MOTIVATION & GOALS

Unify

Parameterize

Share & Reuse

Customize

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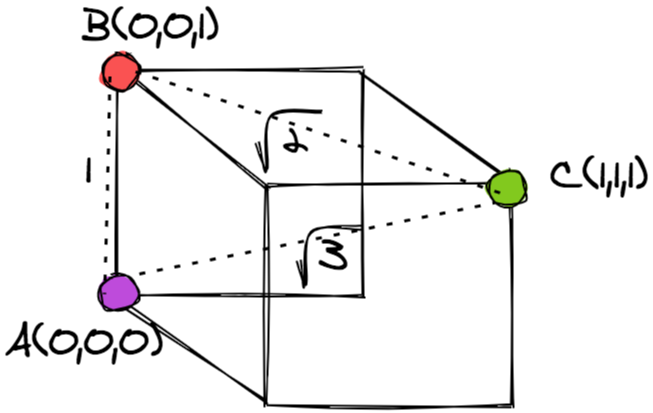
SIMILARITIES BETWEEN METHODS

- MDS
- Isomap
- t-SNE
- LargeVis
- UMAP



https://stackabuse.com/guide-to-multidimensional-scaling-in-python-with-scikit-learn/

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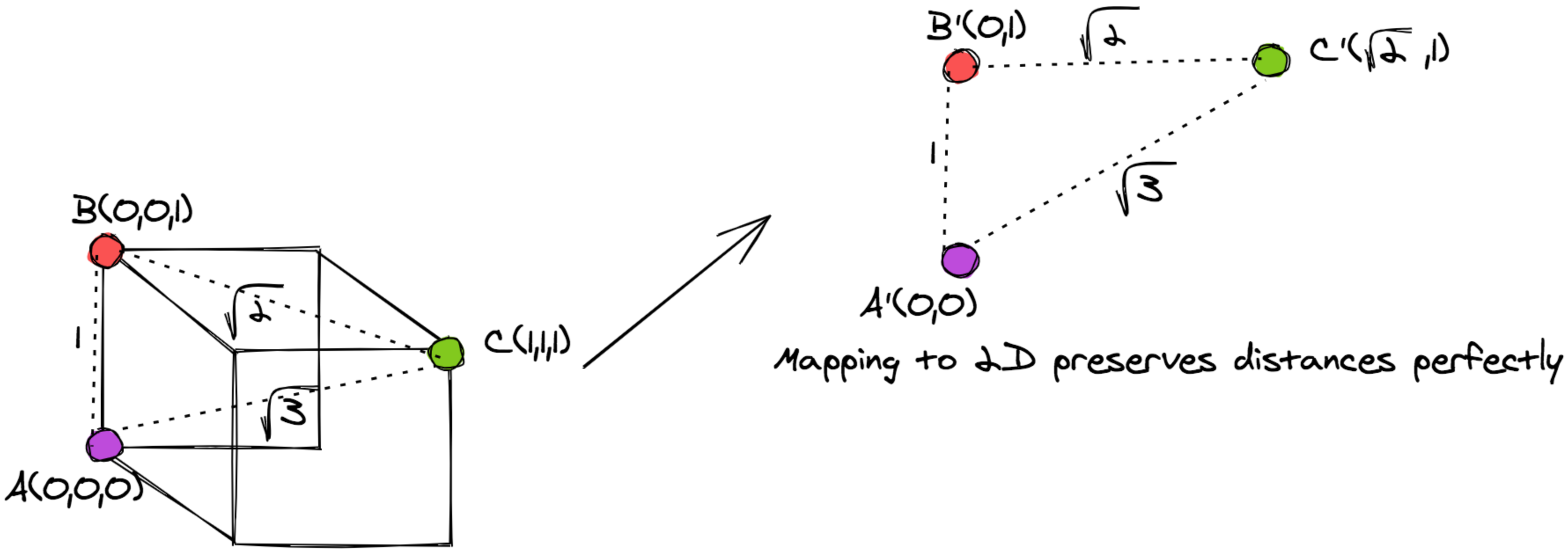

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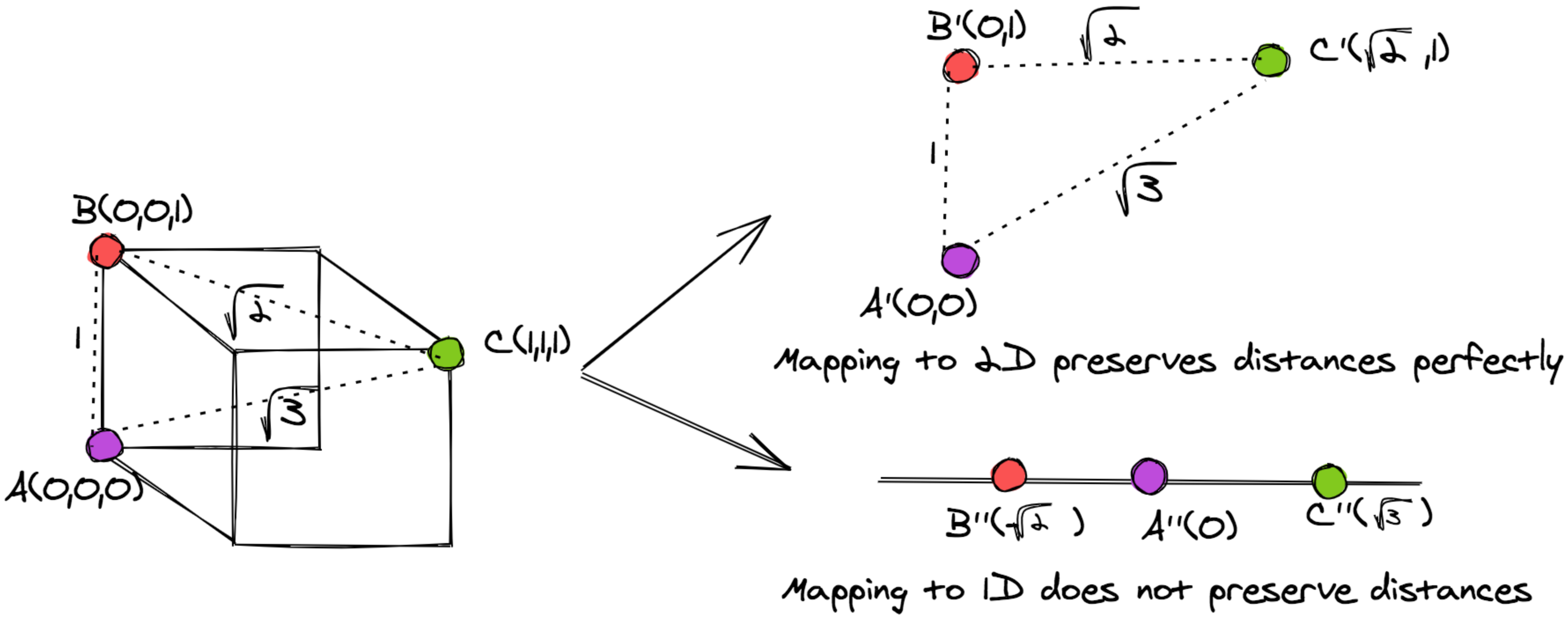

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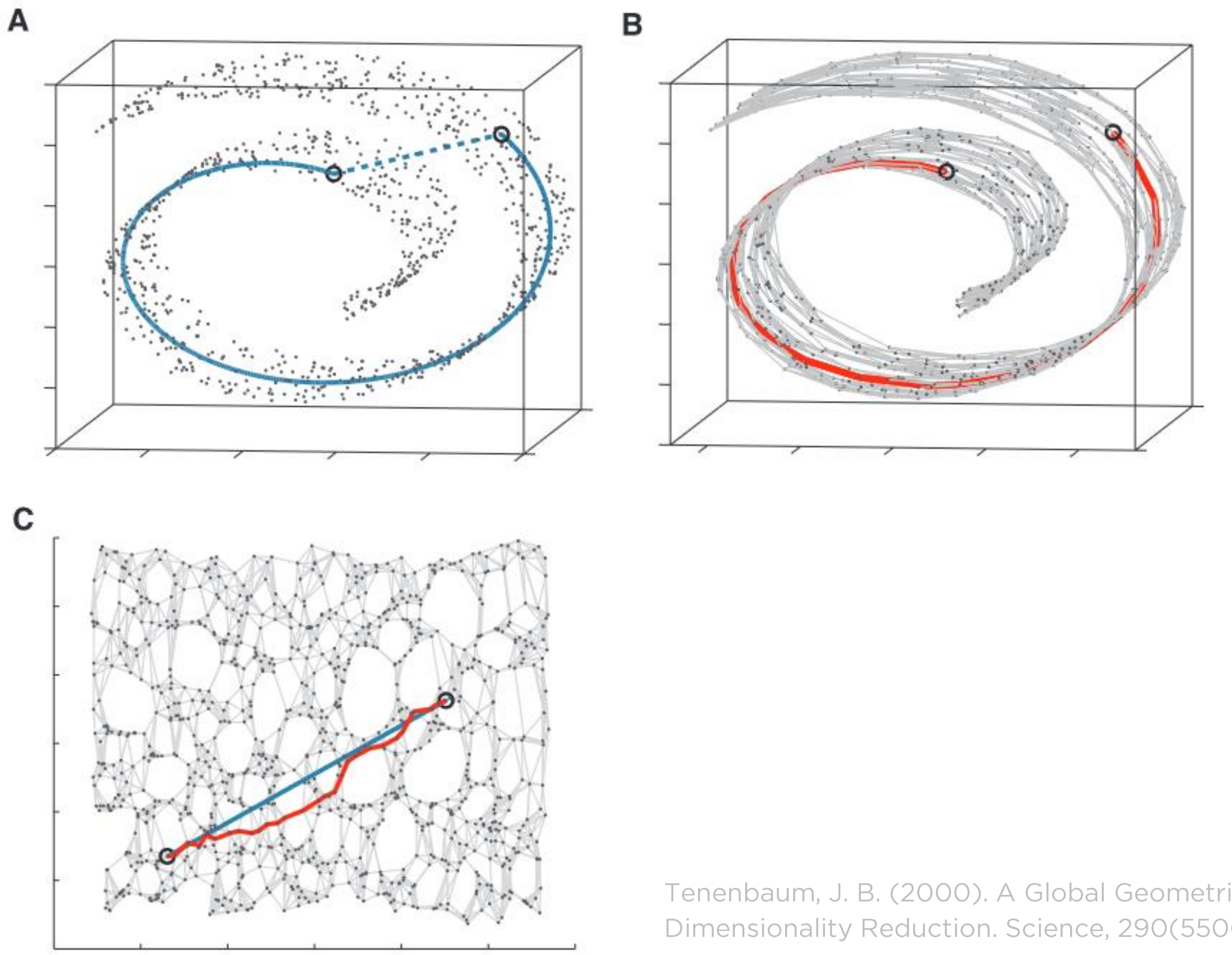

Tenenbaum, J. B. (2000). A Global Geometric Framework for Nonlinear Dimensionality Reduction. Science, 290(5500), 2319–2323.

SIMILARITIES BETWEEN METHODS

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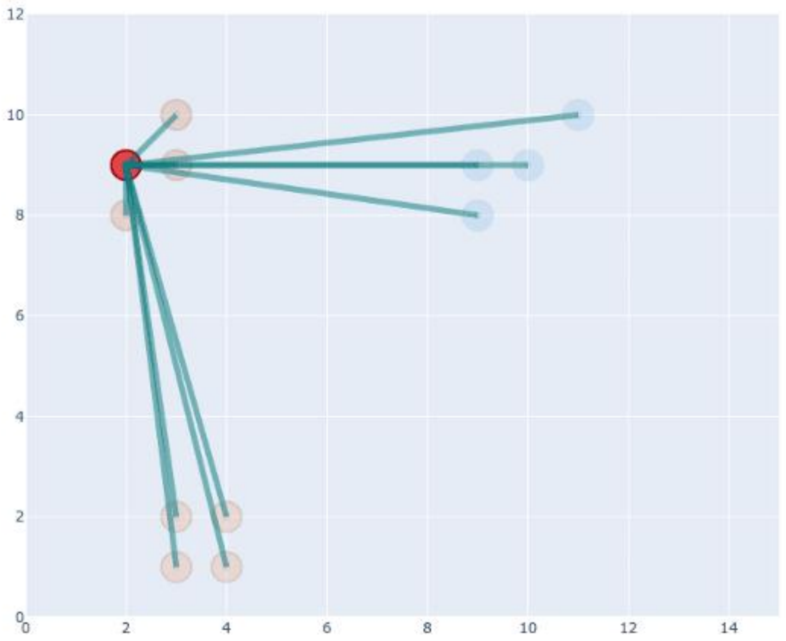

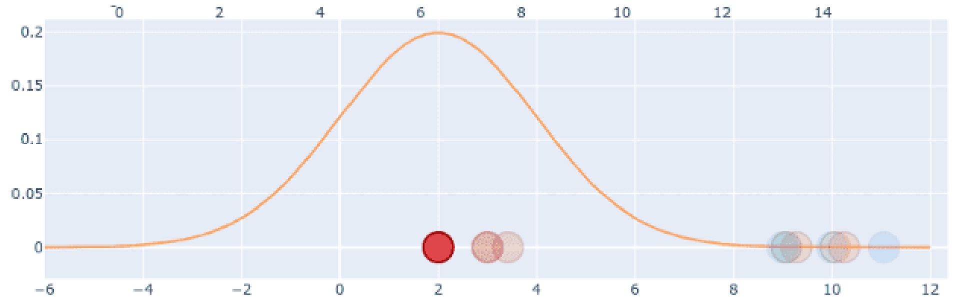

https://towardsdatascience.com/t-sne-clearly-explained-d84c537f53a

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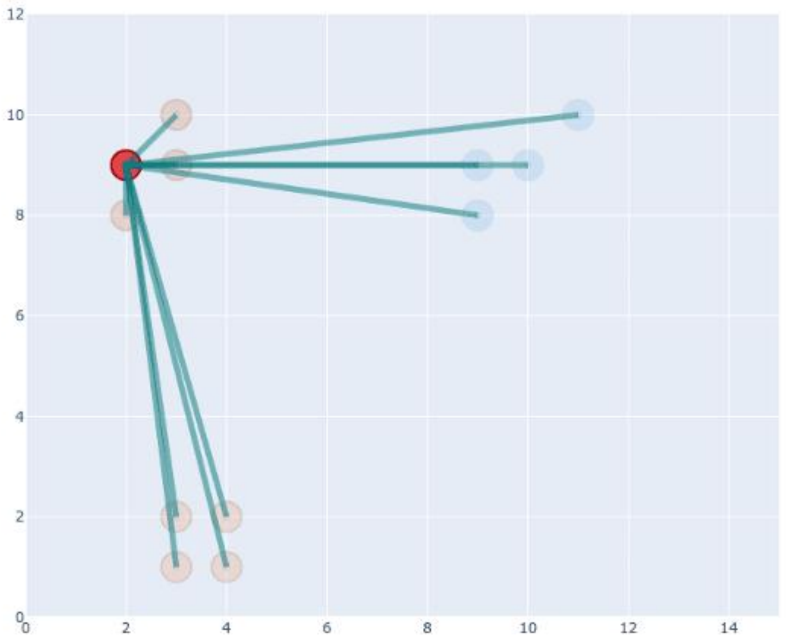

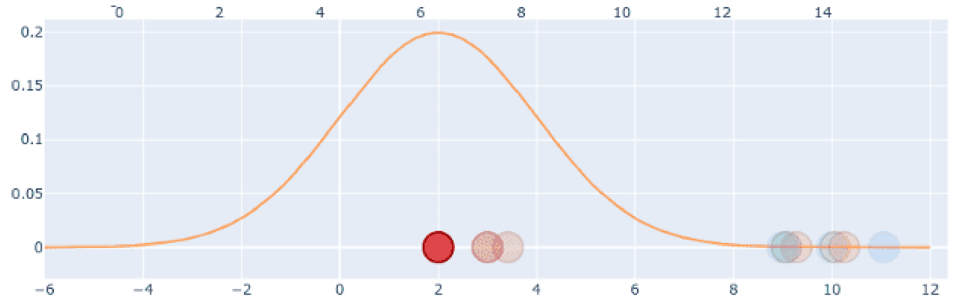

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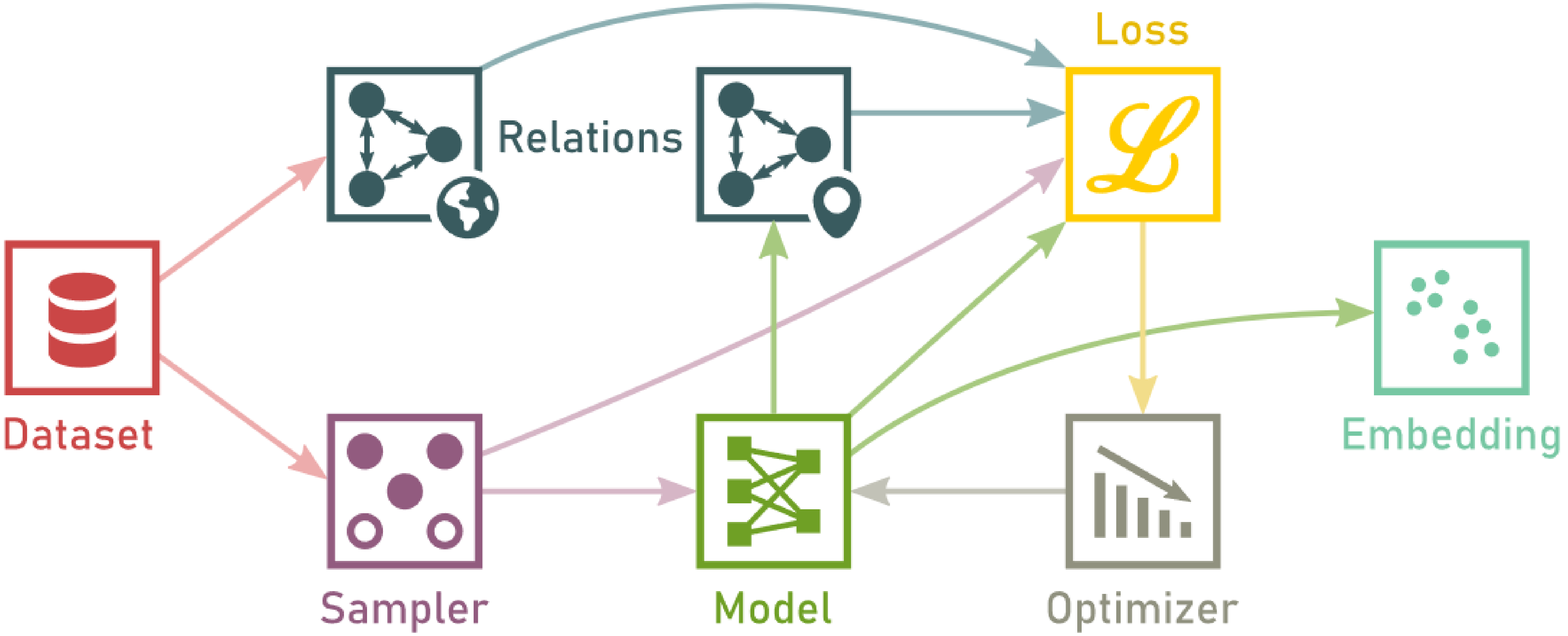
Summary

1. Compute distances in high-dimensional space
2. Optionally transform HD distances
3. Arrange points in low-dimensional space and compute distances
4. Optionally transform LD distances
5. Make (transformed) distances match

DATA FLOW


Loss
Relations
Dataset
Embedding
Sampler
Model
Optimizer

MOTIVATION & GOALS

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PARAMETRIC EMBEDDINGS

- Non-parametric embeddings:

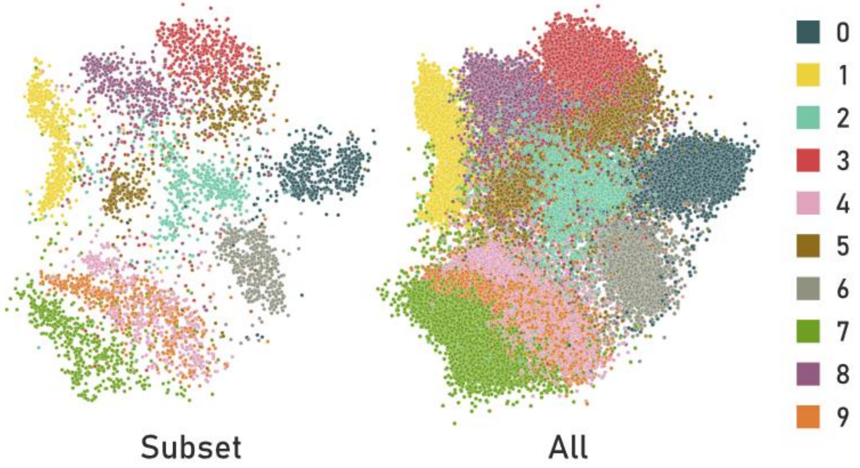
$$\mathrm{DR}(\{x_1, \ldots, x_n\}) = \arg\min_{y_i \in \mathbb{R}^k} \mathcal{L}\big(\{x_1, \ldots, x_n\}, \{y_1, \ldots, y_n\}\big)$$

- **Parametric** embeddings:

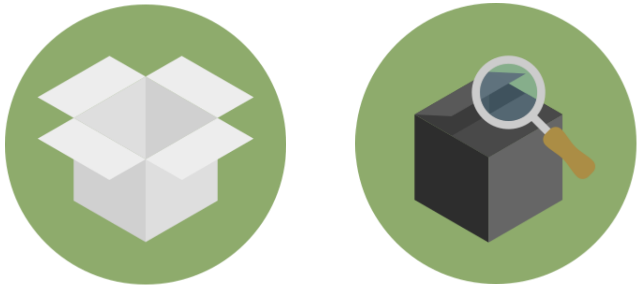
$$\mathrm{DR}_{\text{param}}(\{x_1, \ldots, x_n\}) = \arg\min_{f \in F} \mathcal{L}\big(\{x_1, \ldots, x_n\}, \{f(x_1), \ldots, f(x_n)\}\big)$$

PARAMETRIC EMBEDDINGS

- Out-of-sample extension



- Potentially explainable



- Modern infrastructure

PyTorch

TensorFlow

- Differentiable

$$\frac{\partial f}{\partial x}$$

- Customizable

$$\mathcal{L} = \sum_{i=1}^{n} w_i \times \mathcal{L}_i$$

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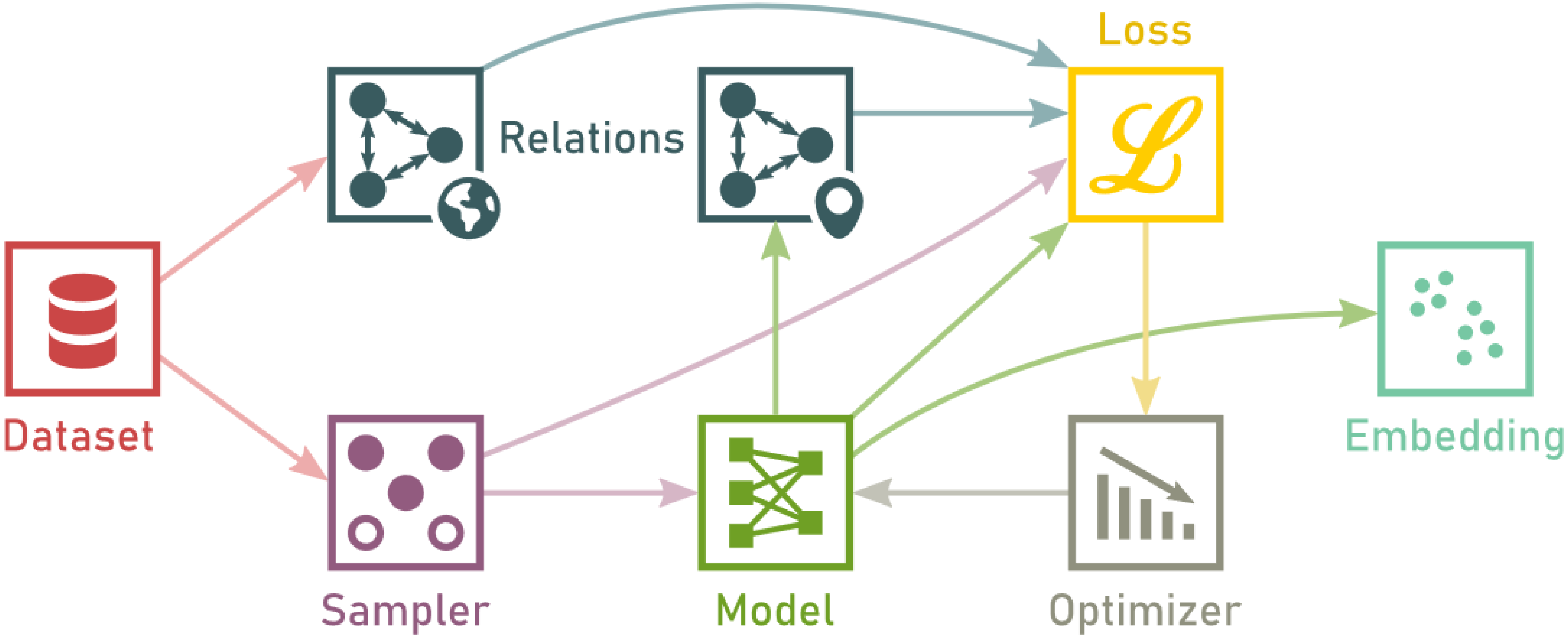
DATA FLOW



Loss
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GRAMMAR & SPECIFICATIONS

```
relations:
```

```
losses:


training phases:
```

GRAMMAR & SPECIFICATIONS

```yaml
relations:
  - name: dists hd
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```yaml
losses:
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    type: relation
    func: mse
    keys:
      rels:
        - dists hd
        - dists ld
training phases:
  - loss:
      components: mds
```
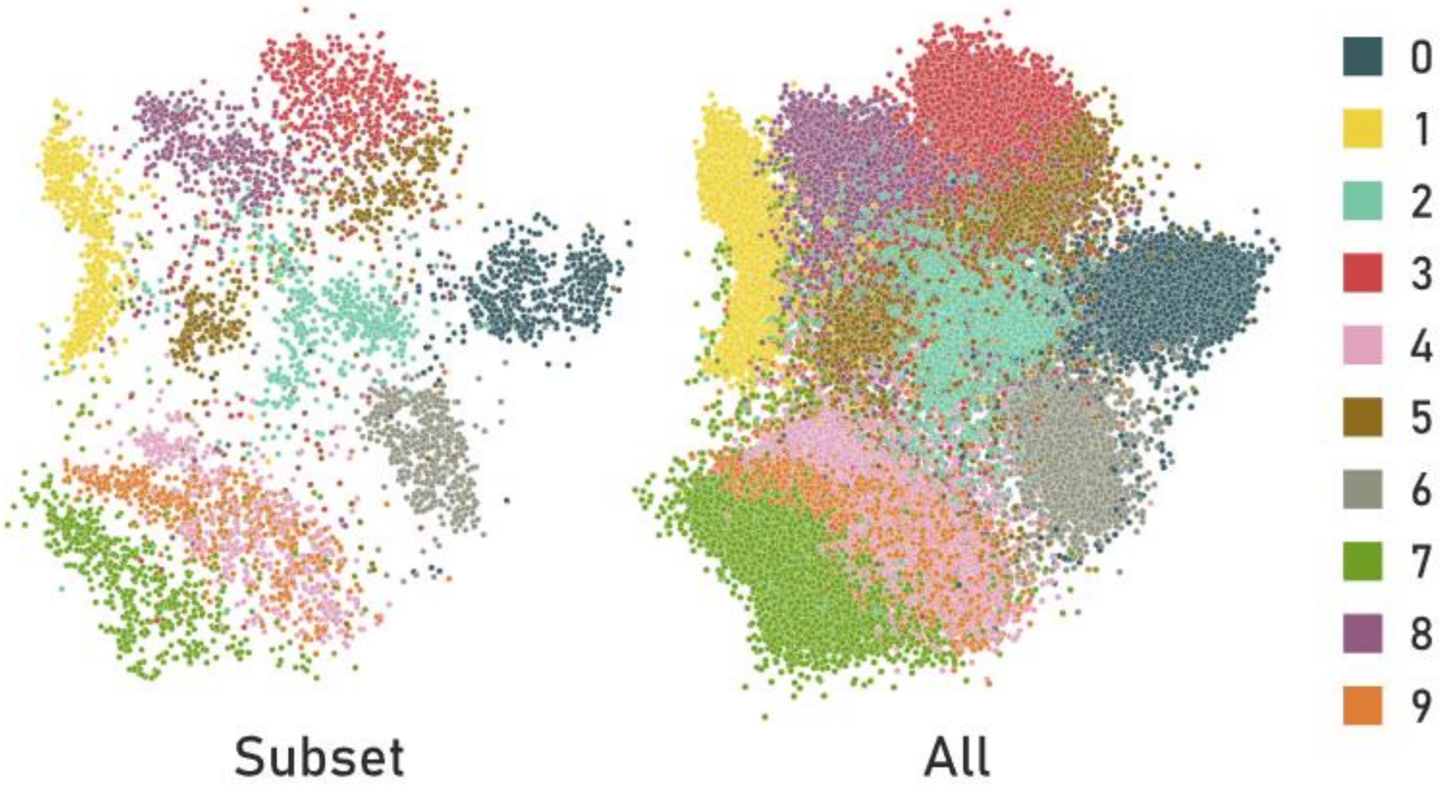

GRAMMAR & SPECIFICATIONS

```yaml
derived data:
  - name: pca
    data func: pca
    keys: [[data, main]]
relations:
  - name: p
    level: global
    type: neighbor
    data: main
    options:
      metric: euclidean
    transforms:
      - type: perplexity
        options:
          perplexity: <p>
      - type: symmetrize
      - type: normalize
  - name: q
    level: batch
    type: pairwise
    data: main
    options:
      metric: euclidean
    transforms:
      - type: t-dist
        options:
          alpha: 1.
      - type: normalize
losses:
  - name: init
    type: position
    func: mse
    keys:
      data: [main, pca]
  - name: emb
    type: relation
    func: kl div
    keys:
      rels: [p, q]
training phases:
  # pca initialization
  - loss:
      components: [init]
      sampling:
        type: item
  # main embedding
  - loss:
      components: [emb]
      sampling:
        type: item
```



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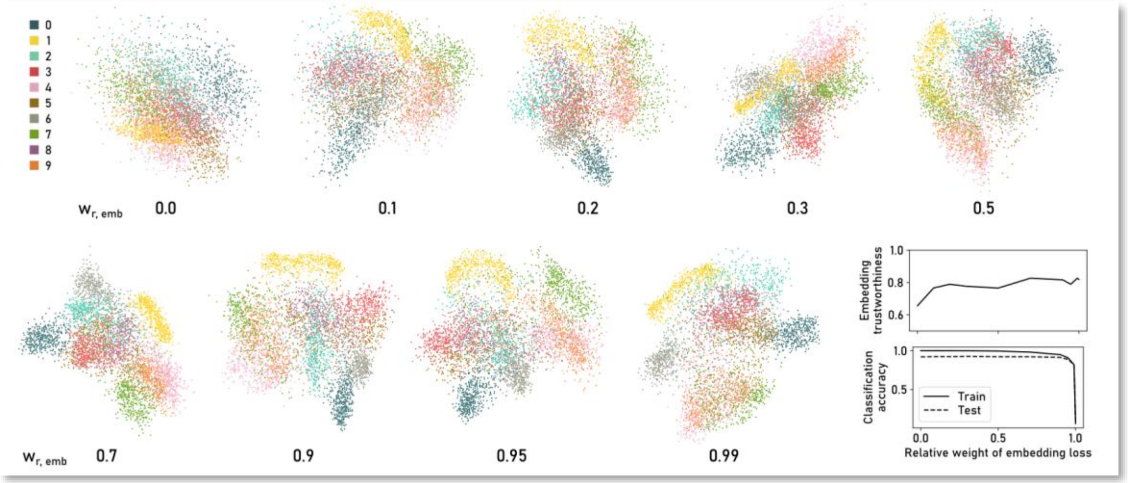
CUSTOMIZATION EXAMPLES

- Hybrid/multitask routines
  - Classification
  - Reconstruction

```
relations: <UMAP relation specs>
losses: [<UMAP loss>, <classification loss>]
training phases:
  - loss:
      components: [umap, class]
      weights: <w>
```

- Multi-phase routines
- Supervised routines



Forest covertype Dataset



SUPERVISED DR – TRIPLETS

- Aspen
- Cottonwood/willow
- Douglas-fir
- Krummholz
- Lodgepole pine
- Ponderosa pine
- Spruce/fir

R = w(t-SNE) / w(Triplet)

Parametric t-SNE (ParaDime)

t-SNE (scikit-learn)

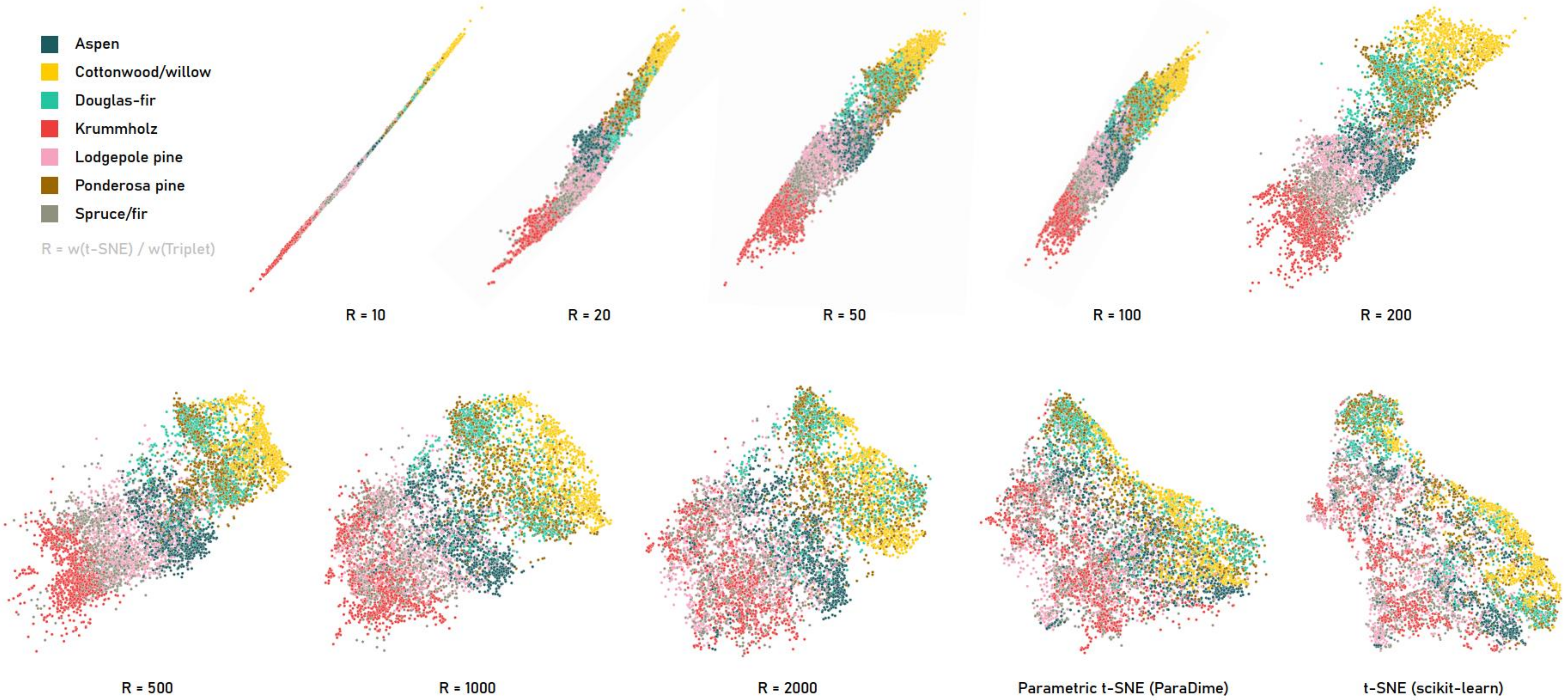
SUPERVISED DR – TRIPLETS

R = 10

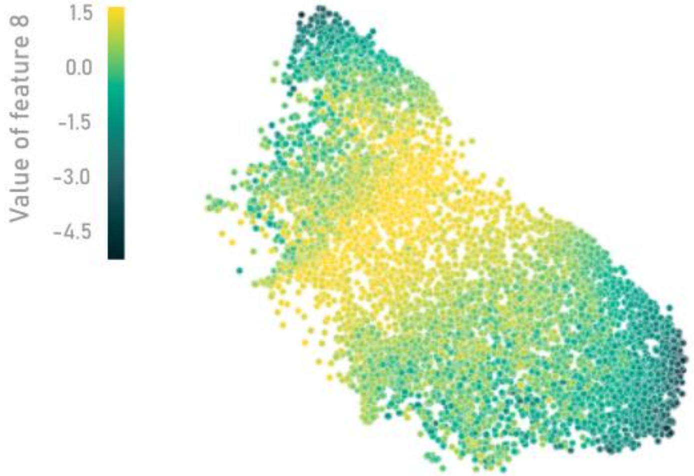
Parametric t-SNE (ParaDime)

t-SNE (scikit-learn)

SUPERVISED DR – TRIPLETS



SUPERVISED DR – CORRELATION



Unguided → Guided

SUPERVISED DR – CORRELATION

SUPERVISED DR – CORRELATION

IMPLEMENTATION & DOCUMENTATION

JKU

PyTorch

python™ Package Index

Read the Docs

Docs » paraDime: A Framework for Parametric Dimensionality Reduction   Edit on GitHub

paraDime

latest

Search docs

USER GUIDE

- Installation
- Simple Usage
- Building Blocks of a paraDime Routine
- Examples

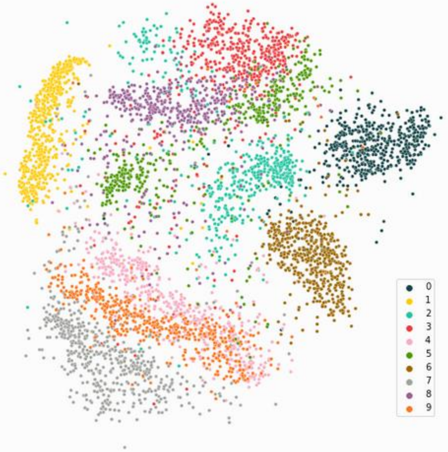
API REFERENCE

- API Reference

paraDime: A Framework for Parametric Dimensionality Reduction

paraDime is a modular framework for specifying and training parametric dimensionality reduction (DR) models. These models allow you to add new data points to existing low-dimensional representations of high-dimensional data. ParaDime DR models are constructed from simple building blocks (such as Relations and Relation Transforms), so that experimentation with novel DR techniques becomes easy.

Here you can see a parametric version of t-SNE [1] trained on a subset of 5000 images of handwritten digits from the MNIST dataset [2]:



The rest of the 60,000 images can then be easily embedded into the same space without retraining the t-SNE:

Read the Docs   v: latest

https://paradime.readthedocs.io/

CONCLUSION

paraDime

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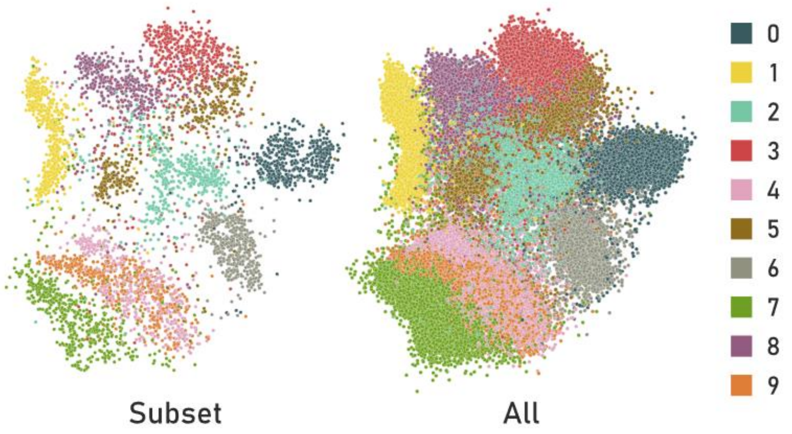
Share



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