The tree autoencoder model,

with application to hierarchical data visualization

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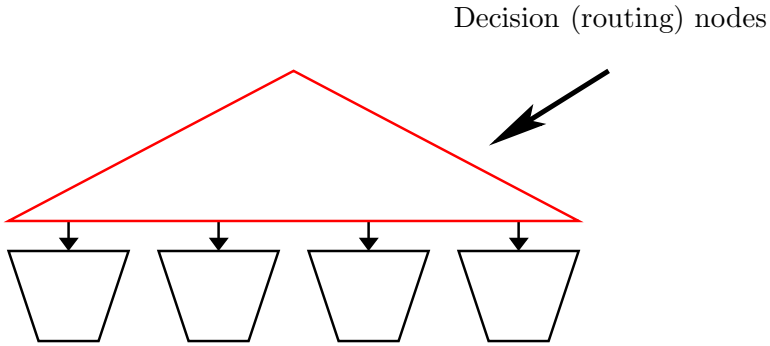
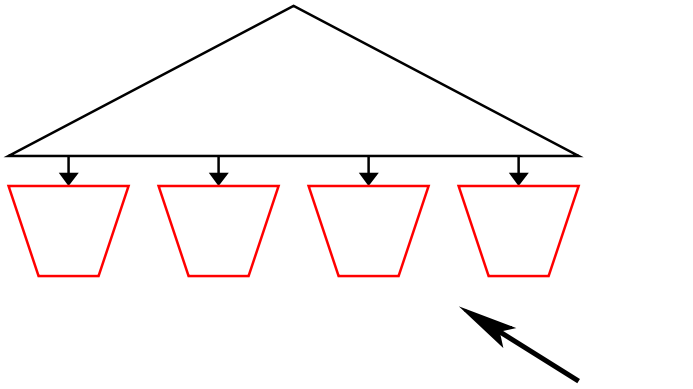
NEURAL INFORMATION PROCESSING SYSTEMS

UCMERCED

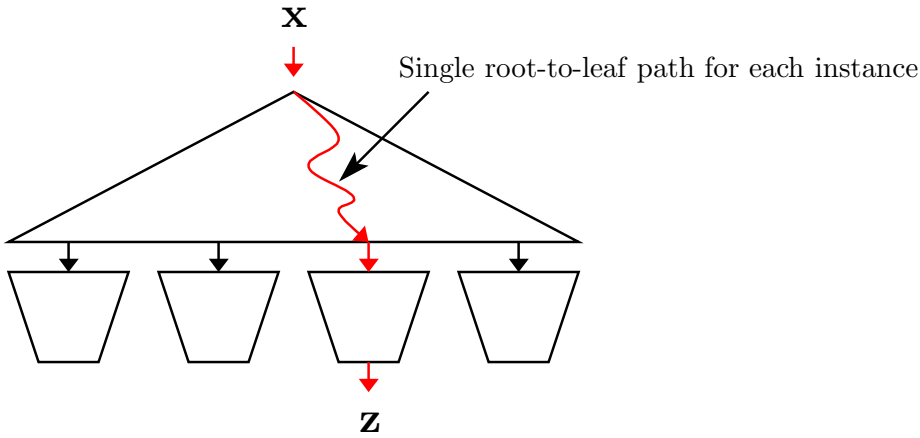
Encoder



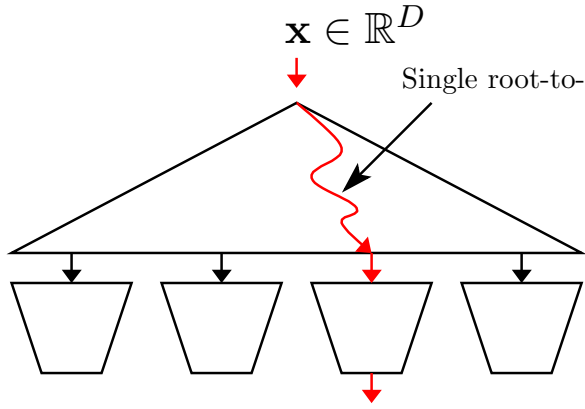
Encoder



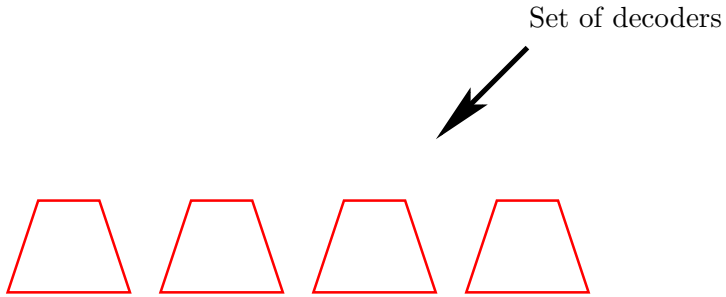
Encoder



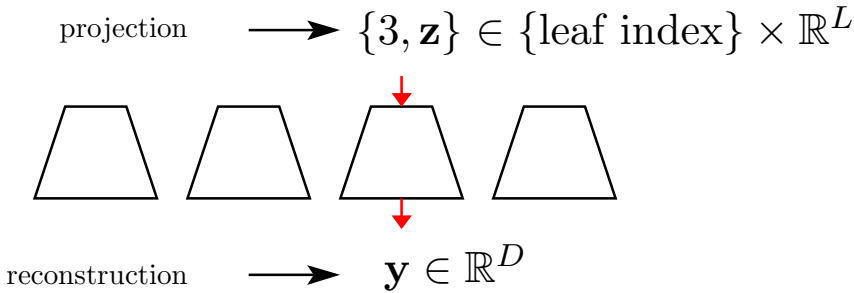
Encoder


$\mathbf{x} \in \mathbb{R}^D$
Single root-to-leaf path for each instance
projection
$\{3, \mathbf{z}\} \in \{\text{leaf index}\} \times \mathbb{R}^L$

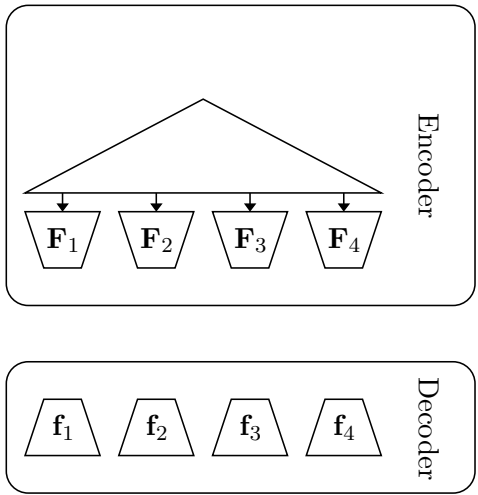
Decoder



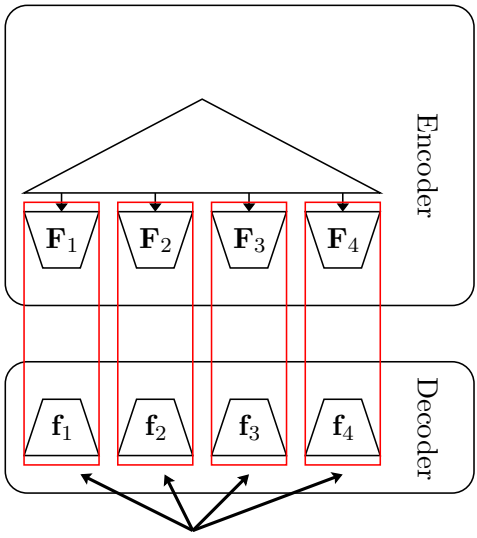
Decoder


projection
$\{3, \mathbf{z}\} \in \{\text{leaf index}\} \times \mathbb{R}^L$
reconstruction
$\mathbf{y} \in \mathbb{R}^D$

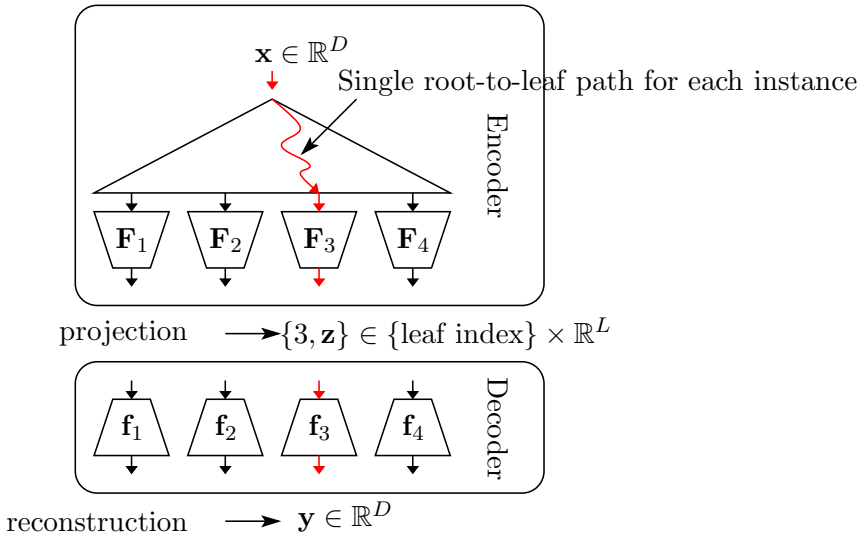
Tree autoencoder



Tree autoencoder



Tree autoencoder



Training

- Objective function:

$$E(\boldsymbol{\Theta}) = \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{T}(\mathbf{x}_n; \boldsymbol{\Theta})\|_2^2 + \lambda \sum_{i \in \text{decision nodes}} \|\mathbf{w}_i\|_1$$

- Since the problem is non-differentiable, gradient descent methods are not applicable
- We use Tree Alternating Optimization

Advantages

- It optimizes a clear objective function – reconstruction error
- It does not require a neighborhood graph
  - Unlike t-SNE or UMAP, which is very costly
- It does not increase distances
  - Distances are preserved or reduced, not artificially increased
- It is highly interpretable
- It has out-of-sample mapping
- It is efficient during inference
  - Logarithmic in the number of leaves
- It is linear in the number of instances.
  - The approximate cost is $\Theta(ND^2)$ for shallow trees and $\mathcal{O}(ND)$ for deep trees

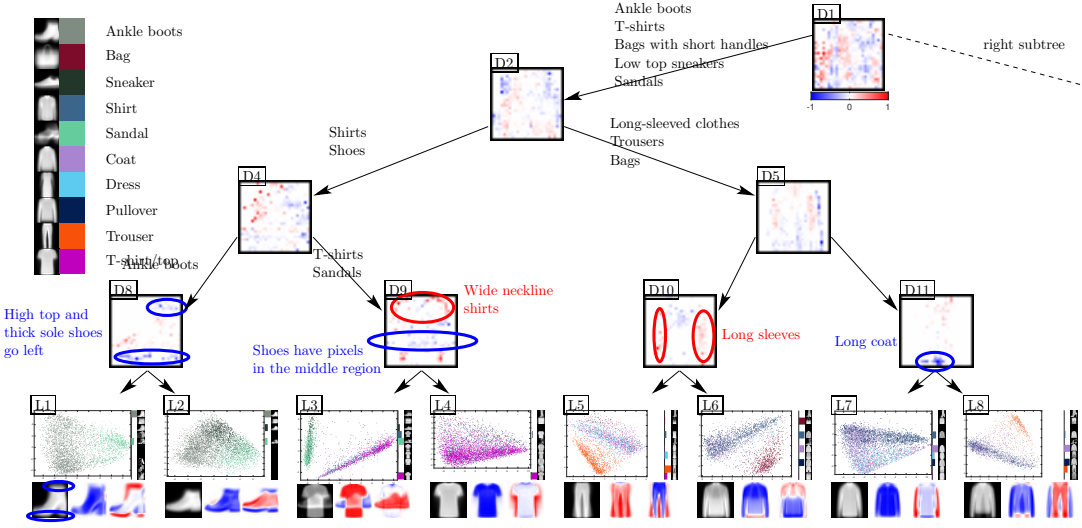
Disadvantages

- It needs access to the explicit feature vectors, unlike graph-based methods, which need instead pairwise affinities.
- The optimization converges to a local optimum, which depends on the initialization
- As with any DR method, PCA trees reveal only some structure, so practitioners should try multiple, complementary methods

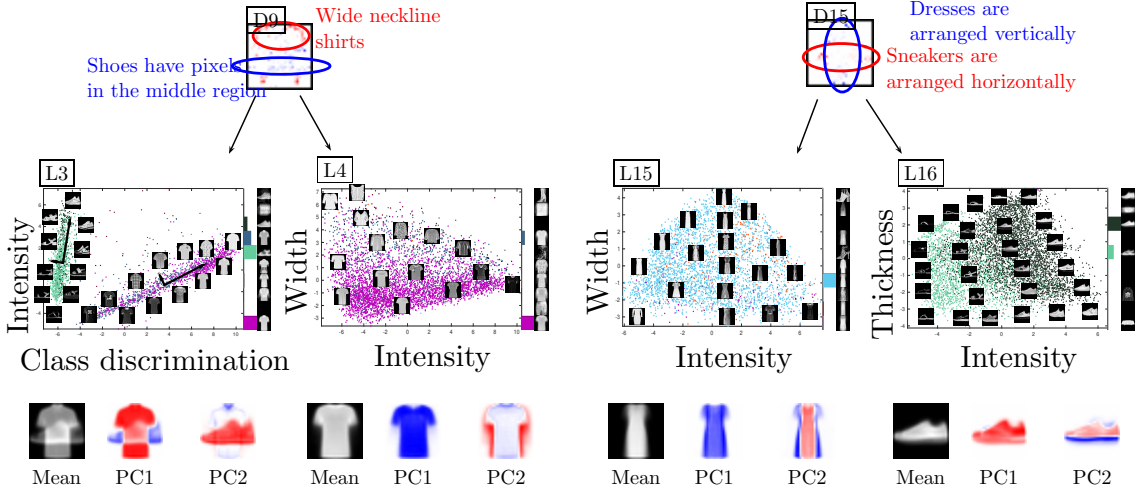
Fashion MNIST

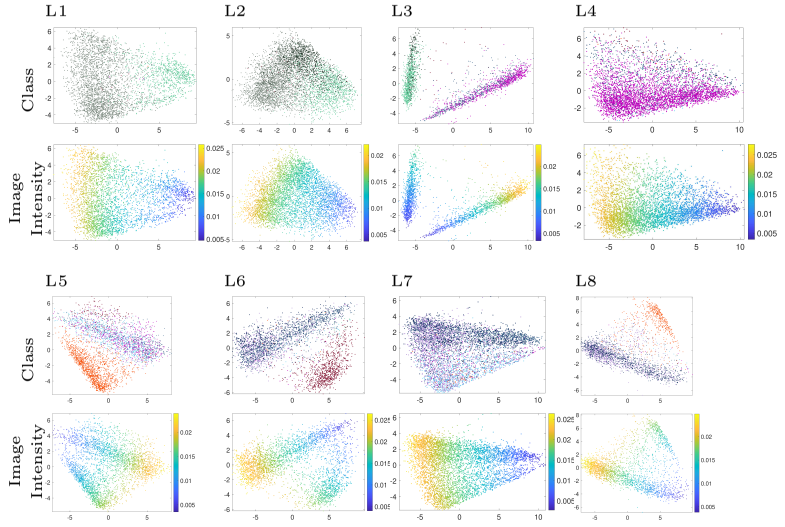
The dataset consists of $60,000$ grayscale images of size 28×28 pixels, organized into 10 classes. Below is an example, where each column corresponds to a different class.

PCA tree in action

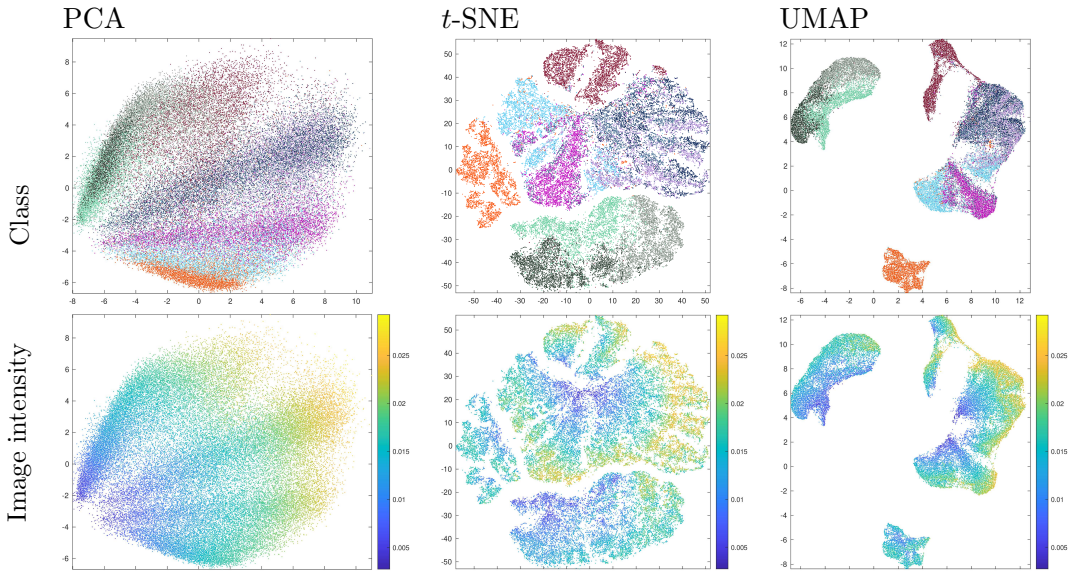


PCA tree in action




L1
L2
L3
L4
L5
L6
L7
L8
Class
Image Intensity

Well established algorithms



Can we trust t-SNE or UMAP?