Machine Learning Course - CS-433

Unsupervised Learning

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ÉCOLE POLYTECHNIQUE
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Unsupervised learning

So far we have assumed that we are given a training set of the form $S_{\text{train}} = \{(\mathbf{x}, y_n)\}_{n=1}^N$ and we are then asked to predict the label y associated to any new feature vector $\mathbf{w}$. This is called *supervised* learning since we are given examples of features *and* labels and are asked to learn from this.
There is a second very important framework in ML called *unsupervised* learning. Here the training set consists exclusively of feature vectors, i.e., $S_{\text{train}} = \{(\mathbf{x})\}_{n=1}^N$. We are asked to learn from the set of features alone without having access to training labels. Unsupervised learning seems to play an important role in how living beings learn.
How can systems learn meaningful information given just the feature vectors?
Two main directions in unsupervised learning are

- representation learning & feature learning and
- density estimation & generative models

These concepts are best explained by means of explicit examples. We will discuss many of these concepts in much more detail later. The idea of this lecture is to take a bird's eye view and to quickly survey some of the existing techniques. This is similar to the overview that we did before talking about specific classification schemes.

Representation Learning & Feature Learning

In feature learning the task is to automatically learn the most important features given a data set. Below is a list of techniques that belong into this category.

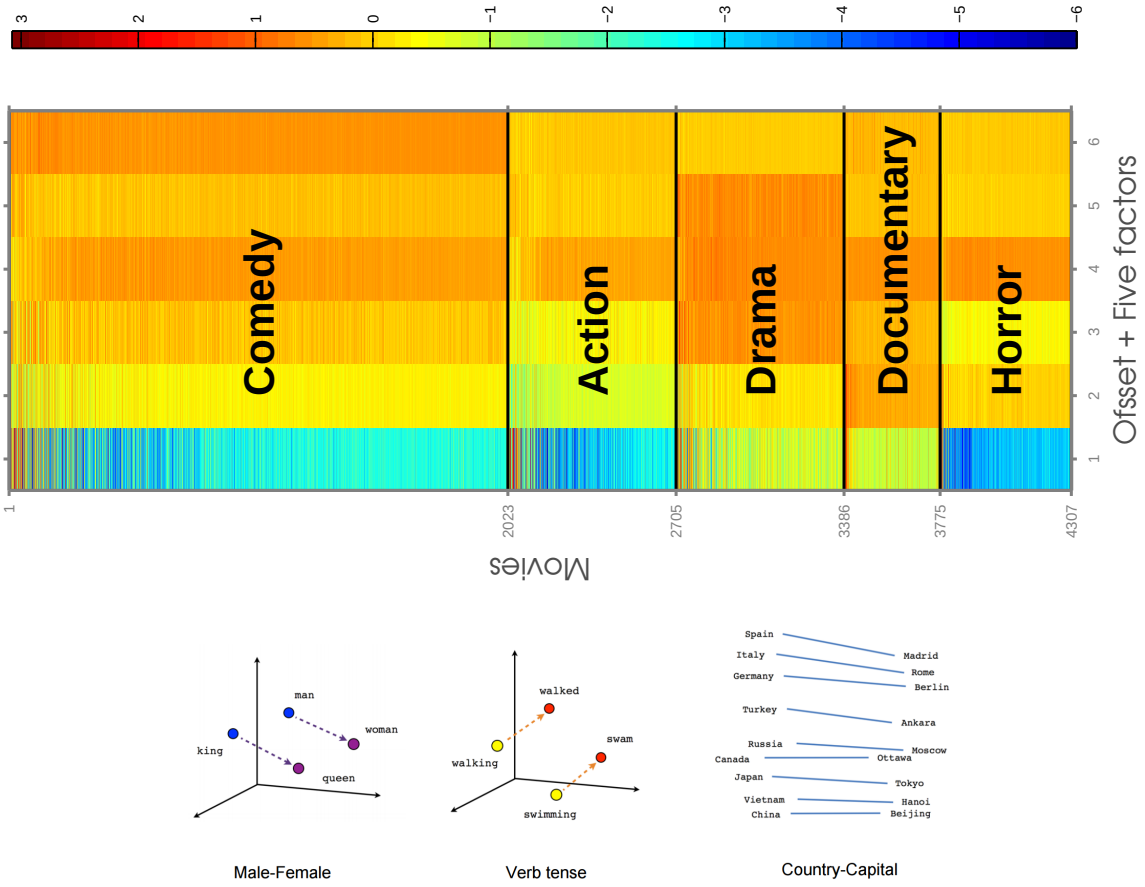
1. **Matrix Factorization:** Matrix factorization can be used both in a supervised fashion as well as an unsupervised fashion. We give one example for each case.

   a) This is an application of matrix factorization in the supervised case. Assume that we are given ratings of movies by viewers. This can be conveniently represented in matrix form, where movies are lets say represented by columns and users by rows. In each row we write the rating (lets say a number between 1 to 5).

   Assume now that we can factorize the matrix reasonably well by a one-dimensional matrix, i.e., an outer product of two vectors. Then implicitly this extracts useful features both for the users and also the movies. E.g., it might implicitly group the movies by "genres" and the users by "types".

   Of course, we can get better approximations by looking at matrix factorizations with higher rank.

   b) **word2vec** A particularly impressive example is `word2vec` (Mikolov et al. 2013). Learning word-representations using matrix-factorizations.



2. **PCA:** The features are typically vectors in $\mathbb{R}^d$ for some d. Assume that we can only keep one number per feature vector. What is the direction onto which we should project our input vectors so that the projected data preserves as much about the original input as possible? One way to formulate this is to ask that the variance of the projected data is as large as possible. We can ask the same question when we are allowed to keep two or more numbers per feature vectors. This view point will lead us to discuss what is called the principal component analysis.

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

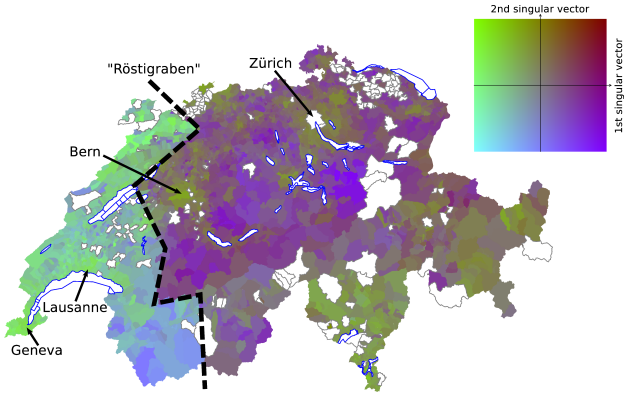
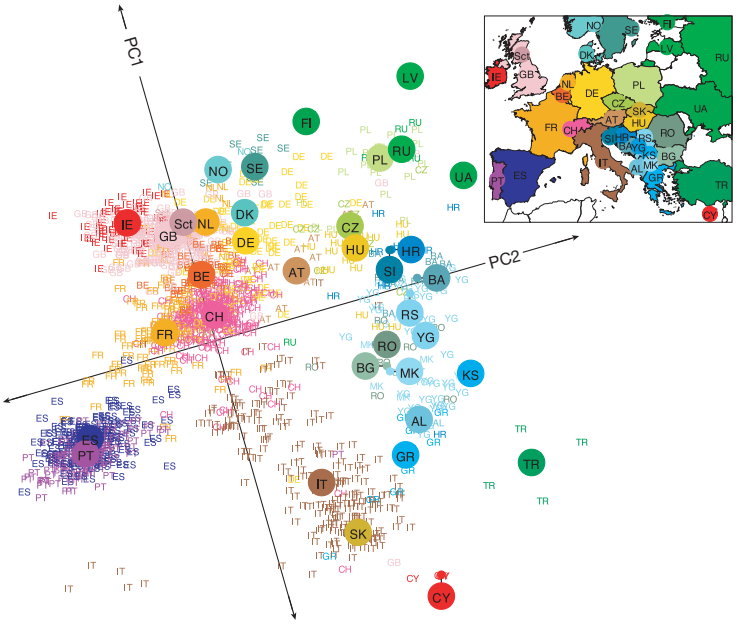


Figure 9: Voting patterns of Swiss municipalities. The color of a municipality is assigned using its location in Figure 8 and the color gradient shown in the upper right corner. Two municipalities with similar colors have similar voting patterns. The *Röstigraben*, corresponding to the cultural difference 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].

b) Genes mirror geography within Europe.



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

3. **Clustering:** One way to reveal structure in the input data is cluster the feature points given some similarity measure between inputs (e.g., like Euclidean distance). Besides the choice of similarity measure we also have a choice of how many clusters we want to create and in addition we can also do this hierarchically.

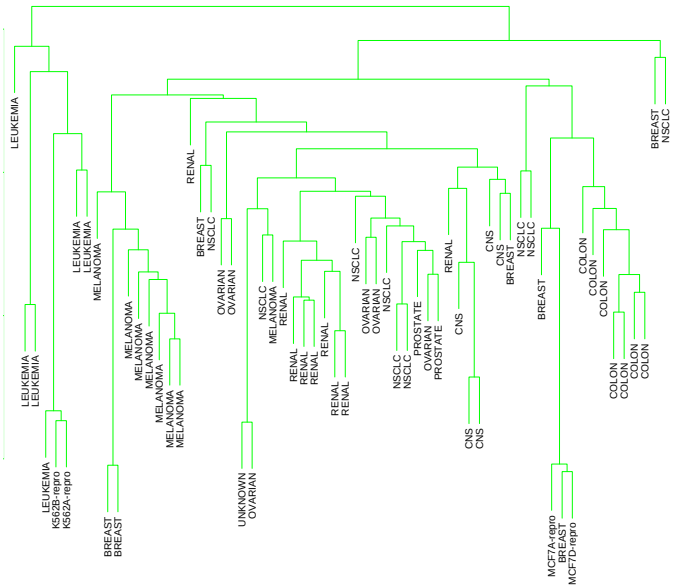


FIGURE 14.12. *Dendrogram from agglomerative hierarchical clustering with average linkage to the human tumor microarray data.*

a)

b) **Clustering:**

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

d) **Clustering:** Clustering articles published in Science (Blei & Lafferty 2007)

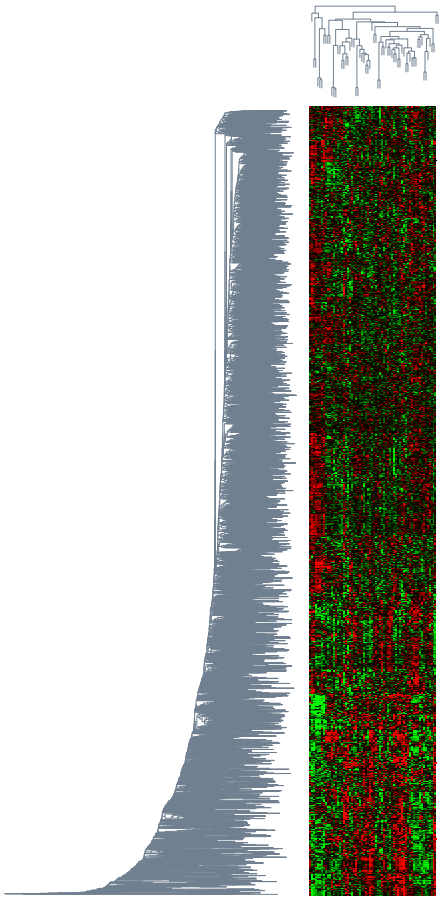
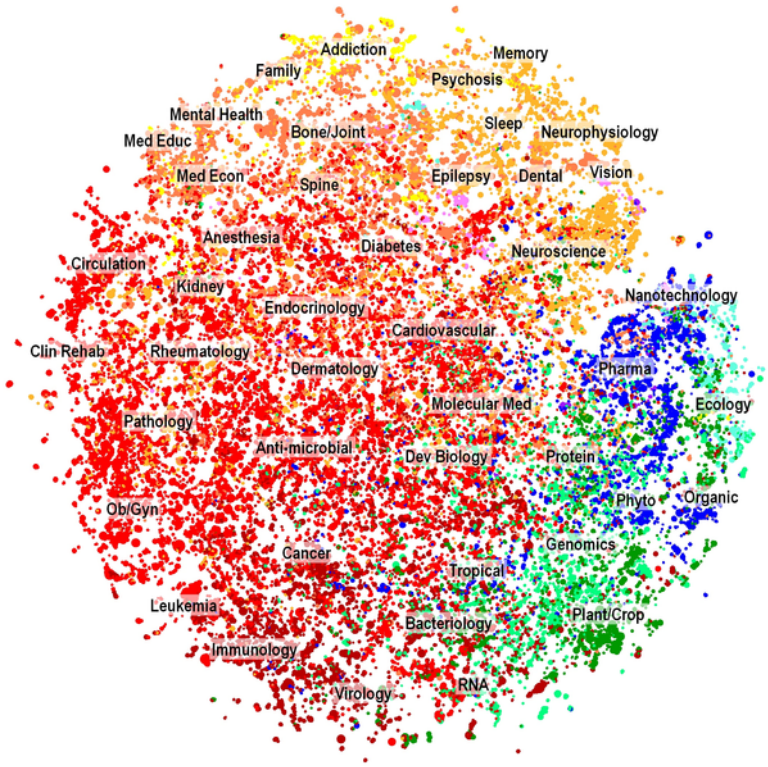


FIGURE 14.14. *DNA microarray data: average linkage hierarchical clustering has been applied independently to the rows (genes) and columns (samples), de-*



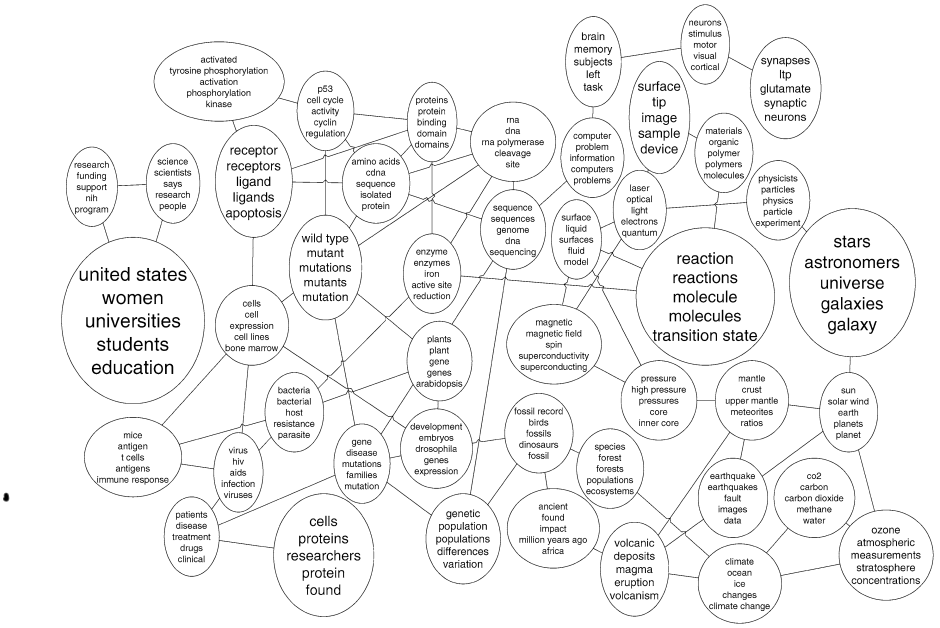


FIG. 2. *A portion of the topic graph learned from* 16,351 *OCR articles from Science* (1990–1999). *Each topic node is labeled with its five most probable phrases and has font proportional to its popularity in the corpus. (Phrases are found by permutation test.) The full model can be found in http://www.cs.cmu.edu/~lemur/science/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

Generative Models: In supervised learning, a generative model, given some data set $S_{\text{train}} = \{(\mathbf{x}_n, y_n)\}$, is a model for the joint distribution of $\mathbf{x}$ and y. But of course, we can also model just the distribution of $\mathbf{x}$.

1. Auto-Encoders: Auto-encoders were invented in the framework of neural nets. But the basic idea can also be applied in other areas. Auto-encoders are a form of a compression algorithm. And we can think of them as a generative model but we can also think of them as a feature learning algorithm.

   Assume that we have a function $f_{\mathbf{w}}$ parametrized by $\mathbf{w}$ that maps a given feature vector $\mathbf{x}$ to a much "smaller" feature vector $\tilde{\mathbf{x}}$ and in addition a second function $g_{\mathbf{w}'}$ that acts like an *inverse map* in the sense that for our given data $(\mathbf{x} - g_{\mathbf{w}'}(f_{\mathbf{w}}(\mathbf{x}))^2$ is small in average.

   Assume at first that there is no error. Then $\tilde{\mathbf{x}}$ is as

useful for a ML task as $\mathbf{x}$ since afterall we can always recover $\mathbf{x}$ from $\tilde{\mathbf{w}}$ by applying the map $g_{\mathbf{w}'}$. But by assumption $\tilde{\mathbf{x}}$ is small. In this sense we have extracted from the original feature vector a smaller feature vector that is as good as the original one irrespective of the task to be learned – we have performed featue selection. Of course, in any real application we will have a small error between $\tilde{\mathbf{w}}$ and its reconstruction $g_{\mathbf{w}'}(\tilde{\mathbf{x}})$. But if this error is small then we can hope not to have lost any essential information. The advantage of this approach is that often we have lots of unlabeled data but only very little labeled data. So we can first apply this approach for the feature selection and then run the learning algorithm on the small feature set.

We can also think of this as a generative model for $\mathbf{x}$. If we truly compressed $\mathbf{x}$ then $\tilde{xv}$ should follow a simple distribution (e.g., if $\tilde{\mathbf{w}}$ is a vector of bits, then it should follow an iid distribution with uniform bits. Otherwise we could compress further.

The above description has be be viewed with some grain of salt. If the vectors $\mathbf{x}$ and $\tilde{\mathbf{x}}$ take on real values then the notion of "compression" is not so clear. But the above explanation still gives a good intuition why autoencoders are useful.

2. Generative Adversarial Networks (GANs)
   GAN's are a fairly recent invention, also again in the framework of neural nets. The idea is to use two neural nets, one that tries to generate samples $\mathbf{x}$ that look like

the data we get, the other one that tries to distinguish real samples from artificially generated samples. These two networks are training alternatively. The aim is so that after sufficient training even a good classifier cannot distinguish real samples from artificially generated ones. If we can achieve this, then this means that we have built a good model for the set of feature vectors we were given.

If we apply this e.g. to photos of rooms, we can then generate many artificial rooms that might even fool a human observer.

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