A Practical Introduction to Machine Learning in Python Day 3 - Wednesday »Unsupervised Machine Learning«

Rupert Kiddle Marieke van Hoof

r.t.kiddle@vu.nl m.vanhoof@uva.nl

September 16, 2024

Today

Automated Content Analysis

Types of Automated Content Analysis

Finding similar variables

An introduction to dimensionality reduction

Principal Component Analysis and Singular Value Decomposition

Finding similar cases

k-means clustering

Hierarchical clustering

Important notes

Automated Content Analysis

Recap: Types of Automated Content Analysis

Automated Content Analysis

Top-down vs. bottom-up

	Methodological approach		
	Counting and Dictionary	Supervised Machine Learning	Unsupervised Machine Learning
Typical research interests and content features	visibility analysis sentiment analysis subjectivity analysis	frames topics gender bias	frames topics
Common statistical procedures	string comparisons counting	support vector machines naive Bayes	principal component analysis cluster analysis latent dirichlet allocation semantic network analysis
	deductive		inductive

Methodological approach

	Counting and Dictionary	Supervised Machine Learning	Unsupervised Machine Learning
Typical research interests and content features	visibility analysis sentiment analysis subjectivity analysis	frames topics gender bias	frames topics
Common statistical procedures	string comparisons counting	ns support vector machines principal component ar naive Bayes cluster analysis latent dirichlet allocatio semantic network analy	
	deductive		inductive

Boumans and Trilling, 2016

The same logic applies to non-textual data

Methodological approach

	Counting and Dictionary	Supervised Machine Learning	Unsupervised Machine Learning
Typical research interests and content features	visibility analysis sentiment analysis subjectivity analysis	frames topics gender bias	frames topics
Common statistical procedures	string comparisons counting	support vector machines naive Bayes	principal component analysis cluster analysis latent dirichlet allocation semantic network analysis
	deductive		inductive

Boumans and Trilling, 2016

The same logic applies to non-textual data!

Automated Content Analysis

0000000000000

Supervised machine learning You have a dataset with both

predictor and outcome (independent and dependent variables; features and labels)
— a labeled dataset. Think of regression: You measured x1, x2, x3 and you want to predict y, which you

Unsupervised machine learning

You have no labels. (You did not measure y)

You might already be familiar with some techniques to figure out whether x1, x2,...x_i co-occur

- Principal Component Analysis (PCA) and Singular Value Decomposition (SVD)
- Cluster analysis
- Topic modelling (Non-negative matrix factorization and Latent Dividuet Allocation)

Automated Content Analysis

000000000000

Supervised machine learning

You have a dataset with both predictor and outcome (independent and dependent variables; features and labels) — a labeled dataset. Think of regression: You measured x1, x2, x3 and you want to predict y, which you also measured

Unsupervised machine learning

measure y)
You might already be familiar with some techniques to figure out

- Principal Component Analysis (PCA) and Singular Value Decomposition (SVD)
- Topic modelling (Non-negative matrix factorization and Latent

Supervised machine learning

You have a dataset with both predictor and outcome (independent and dependent variables; features and labels) — a labeled dataset. Think of

Unsupervised machine learning

Finding similar cases

You have no labels. (You did not

- Principal Component Analysis
- Topic modelling (Non-negative

Supervised machine learning

You have a dataset with both predictor and outcome (independent and dependent variables; features and labels) — a labeled dataset. Think of

Unsupervised machine learning

You have no labels. (You did not measure y)

- Principal Component Analysis
- Topic modelling (Non-negative

Automated Content Analysis

0000000000000

Unsupervised machine learning

You have no labels. (You did not

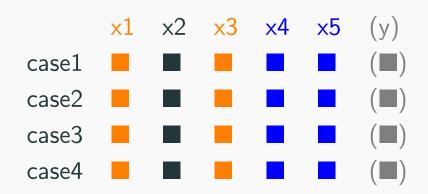
You might already be familiar with some techniques to figure out whether x1, x2,...x_i co-occur

- Principal Component Analysis (PCA) and Singular Value Decomposition (SVD)
- Cluster analysis
- Topic modelling (Non-negative matrix factorization and Latent Dirichlet Allocation)

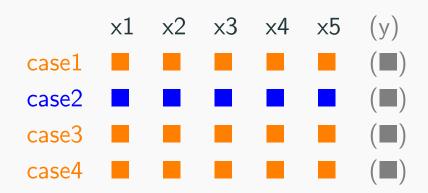
Let's distinguish four use cases...

- 1. Finding similar variables (dimensionality reduction) unsupervised
- 2. Finding similar cases (clustering) unsupervised
- 3. Predicting a continous variable (regression) supervised
- 4. Predicting group membership (classification) supervised

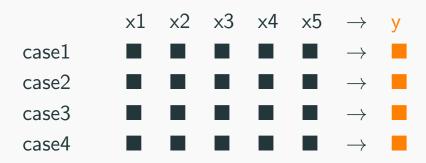
	x1	x2	x3	x4	x5	У
case1						
case2						
case3						
case4						



Dimensionality reduction: finding similar variables (features)



Clustering: finding similar cases



new case lacksquare lacksquare

Regression and classification: learn how to predict y.

Note, again, that the \blacksquare signs can be *anything*. For us, often word counts or $tf \cdot idf$ scores (x) and, for supervised approaches, a topic, a sentiment, or similar (y).

But it could also be pixel colors or clicks on links or anything else.

	×1	x2	x3	×4	x5	У
case1						
case2						
case3						
case4						

A lot of applications and use cases, ...

- ... but we'll distinguish two today:
 - 1. Finding similar variables (dimension reduction)
 - 2. Finding similar cases (clustering)

A lot of applications and use cases, ...

- ... but we'll distinguish two today:
 - 1. Finding similar variables (dimension reduction)
 - 2. Finding similar cases (clustering)

Are we more interested in which features "belong together" or which cases "belong together"?

There are many other techniques than those presented today, and vice versa, those presented today can also be used for other purposes

Finding similar variables

Finding similar variables

An introduction to dimensionality

reduction

Finding similar variables	
An introduction to dimensionality reduction	

Dimensionality reduction

dimensionality = the number of features we have

- (1) Explorative data analysis and visualization
 - No good way to visualize 10,000 dimensions (or even 4)

- We need more training cases to increase the likelihood that the

Dimensionality reduction

dimensionality = the number of features we have

- (1) Explorative data analysis and visualization
 - No good way to visualize 10,000 dimensions (or even 4)
- (2) The curse of dimensionality

More features means more data (good!), but:

- Too many features can lead to unfeasible computation times
- We need more training cases to increase the likelihood that the possible combinations actually occur

Dimensionality reduction

First approach: feature selection

Only choose the features that are really relevant

Example: Exclude all terms that occur in more than 50% of the documents, or in less than n = 5 documents:

```
vec = CountVectorizer(max df=0.5, min df=5)
```

https://scikit-learn.org/stable/modules/generated/sklearn.feature extraction.text.CountVectorizer.html

Dimensionality reduction

Second approach: feature extraction

- Create a smaller set of features
- ullet E.g.: 1,000 features o PCA to reduce to 50 components oSML with these 50 component scores as features

Dimensionality reduction

So, we can use unsupervised ML as a dimension reduction step in a supervised ML pipeline. But it can also be a goal in itself, to

understand the data better or to visualize them.

Finding similar variables

Principal Component Analysis and Singular Value Decomposition

Finding similar variables

Principal Component Analysis (PCA) and Singular Value

Decomposition (SVD)

- related to and often confused with Factor Analysis (same menu item in SPSS – many people who believe they run FA actually run PCA!)
- Components are ordered (first explains most variance)
- Components do not necessarily carry a meaningful interpretation

Preparation: Import modules and get some texts

```
from sklearn import datasets
1
    from sklearn.decomposition import PCA
    from sklearn.decomposition import TruncatedSVD
    from sklearn.feature_extraction.text import CountVectorizer
    from sklearn.pipeline import make_pipeline
6
    from sklearn.preprocessing import FunctionTransformer
    import matplotlib.pyplot as plt
7
8
    autotexts = datasets.fetch_20newsgroups('rec.autos', remove=('headers',
         'footers', 'quotes'), subset='train')['data']
    religiontexts = datasets.fetch_20newsgroups('soc.religion.christian',
10
        remove=('headers', 'footers', 'quotes'), subset='train')['data']
11
    texts = autotexts[:20] + religiontexts[:20]
12
```

Running PCA

PCA does not accept a *sparse matrix* as input (but the CountVectorizer gives one as output), so we need to transform it into a *dense matrix*.

```
myvec = CountVectorizer(max_df=.5, min_df=5)
mypca = PCA(n_components=2)

mypipe = make_pipeline(myvec, FunctionTransformer(lambda x:
np.asarray(x.todense()), accept_sparse=True), mypca)

r = mypipe.fit_transform(texts)
```

Singular value decomposition

The need to use a dense matrix is *really* a problem for large feature sets (which we have in NLP).

Singular value decomposition

The need to use a dense matrix is *really* a problem for large feature sets (which we have in NLP).

We therefore can better use SVD, which is essentially* the same and very simple to use:

```
mysvd = TruncatedSVD(n_components=2)
mypipe = make_pipeline(myvec, mysvd)
r = mypipe.fit_transform(texts)
```

```
(In this specific case, we even get exactly the same plot...)
```

* It's mathematically different, but SVD is even used "under the hood" by several PCA modules to solve PCA problems.

More info and background: https:

//towardsdatascience.com/pca-and-svd-explained-with-numpy-5d13b0d2a4d8

Finding similar cases	
k-means clustering	

Grouping features vs grouping cases

Let's consider a corpus of several thousand user comments.

We could use SVD, MDS, or similar techniques to

- figure out relationships between features
- see which features stand out.
- get a first sense what topics are in the corpus.

Grouping features vs grouping cases

Let's consider a corpus of several thousand user comments.

We could use SVD, MDS, or similar techniques to

- figure out relationships between features
- see which features stand out.
- get a first sense what topics are in the corpus.

- We do not learn anything about which texts (cases) belong to which topic
- We could use the component scores returned by

Grouping features vs grouping cases

Let's consider a corpus of several thousand user comments.

We could use SVD, MDS, or similar techniques to

- figure out relationships between features
- see which features stand out.
- get a first sense what topics are in the corpus.

- We do not learn anything about which texts (cases) belong to which topic
- We could use the component scores returned by .fit_transform() to then group our cases

Grouping features vs grouping cases

Let's consider a corpus of several thousand user comments.

We could use SVD, MDS, or similar techniques to

- figure out relationships between features
- see which features stand out.
- get a first sense what topics are in the corpus.

- We do not learn anything about which texts (cases) belong to which topic
- We could use the component scores returned by .fit_transform() to then group our cases

Grouping features vs grouping cases

Let's consider a corpus of several thousand user comments.

We could use SVD, MDS, or similar techniques to

- figure out relationships between features
- see which features stand out.
- get a first sense what topics are in the corpus.

- We do not learn anything about which texts (cases) belong to which topic
- We could use the component scores returned by .fit_transform() to then group our cases
- ⇒ Alternative: Choose the opposite approach and first find out which cases are most similar, then describe what features characterize each group of cases

- Goal: group cases into k clusters
- k is set in advance
- Algorithm to determine k centroids (points in the middle of
- non-deterministic: starts with a randomly choosen centroids
- Cheap to compute: works even with large number of cases
- We can run PCA first to reduce the number of features if we

- Goal: group cases into k clusters
- k is set in advance
- Algorithm to determine k centroids (points in the middle of
- non-deterministic: starts with a randomly choosen centroids
- Cheap to compute: works even with large number of cases
- We can run PCA first to reduce the number of features if we

- Goal: group cases into k clusters
- k is set in advance
- Algorithm to determine k centroids (points in the middle of the cases that belong to it) such that the distances between the cases and their centroids are minimized
- non-deterministic: starts with a randomly choosen centroids
- Cheap to compute: works even with large number of cases
- We can run PCA first to reduce the number of features if we

- Goal: group cases into k clusters
- k is set in advance
- Algorithm to determine k centroids (points in the middle of the cases that belong to it) such that the distances between the cases and their centroids are minimized
- non-deterministic: starts with a randomly choosen centroids (there are other versions)
- Cheap to compute: works even with large number of cases
- We can run PCA first to reduce the number of features if we

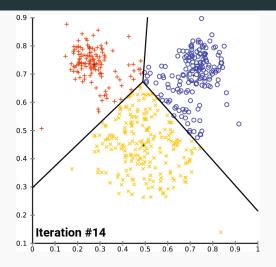
- Goal: group cases into k clusters
- k is set in advance
- Algorithm to determine k centroids (points in the middle of the cases that belong to it) such that the distances between the cases and their centroids are minimized
- non-deterministic: starts with a randomly choosen centroids (there are other versions)
- Cheap to compute: works even with large number of cases
- We can run PCA first to reduce the number of features if we

k-means clustering

Automated Content Analysis

- Goal: group cases into k clusters
- k is set in advance
- Algorithm to determine k centroids (points in the middle of the cases that belong to it) such that the distances between the cases and their centroids are minimized
- non-deterministic: starts with a randomly choosen centroids (there are other versions)
- Cheap to compute: works even with large number of cases
- We can run PCA first to reduce the number of features if we want/need to

k-means clustering



https://upload.wikimedia.org/wikipedia/commons/e/ea/K-means convergence.gif

Notice the big symbols indicating the centroids.

```
from sklearn.feature_extraction.text import TfidfVectorizer
from sklearn.cluster import KMeans

k = 5

texts = ['text1 ejkh ek ekh', 'ekyerykel'] # a list of texts

vec = TfidfVectorizer(min_df=5, max_df=.4)
features = vec.fit_transform(texts)
km = KMeans(n_clusters=k, init='k-means++', max_iter=100, n_init=1)
predictions = km.fit_predict(features)
```

That's it!

- predictions is a list of integers indicated the predicted cluster number. We can thus use zip(predictions, texts) to put them together.
- We could also use .fit() and .transform() sperately and use our km to predict clusters for additional cases we have no used to train the model

```
from sklearn.feature_extraction.text import TfidfVectorizer
from sklearn.cluster import KMeans

k = 5

texts = ['text1 ejkh ek ekh', 'ekyerykel'] # a list of texts

vec = TfidfVectorizer(min_df=5, max_df=.4)
features = vec.fit_transform(texts)
km = KMeans(n_clusters=k, init='k-means++', max_iter=100, n_init=1)
predictions = km.fit_predict(features)
```

That's it!

- predictions is a list of integers indicated the predicted cluster number. We can thus use zip(predictions, texts) to put them together.
- We could also use .fit() and .transform() sperately and use our km to predict clusters for additional cases we have not used to train the model

Finding the optimal k

- The only way to find k is to estimate multiple models with different ks
- No single best solution; finding a balance between error within clusters (distances from centroid) and low number of clusters.
- An elbow plot can be helpful (see example in Burscher et al, 2016)

Finding the optimal k

Automated Content Analysis

- The only way to find k is to estimate multiple models with different ks
- No single best solution; finding a balance between error within clusters (distances from centroid) and low number of clusters.
- An elbow plot can be helpful (see example in Burscher et al, 2016)

Code-example for creating an elbow plot:

https://pythonprogramminglanguage.com/kmeans-elbow-method/

Burscher, B., Vliegenthart, R., & de Vreese, C. H. (2016). Frames beyond words: Applying cluster and sentiment analysis to news coverage of the nuclear power issue. Social Science Computer Review, 34(5), 530-545. doi:10.1177/0894439315596385

Hierarchical clustering

Finding similar cases		
Hierarchical clustering		

Downsides of k-means clustering

k-means is fast, but has problems:

- k can only be determined by fitting multiple models and comparing them
- bad results if the wrong k is chosen
- bad results if the (real) clusters are non-spherical
- bad results if the (real) clusters are not evenly sized

Hiearchical clusttering

General idea

- To start, each case has its own cluster
- Merge the two clusters that are most similar
- Repeat until desired number of clusters is reached

- Stopping criterion: based on numerical statistic (e.g.,
- Linkage: how to determine which two clusters should be

Hiearchical clusttering

General idea

- To start, each case has its own cluster
- Merge the two clusters that are most similar
- Repeat until desired number of clusters is reached

Different options

- Stopping criterion: based on numerical statistic (e.g., Duda-Hart) or dendrogram
- Linkage: how to determine which two clusters should be merged?

Let's look into some options

https://scikit-learn.org/stable/modules/clustering.html# hierarchical-clustering

⇒ Ward's linkage is a good default all-rounder choice, especially if you encounter the problem that other linkages lead to almost all cases ending up in one cluster.

Hierarchical clustering takeaway

Automated Content Analysis

- The main reason not to use hierarchical methods (but k-means) is their computational cost: when clustering survey data of media users, never use k-means!
- But for NLP/ML, costs may be too high (if not used carefully)
- Very much worth considering, though, if you are really into grouping cases!





Important notes

Automated Content Analysis

Consider the scales of measurement

Clustering is based on distances – if your features are not measured on the same scale, or if it is not meaningful to calculate a numerical distance, it won't produce meaningful results!

Consider standardizing/whitening your features!

Important notes

Consider the scales of measurement

Clustering is based on distances – if your features are not measured on the same scale, or if it is not meaningful to calculate a numerical distance, it won't produce meaningful results!

Consider standardizing/whitening your features!

Pay attention outliers/extreme cases

Extreme cases or outliers can have a strong influence.

Important notes

Consider the scales of measurement

Clustering is based on distances – if your features are not measured on the same scale, or if it is not meaningful to calculate a numerical distance, it won't produce meaningful results!

Consider standardizing/whitening your features!

Pay attention outliers/extreme cases

Extreme cases or outliers can have a strong influence.

Do proper pre-processing

To reduce the number of features, but also to have meaningful features (dimensions on which you expect high distances between the clusters).

Exercise

- 1. Go to https://figshare.com/articles/News-Processed-Dataset/5296357 and download WSJ_20170607_to_20170726_10AmTo4Pm.json (the small file of 9 MB)
- 2. You can read the file as follows:1

```
import json
with open('WSJ_20170607_to_20170726_10AmTo4Pm.json') as f:
texts = [json.loads(line)['content'] for line in f]
```

3. Use unsupervised machine learning techniques (and/or other techniques) to draw inferences about topics of (groups of) texts!

¹It's a json-lines file with one json object per line (see slides yesterday), and we only need what's withinthe ['content'] key, the rest is some metadata – try out what happens if you leave away the ['content']

This afternoon we will discuss one of the most popular
unsupervised methods of the moment – topic modeling.