annotated version

Machine Learning Course - CS-433

Unsupervised Learning

Nov 19, 2020

changes by Martin Jaggi 2020, 2019, changes by Rüdiger Urbanke 2018, changes by Martin Jaggi 2016, 2017 ©Mohammad Emtiyaz Khan 2015

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EPFL

Unsupervised learning

How can systems learn when there are no labels available? How to learn a meaningful internal representation for data examples? I.e., to represent them in a way that reflects the semantic structure of the overall collection of input patterns? This question is the central focus of unsupervised learning.

In unsupervised learning, our data consists only of features (or inputs) $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$, vectors in $\mathbb{R}^D$, and there are **no outputs** y_n available.

Unsupervised learning seems to play an important role in how living beings learn. Variants of it seem to be more common in the brain than supervised learning.

Two main directions in unsupervised learning are

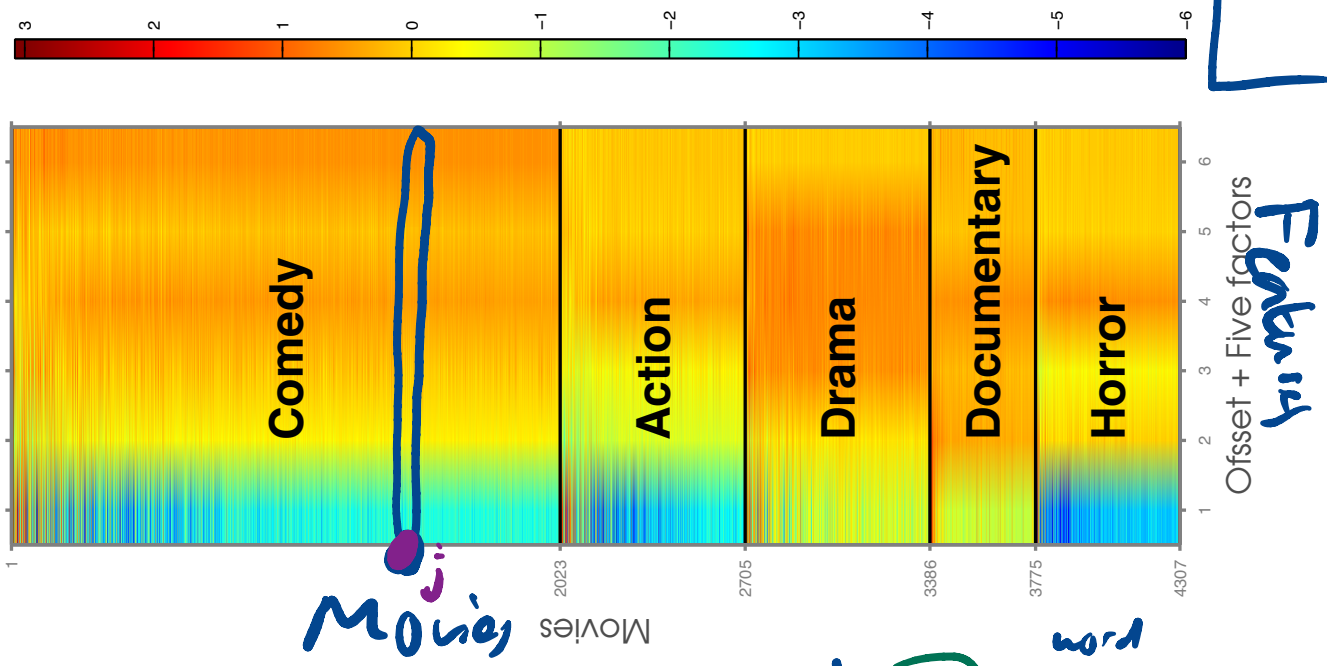
- representation learning and
- density estimation & generative models

Examples

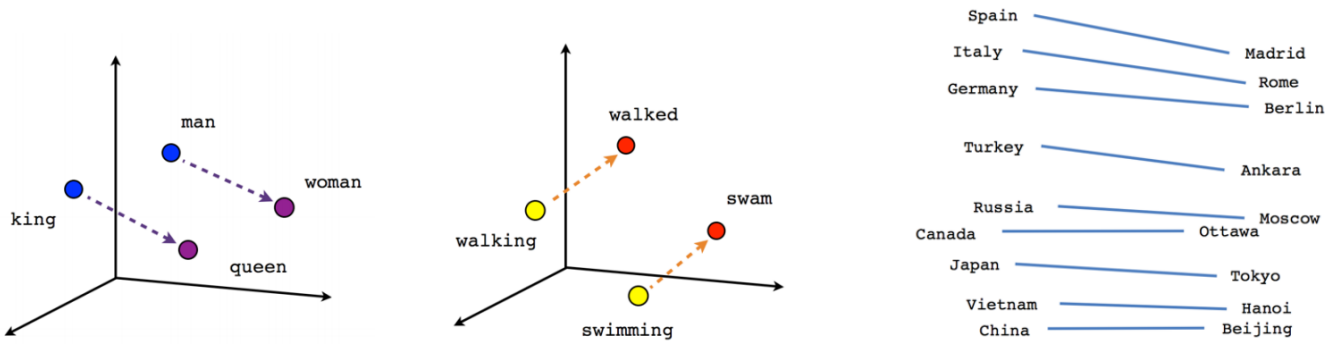
Examples for Representation Learning

Rec. Sys.

Given ratings of movies and viewers, we use matrix factorization to extract useful features (see e.g. Netflix Prize).



Learning word-representations using matrix-factorizations, `word2vec` (Mikolov et al. 2013).



Male-Female | Verb tense | Country-Capital

Given voting patterns of regions across Switzerland, we use PCA to extract useful features (Etter et al. 2014).

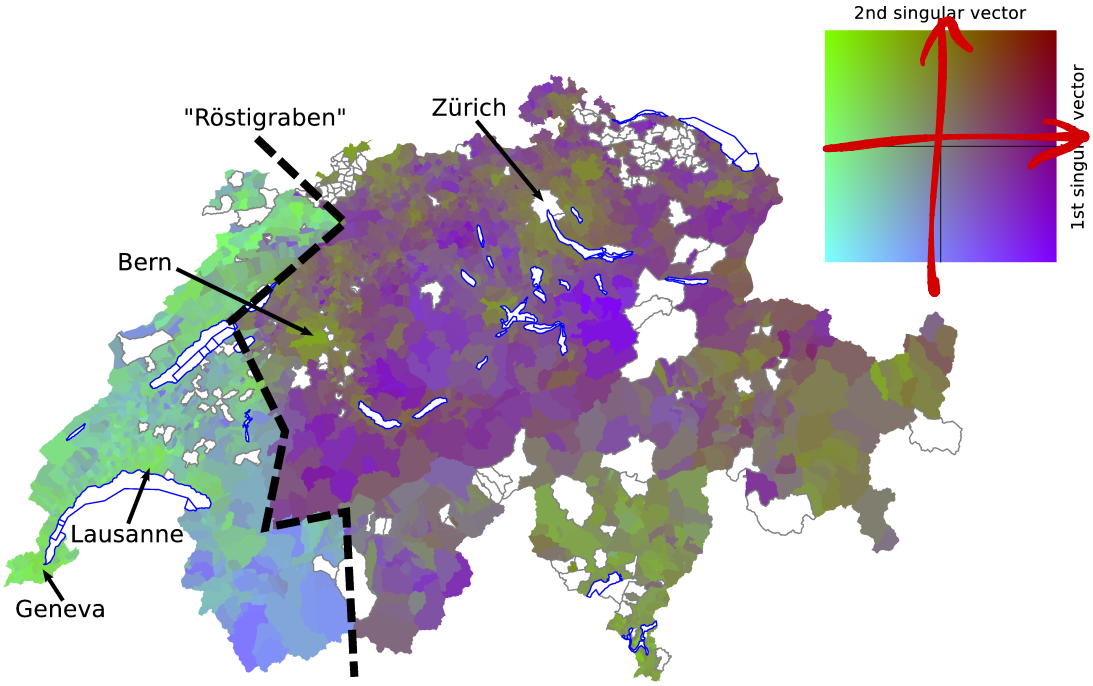
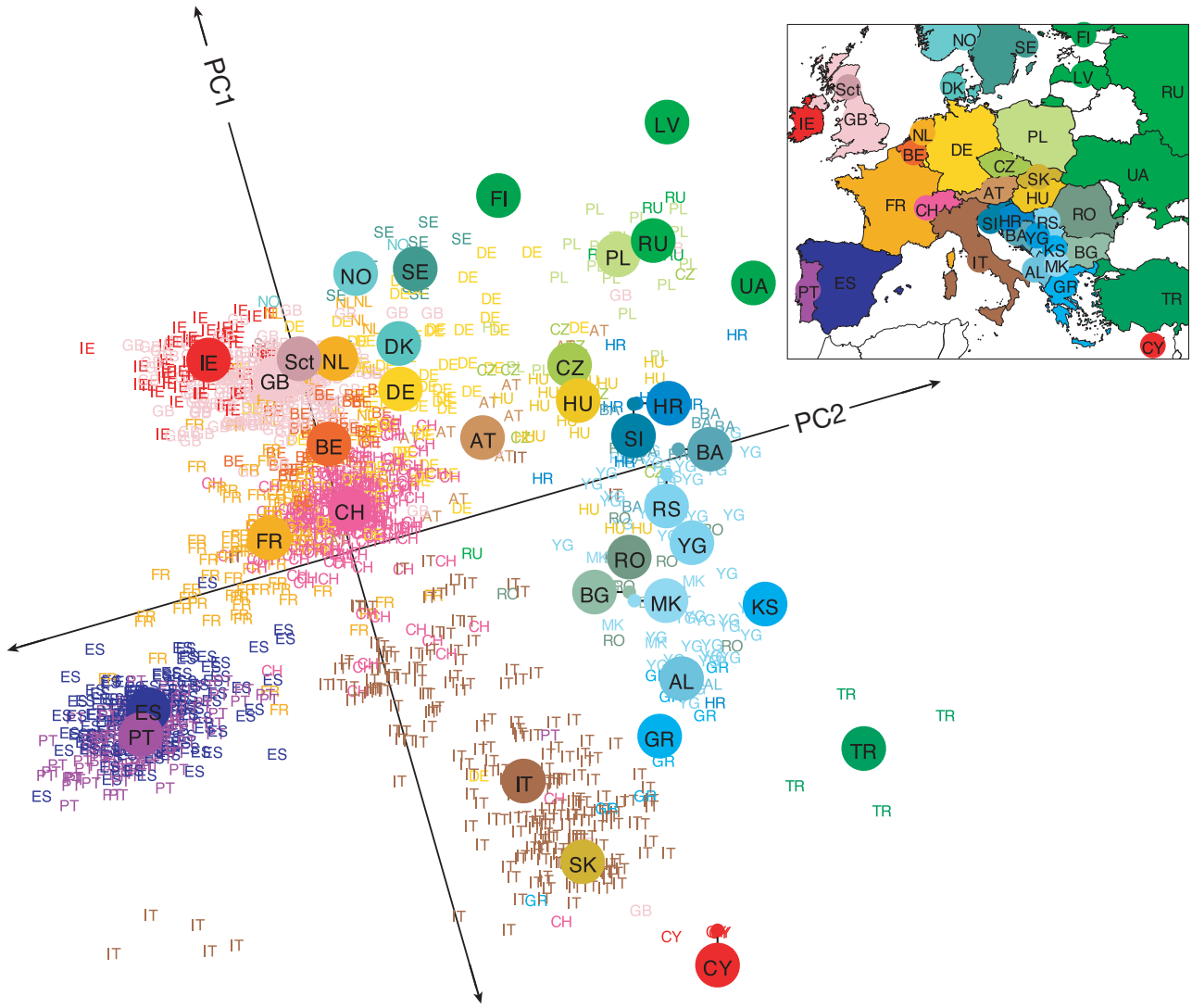


Figure 9: Voting patterns of Swiss municipalities. The color of a municipality is assigned using its location in Figure 8 and the color gradient shown in the upper right corner. Two municipalities with similar colors have similar voting patterns. The *Röstigraben*, corresponding to the cultural difference between French-speaking municipalities and German-speaking ones, is clearly visible from the difference in voting patterns. Regions shown in white are lakes or municipalities for which some vote results are missing (due to a merging of municipalities, for example). A more detailed map can be found online [2].

PCA Example 2: Genes mirror geography



Nature 2008, http://dx.doi.org/10.1038/nature07331

Examples for Clustering

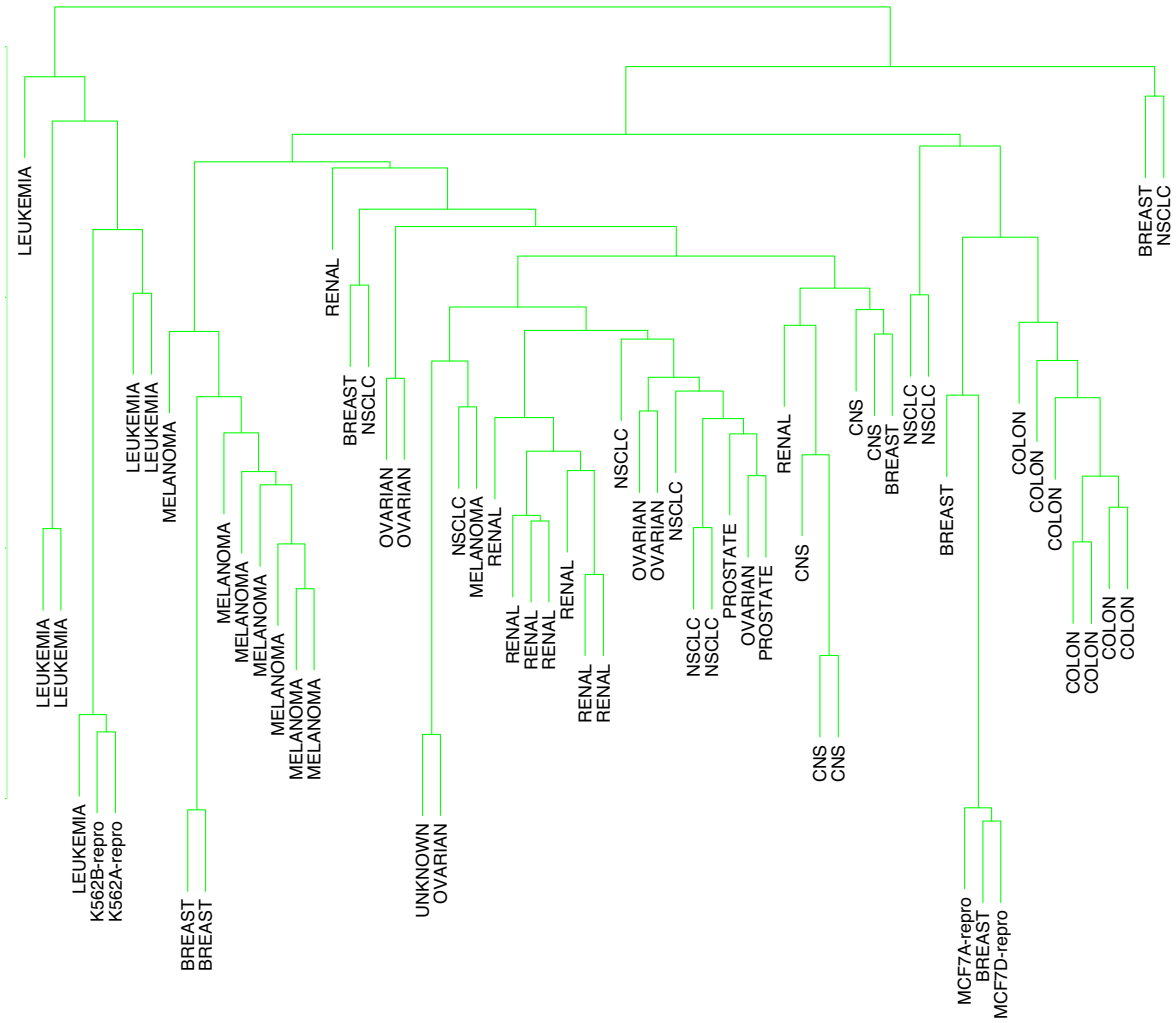
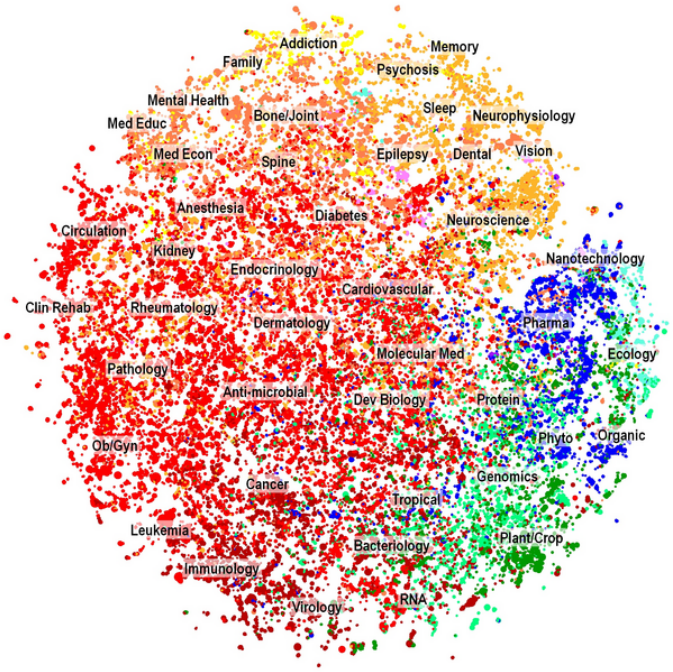


FIGURE 14.12. *Dendrogram from agglomerative hierarchical clustering with average linkage to the human tumor microarray data.*

Clustering more than two million biomedical publications (Kevin Boyack et.al. 2011)



Clustering articles published in Science (Blei & Lafferty 2007)

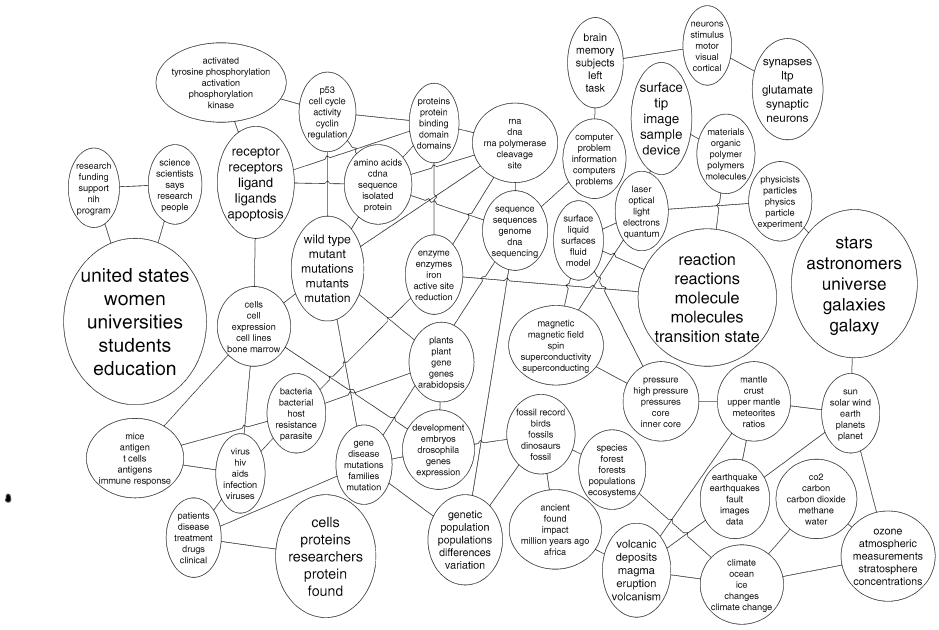


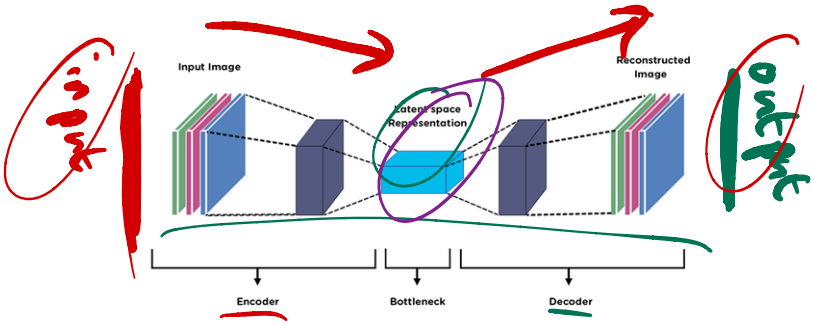
FIG. 2. *A portion of the topic graph learned from* 16,351 *OCR articles from Science* (1990–1999). *Each topic node is labeled with its five most probable phrases and has font proportional to its popularity in the corpus.* (*Phrases are found by permutation test.*) *The full model can be found in http://www.cs.cmu.edu/~lemur/science/ and on STATLIB.*

Unsupervised Representation Learning & Generation

How does it work?

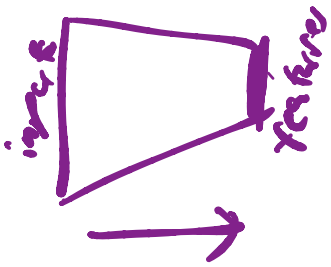
Define a unsupervised or self-supervised loss function, for

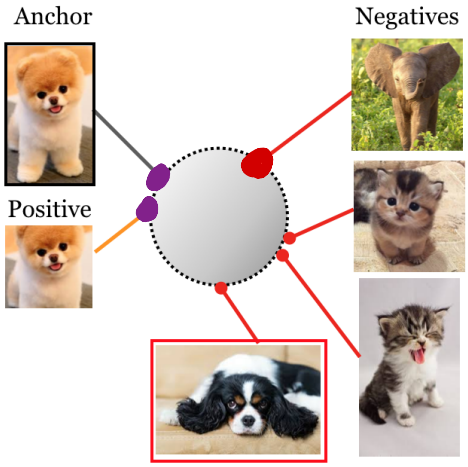
- Compression & Reconstruction
  (e.g. Auto-Encoder)



. image: Deepak Birla

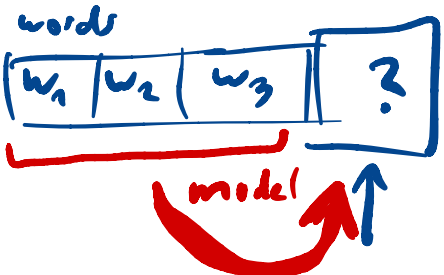
- Consistency & Contrastive Learning
  (e.g. Noise-contrastive estimation)





. image: arxiv.org/pdf/2004.11362

- Generation
  (e.g. Auto-Encoder, Gaussian Mixture Model)



Language model

Examples:

(G = can be used as a generative model)

- Auto-Encoders (G)
  Invertible networks, learned compression, normalizing flows

- Image Representation Learning
  combining unsupervised representation learning (pre-training) with supervised learning

- Language models & sequential data GPT-3
  text generation (G), or sequence continuation (G), BERT (G)
  video, audio & timeseries (auto-regressive, contrastive or G)

- Generative Adversarial Networks (GAN) (G)
  see also *predictability minimization*

"Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Network", ICLR 2016, https://arxiv.org/abs/1511.06434