Curs 7: Preprocesarea datelor si invatare nesupervizata

Invatarea nesupervizata a datelor trateaza cazul in care datele nu sunt etichetate, adica nu au nicio indicatie - fie ea de natura continua sau discreta - asociata. Orice problema de clasificare sau de regresie se poate transforma intr-o problema de invatare de tip nesupervizat, prin inlaturarea etichetei aferente fiecarei inregistrari.

Discutam in acest curs doua tipuri de invatare nesupervizata:

- transformare nesupervizata a datelor
- clustering

Aceste operatii se folosesc frecvent in etapa de explorare a datelor, de exemplu pentru a capata rapid o idee despre structura datelor. In alte cazuri se aplica pe post de metode de preprocesare, de exemplu pentru a aduce valorile de pe dimensiuni diferite la aceleasi scale sau pentru a micsora numarul de date.

7.1 Transformarea nesupervizata a datelor

Transformarea nesupervizata a datelor vizeaza obtinerea unei noi reprezentari a setului initial cu scopul de a le face mai usor de inteles de oameni sau mai utile pentru un algoritm de ML. De exemplu, reducerea de la un numar mare de dimensiuni la 2 sau 3 dimensiuni permite reprezentarea grafica si obtinerea rapida a unei vederi initiale bune asupra datelor.

7.1.1. Scalarea datelor

Anumiti algoritmi, precum cei bazati pe calcul de distante sau cei ce lucreaza cu stochastic gradient descent sunt senzitivi la scala datelor: ei necesita ca datele sa fie cu acelasi odin de marime. De exemplu, pentru cazul in care pentru doi vectori n-dimensionali $\mathbf{x} = (x_1, \ldots, x_n)$ respectiv $\mathbf{y} = (y_1, \ldots, y_n)$ se calculeaza distanta dintre ei cu metrica Euclidiana:

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

daca pentru primul indice (prima dimensiune) valorile sunt de ordinul sutelor iar pentru restul dimensiunilor valorile sunt de ordinul zecilor de unitati, atunci valoarea distantei este practic determinata doar de diferenta intre prima dimensiune a fiecarui vector; celelalte dimensiuni au influenta mult redusa (comparati sutimi de unitati cu zeci de mii de unitati).

Exista urmatoarele metode populare de scalare:

1. scalarea min-max: toate trasaturile (dimensiunile) sunt transformate in mod independent, astfel incat valorile minime si maxime pe respectiva trasatura sa fie intre un minim si un maxim date. Implementarea e simpla, se calculeaza pentru fiecare dimensiune minimul si maximul, apoi diferenta dintre fiecare valoare si minimul seriei sale este impartita la diferenta intre maximul si minimul seriei din care face parte;
2. standardizarea: fiecare dimensiune e astfel transformata incat sa aiba media zero si deviatia standard 1; aceasta se obtine prin: se calculeaza media si deviatia standard pentru fiecare dimensiune; fiecare serie (dimensiune) se transforma prin impartirea diferentei dintre valorile din seria originara si media seriei la deviatia standard;
3. scalarea robusta: ca la punctul anterior, dar se folosesc mediana si quartile ale datelor din fiecare serie, independent;
4. normalizarea: se imparte orice vector (presupus nenul) la norma sa. Norma se alege convenabil. In urma transformarii, orice vector va avea norma 1 si se va gasi pe hipersfera de raza 1 centrata in origine.

In [1]:
```
%matplotlib inline
import matplotlib.pyplot as plt
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
import numpy as np
import pandas as pd
```

In [2]:
```
data_cancer = load_breast_cancer()
data_names = data_cancer.feature_names
print(data_names)
```

```
['mean radius' 'mean texture' 'mean perimeter' 'mean area'
 'mean smoothness' 'mean compactness' 'mean concavity'
 'mean concave points' 'mean symmetry' 'mean fractal dimension'
 'radius error' 'texture error' 'perimeter error' 'area error'
 'smoothness error' 'compactness error' 'concavity error'
 'concave points error' 'symmetry error' 'fractal dimension error'
 'worst radius' 'worst texture' 'worst perimeter' 'worst area'
 'worst smoothness' 'worst compactness' 'worst concavity'
 'worst concave points' 'worst symmetry' 'worst fractal dimension']
```

In [3]:
```
df_cancer = pd.DataFrame(data_cancer.data, columns=data_names)
df_cancer.head()
```

Out[3]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	sy
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	0.2
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	0.1
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	0.2
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	0.2
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	0.1

5 rows × 30 columns

In [4]:
```
df_cancer.describe()
```

Out[4]:

	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	c
count	569.000000	569.000000	569.000000	569.000000	569.000000	569.000000	569
mean	14.127292	19.289649	91.969033	654.889104	0.096360	0.104341	0.0
std	3.524049	4.301036	24.298981	351.914129	0.014064	0.052813	0.0
min	6.981000	9.710000	43.790000	143.500000	0.052630	0.019380	0.0
25%	11.700000	16.170000	75.170000	420.300000	0.086370	0.064920	0.0
50%	13.370000	18.840000	86.240000	551.100000	0.095870	0.092630	0.0
75%	15.780000	21.800000	104.100000	782.700000	0.105300	0.130400	0.1
max	28.110000	39.280000	188.500000	2501.000000	0.163400	0.345400	0.4

8 rows × 30 columns

Se observa discrepantele majore intre valorile minime si maxime:

In [5]:
```
df_cancer.describe().loc[['min', 'max']]
```

Out[5]:

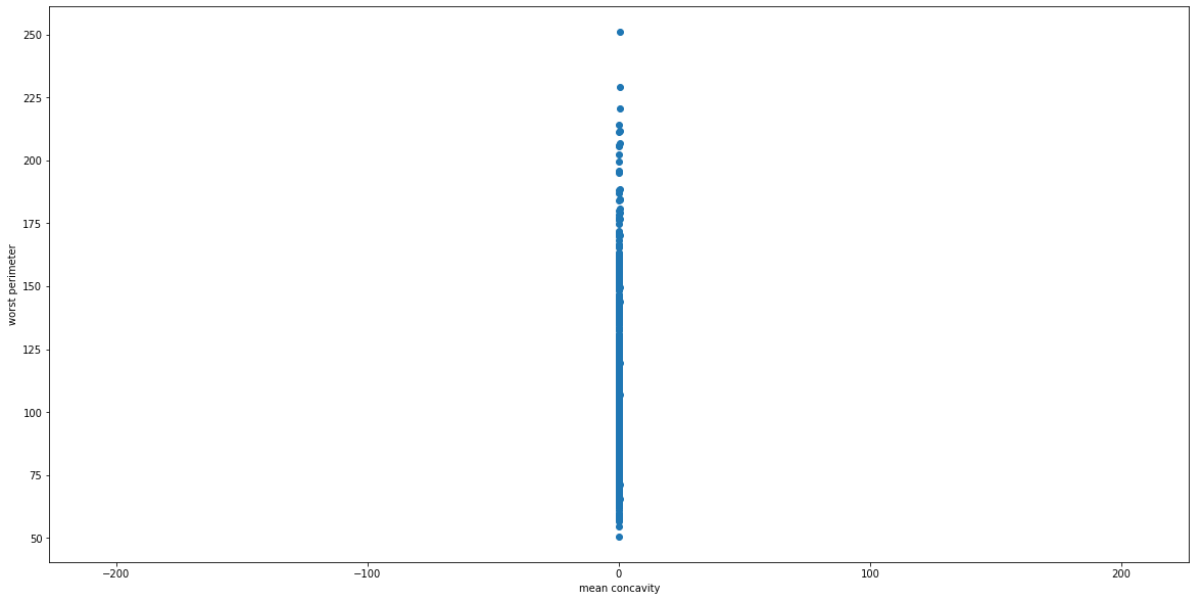
	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points
min	6.981	9.71	43.79	143.5	0.05263	0.01938	0.0000	0.0000
max	28.110	39.28	188.50	2501.0	0.16340	0.34540	0.4268	0.2012

2 rows × 30 columns

Reprezentare grafica:

In [6]:
```
feature1 = 'mean concavity'
feature2 = 'worst perimeter'
plt.figure(figsize=(20, 10))
plt.axis('equal')
plt.xlabel(feature1)
plt.ylabel(feature2)
plt.scatter(df_cancer[feature1], df_cancer[feature2])
```

Out[6]: <matplotlib.collections.PathCollection at 0xb764da0>



In [7]:
```
# import seaborn as sns
# sns.set(style="ticks")
# sns.pairplot(df_cancer)
```

In cazul in care setul de date esta impartit in set de antrenare si set de validare sau de testare, parametrii folositi pentru transformarea datelor trebuie sa fie retinuti si reutilizati pentru a face aceleasi transformari pe setul exterior celui de antrenare. Este gresit ca seturile de testare sau de validare sa fie transformate cu alte valori, pentru ca modelul (de clasificare/regresie/clustering) determinat pe setul de antrenare are sanse reale sa nu functioneze pe date din cu totul alte intervale.

Exemple de aplicare a transformarilor:

In [8]:
```
#etichetele y_* sunt utile pentru a demonstra utilitatea scalarii
X_train, X_test, y_train, y_test = train_test_split(data_cancer.data, data_can
cer.target, test_size=1/3)
print(X_train.shape)
print(X_test.shape)
```

```
(379, 30)
(190, 30)
```

In [9]:
```
from sklearn.preprocessing import MinMaxScaler
```

In [10]:
```
min_max_scaler = MinMaxScaler()
min_max_scaler.fit(X_train)
#se observa ca datele din X_train nu sunt modificare
print(np.min(X_train, axis=0))
```

```
[  6.98100000e+00   9.71000000e+00   4.37900000e+01   1.43500000e+02
   6.25100000e-02   1.93800000e-02   0.00000000e+00   0.00000000e+00
   1.06000000e-01   4.99600000e-02   1.11500000e-01   3.60200000e-01
   7.71400000e-01   6.80200000e+00   1.71300000e-03   2.25200000e-03
   0.00000000e+00   0.00000000e+00   7.88200000e-03   8.94800000e-04
   7.93000000e+00   1.20200000e+01   5.04100000e+01   1.85200000e+02
   7.11700000e-02   2.72900000e-02   0.00000000e+00   0.00000000e+00
   1.56500000e-01   5.50400000e-02]
```

In [11]:
```
#dar obiectul de scalare castiga in starea lui valorile minime si maxime pe fi
ecare trasatura:
print(min_max_scaler.data_min_ == np.min(X_train, axis=0))
print(min_max_scaler.data_max_ == np.max(X_train, axis=0))
```

```
[ True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True]
[ True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True  True  True  True  True  True  True
  True  True  True  True  True  True]
```

In [12]:
```
X_train_scaled = min_max_scaler.transform(X_train)
print(np.min(X_train_scaled, axis=0), '\n', np.max(X_train_scaled, axis=0), se
p='')
```

```
[ 0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.]
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.
  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]
```

Frecvent se cere atat determinarea parametrilor de transfromare, cat si aplicarea transformarii pe un acelsi set de date:

In [13]:
```
X_train_scaled = min_max_scaler.fit_transform(X_train)
```

Transformarea setului de testare se face folosind acelasi obiect de scalare obtinut (fitted) pe setul de antrenare

In [14]:
```
X_test_scaled = min_max_scaler.transform(X_test)
```

Daca setul de testare face parte din aceeasi distributie ca si cel de antrenare, ar trebui ca valorile minima si maxime obtinute pe setul de testare sa fie aproximativ 0 si 1:

In [15]:
```
#minim pe setul de testare, pe fiecare trasatura
np.min(X_test_scaled, axis = 0)
```

Out[15]:
```
array([ 0.03849004,  0.03990531,  0.02986046,  0.01780204, -0.09792844,
        0.02691668,  0.        ,  0.        ,  0.14090909,  0.00610783,
        0.00230433,  0.01768034, -0.00155196,  0.00302195,  0.03824319,
        0.01095022,  0.        ,  0.        ,  0.04494382,  0.00742993,
        0.04103175,  0.01252665,  0.03829169,  0.01869588,  0.08531995,
        0.01550388,  0.        ,  0.        ,  0.01636113,  0.00111505])
```

In [16]:
```
#maxim pe setul de testare, pe fiecare trasatura
np.max(X_test_scaled, axis = 0)
```

Out[16]:
```
array([ 1.0439745 ,  0.72404464,  1.04627287,  1.119155  ,  0.81464962,
        1.2324966 ,  1.00093809,  1.05175118,  0.93232323,  0.90564448,
        2.1942789 ,  0.70893741,  2.28575432,  3.08768267,  0.7348472 ,
        0.71956019,  1.30348914,  1.34428317,  1.32643996,  1.31777539,
        1.11547619,  0.93656716,  1.1224216 ,  1.33455786,  0.97226441,
        0.88347838,  0.93450479,  0.98522337,  0.78710822,  0.56316411])
```

Exemplul de mai sus se aplica cu mimime modificari altor metode de scalare:

In [17]:
```
from sklearn.preprocessing import StandardScaler

standard_scaler = StandardScaler()
X_train_std = standard_scaler.fit_transform(X_train)
print('valori medii: ', np.mean(X_train_std, axis = 0))
print('deviatie standard: ', np.std(X_train_std, axis = 0))
```

```
valori medii:  [ -2.59745318e-15   2.56391214e-15   6.04148804e-15   4.713321
50e-16
   2.54062382e-15  -1.20689152e-16  -9.26845818e-16  -5.76788690e-16
  -2.19056670e-15   1.62716147e-16   1.18111325e-15   3.21642449e-16
   2.26731562e-16   7.20619694e-16  -1.36712687e-15   2.75944615e-16
   1.74003292e-16   1.33314643e-15  -2.62762547e-15  -5.97879998e-16
  -2.54326024e-15   6.19850111e-16   1.06393932e-15  -6.60568053e-16
  -1.80154924e-15  -1.31820676e-16  -5.92314236e-16   3.89603331e-17
   1.85251990e-15   3.43319627e-15]
deviatie standard:  [ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.
1.  1.  1.  1.
  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]
```

Utilitatea aplicarii unei astfel de preprocesari este data mai jos:

In [18]:
```
from sklearn.neighbors import KNeighborsClassifier
```

In [19]:
```
#varianta cu date nescalate

knn = KNeighborsClassifier(n_neighbors=3)
knn.fit(X_train, y_train)
knn.score(X_test, y_test)
```

Out[19]: 0.91578947368421049

In [20]:
```
knn_scaled = KNeighborsClassifier(n_neighbors=3)
knn_scaled.fit(X_train_scaled, y_train)
knn_scaled.score(X_test_scaled, y_test)
```

Out[20]: 0.97894736842105268

Desigur, putem constata si efectul pe datele standardizate:

In [21]:
```
knn_std = KNeighborsClassifier(n_neighbors=3)
knn_std.fit(X_train_std, y_train)
X_test_std = standard_scaler.transform(X_test)
knn_std.score(X_test_std, y_test)
```

Out[21]: 0.98421052631578942

7.1.2. Reducerea dimensionalitatii

Frecvent, datele disponibile au un numar mare de dimensiuni. In destule cazuri se poate renunta la unele din ele, fara a peirde informatie esentiala. In plus, se castiga in viteza de calcul, deoarece se ajunge sa se lucreze cu mai putine trasaturi. In destule situatii se poate ajunge la doua trasaturi numerice care pot fi reprezentate in plan, dand posibilitatea unei explorari initiale.

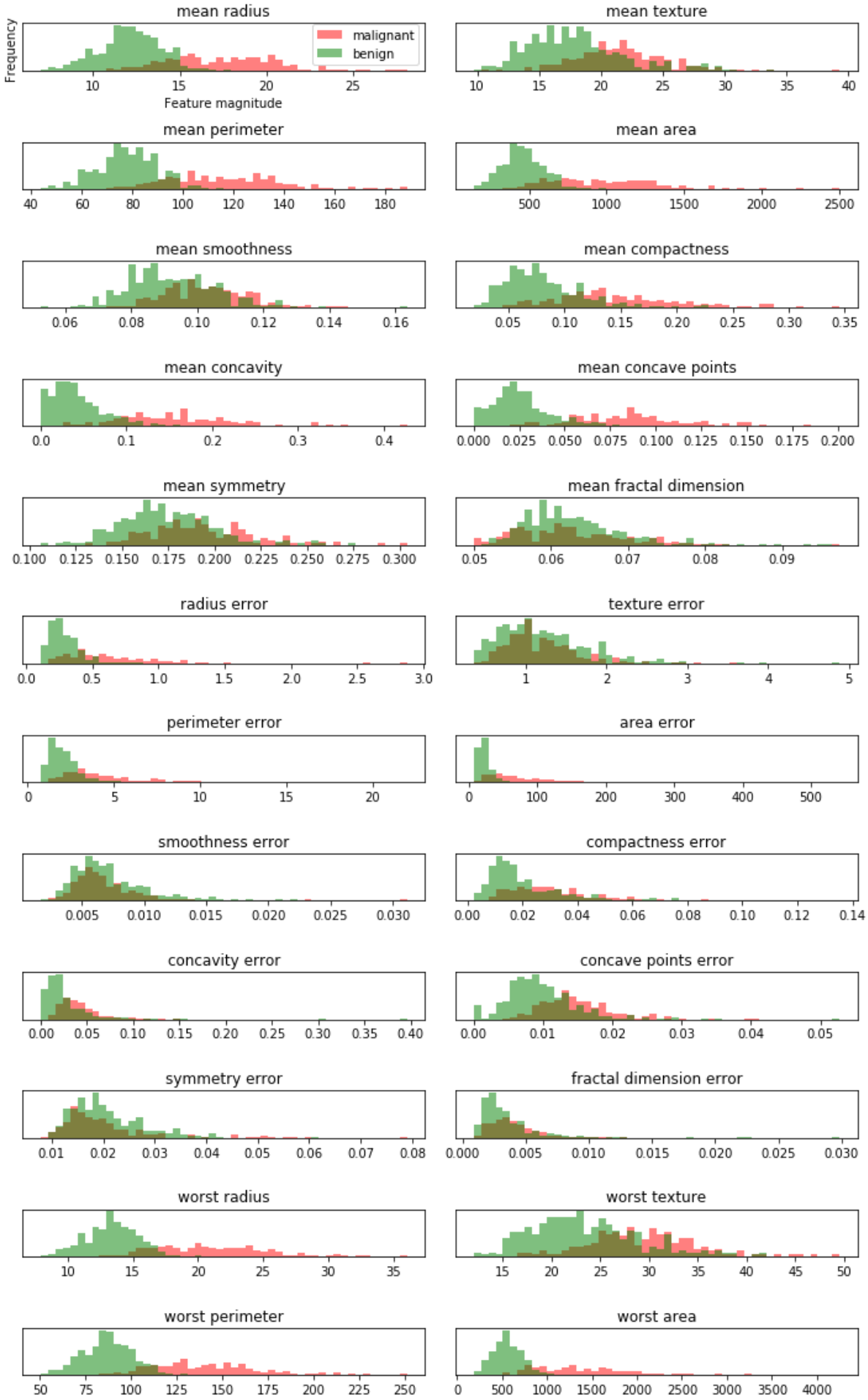
Cea mai populara transformare este analiza componentelor principale (Principal Component Analysis, PCA) care se obtine prin metode algebrice relativ simple.

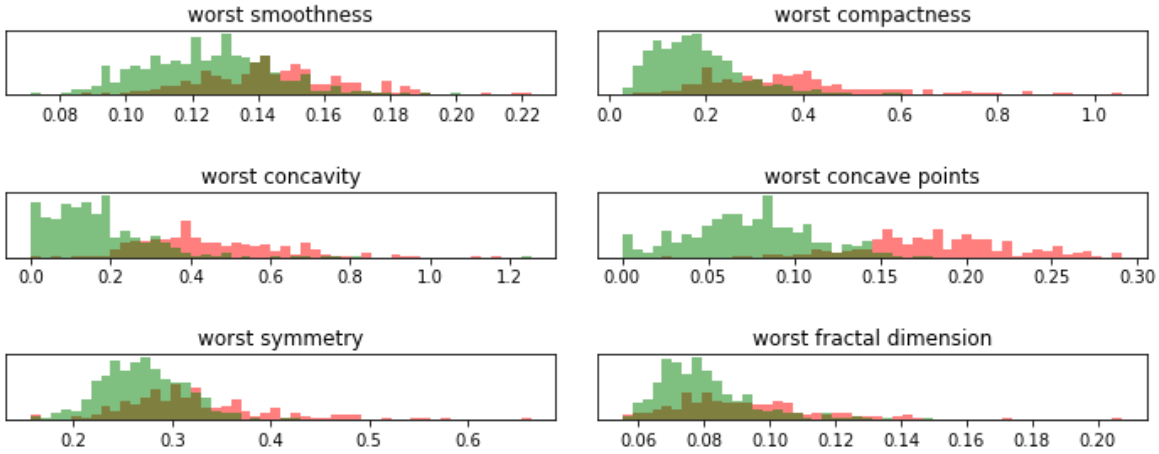
Bibliografie recomandata pentru prezentare matematica este:

1. A tutorial on Principal Components Analysis (http://www.cs.otago.ac.nz/cosc453/student_tutorials/principal_components.pdf)
2. A Tutorial on Principal Component Analysis (https://arxiv.org/abs/1404.1100)
3. PCA Whitening (http://ufldl.stanford.edu/tutorial/unsupervised/PCAWhitening/)

In [22]:
```
#sursa: Introduction to Machine Learning with Python, chapter 03

fig, axes = plt.subplots(15, 2, figsize=(10, 20))
malignant = data_cancer.data[data_cancer.target == 0]
benign = data_cancer.data[data_cancer.target == 1]
ax = axes.ravel()
for i in range(30):
    _, bins = np.histogram(data_cancer.data[:, i], bins=50)
    ax[i].hist(malignant[:, i], bins=bins, color='red', alpha=.5)
    ax[i].hist(benign[:, i], bins=bins, color='green', alpha=.5)
    ax[i].set_title(data_cancer.feature_names[i])
    ax[i].set_yticks(())
ax[0].set_xlabel("Feature magnitude")
ax[0].set_ylabel("Frequency")
ax[0].legend(["malignant", "benign"], loc="best")
fig.tight_layout()
```


mean radius
malignant
benign
Frequency
Feature magnitude
mean texture
mean perimeter
mean area
mean smoothness
mean compactness
mean concavity
mean concave points
mean symmetry
mean fractal dimension
radius error
texture error
perimeter error
area error
smoothness error
compactness error
concavity error
concave points error
symmetry error
fractal dimension error
worst radius
worst texture
worst perimeter
worst area



In histogramele anterioare se observa ca diferite trasaturi individuale au o putere discriminativa mai mica sau mai mare. Ne intereseaza sa consideram doua tarsaturi (nu neaparat din cele originare, pot fi si combinatii liniare ale acestora) astfel incat separarea intre malign si benign sa fie mai clara.

In [23]:
```
X_cancer, y_cancer = data_cancer.data, data_cancer.target

#se aplica in prealabil o scalare a datelor de intrare
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X_cancer)
```

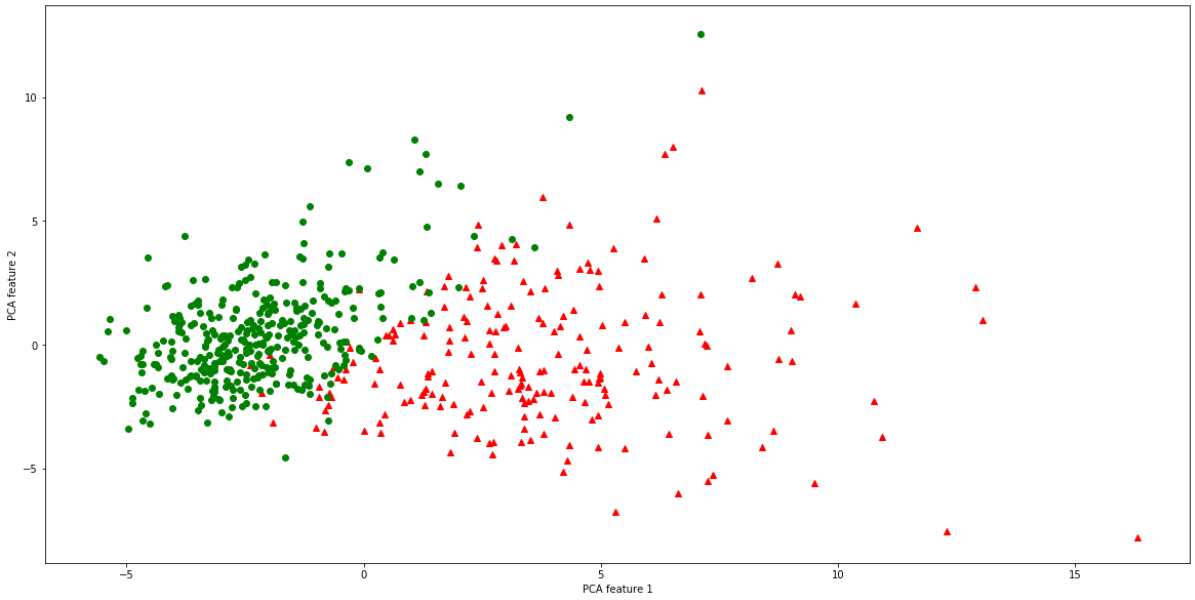
In [24]:
```
#aplicarea PCA
from sklearn.decomposition import PCA
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_scaled)
print(X_scaled.shape)
print(X_pca.shape)
```

```
(569, 30)
(569, 2)
```

In [25]:
```
X_pca_malign = X_pca[y_cancer == 0]
X_pca_benign = X_pca[y_cancer == 1]

plt.figure(figsize=(20, 10))
plt.scatter(X_pca_malign[:, 0], X_pca_malign[:, 1], c='r', marker='^')
plt.scatter(X_pca_benign[:, 0], X_pca_benign[:, 1], c='g', marker='o')
plt.xlabel('PCA feature 1')
plt.ylabel('PCA feature 2')
```

Out[25]: Text(0,0.5,'PCA feature 2')



Trasaturile determinate de PCA sunt obtinute pe baza unor transformari liniare ale trasaturilor din setul originar. Se pot afisa coeficientii transformarii liniare:

In [26]:
```
print('Coeficientii pentru PCA feature 1, respectiv PCA feature 2:', pca.compo
nents_)
```

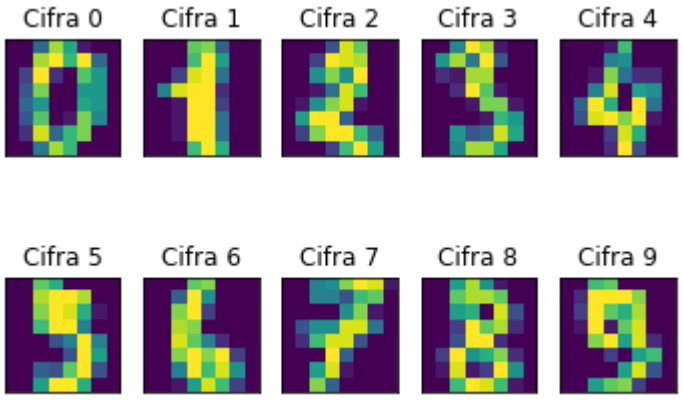
```
Coeficientii pentru PCA feature 1, respectiv PCA feature 2: [[ 0.21890244  0.
10372458  0.22753729  0.22099499  0.14258969  0.23928535
   0.25840048  0.26085376  0.13816696  0.06436335  0.20597878  0.01742803
   0.21132592  0.20286964  0.01453145  0.17039345  0.15358979  0.1834174
   0.04249842  0.10256832  0.22799663  0.10446933  0.23663968  0.22487053
   0.12795256  0.21009588  0.22876753  0.25088597  0.12290456  0.13178394]
 [-0.23385713 -0.05970609 -0.21518136 -0.23107671  0.18611302  0.15189161
   0.06016536 -0.0347675   0.19034877  0.36657547 -0.10555215  0.08997968
  -0.08945723 -0.15229263  0.20443045  0.2327159   0.19720728  0.13032156
   0.183848    0.28009203 -0.21986638 -0.0454673  -0.19987843 -0.21935186
   0.17230435  0.14359317  0.09796411 -0.00825724  0.14188335  0.27533947]]
```

O alta metoda destul de populara pentru extragerea de trasaturi este t-SNE. O excelenta prezentare a unuia din autorii algoritmului, Laurens van der Maaten, este aici (https://www.youtube.com/watch?v=RJVL80Gg3lA). Articolele care prezinta variante ale algoritmului sunt pe siteul autorului (https://lvdmaaten.github.io/tsne/). Exemplificarea se face pe setul de date `digits` din sklearn:

In [27]:
```
from sklearn.datasets import load_digits
digits = load_digits()
digits.DESCR
```

Out[27]:
```
"Optical Recognition of Handwritten Digits Data Set\n===================
============================\n\nNotes\n-----\nData Set Characteristics:\n    :
Number of Instances: 5620\n    :Number of Attributes: 64\n    :Attribute Info
rmation: 8x8 image of integer pixels in the range 0..16.\n    :Missing Attrib
ute Values: None\n    :Creator: E. Alpaydin (alpaydin '@' boun.edu.tr)\n    :
Date: July; 1998\n\nThis is a copy of the test set of the UCI ML hand-written
digits datasets\nhttp://archive.ics.uci.edu/ml/datasets/Optical+Recognition+o
f+Handwritten+Digits\n\nThe data set contains images of hand-written digits:
 10 classes where\neach class refers to a digit.\n\nPreprocessing programs ma
de available by NIST were used to extract\nnormalized bitmaps of handwritten
 digits from a preprinted form. From a\ntotal of 43 people, 30 contributed to
the training set and different 13\nto the test set. 32x32 bitmaps are divided
into nonoverlapping blocks of\n4x4 and the number of on pixels are counted in
each block. This generates\nan input matrix of 8x8 where each element is an i
nteger in the range\n0..16. This reduces dimensionality and gives invariance
 to small\ndistortions.\n\nFor info on NIST preprocessing routines, see M. D.
Garris, J. L. Blue, G.\nT. Candela, D. L. Dimmick, J. Geist, P. J. Grother,
 S. A. Janet, and C.\nL. Wilson, NIST Form-Based Handprint Recognition Syste
m, NISTIR 5469,\n1994.\n\nReferences\n----------\n  - C. Kaynak (1995) Method
s of Combining Multiple Classifiers and Their\n    Applications to Handwritte
n Digit Recognition, MSc Thesis, Institute of\n    Graduate Studies in Scienc
e and Engineering, Bogazici University.\n  - E. Alpaydin, C. Kaynak (1998) Ca
scading Classifiers, Kybernetika.\n  - Ken Tang and Ponnuthurai N. Suganthan
 and Xi Yao and A. Kai Qin.\n    Linear dimensionalityreduction using relevan
ce weighted LDA. School of\n    Electrical and Electronic Engineering Nanyang
Technological University.\n    2005.\n  - Claudio Gentile. A New Approximate
 Maximal Margin Classification\n    Algorithm. NIPS. 2000.\n"
```

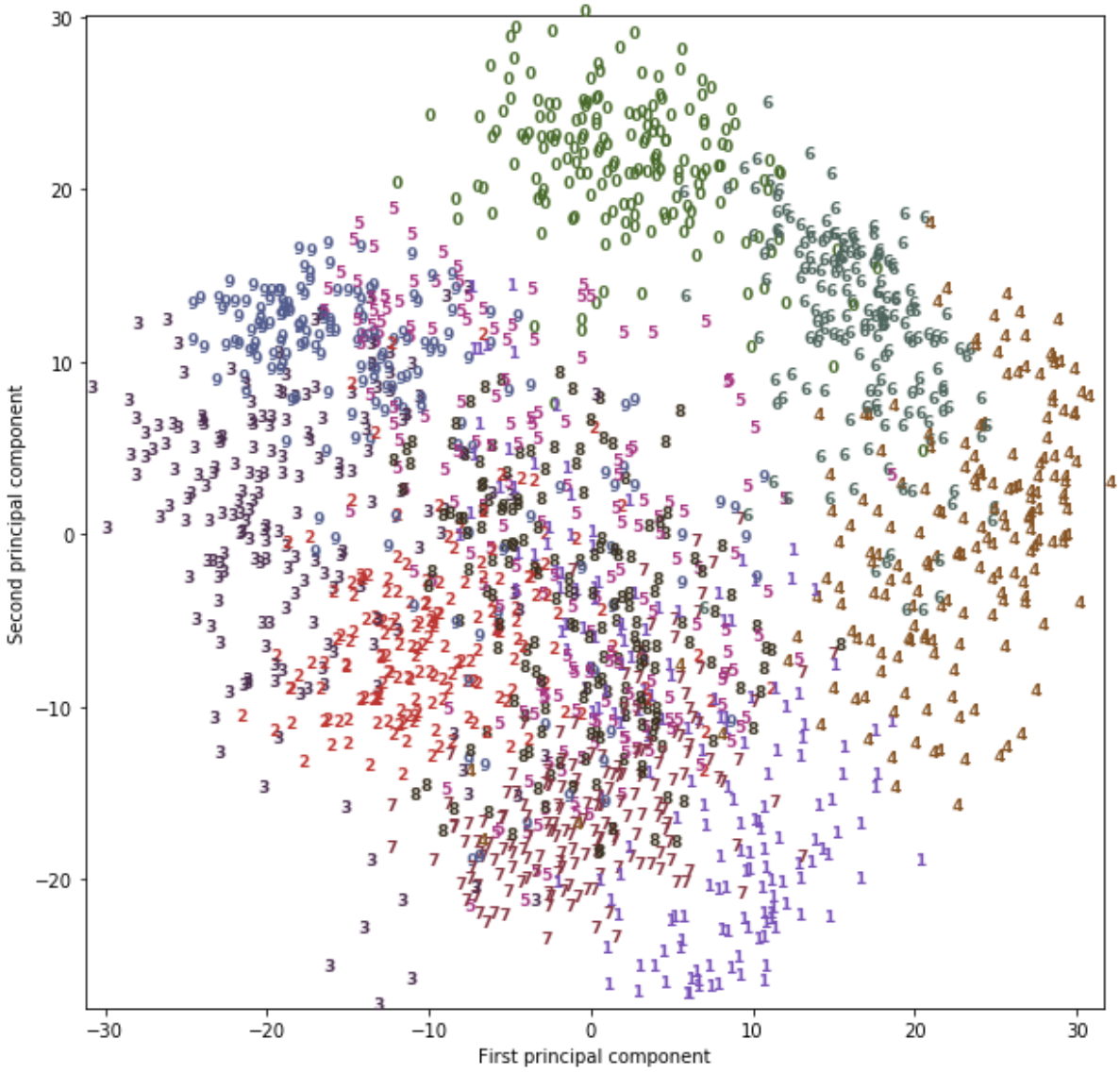
In [28]:
```
fig, axes = plt.subplots(2, 5, subplot_kw = {'xticks':(), 'yticks':()})
for ax, img, img_cls in zip(axes.ravel(), digits.images, digits.target_names):
    ax.imshow(img)
    ax.set_title('Cifra ' + str(img_cls))
```



In [29]:
```
#sursa: https://github.com/amueller/introduction_to_ml_with_python/blob/master/03-unsupervised-learning.ipynb

# build a PCA model
pca = PCA(n_components=2)
pca.fit(digits.data)
# transform the digits data onto the first two principal components
digits_pca = pca.transform(digits.data)
colors = ["#476A2A", "#7851B8", "#BD3430", "#4A2D4E", "#875525",
          "#A83683", "#4E655E", "#853541", "#3A3120", "#535D8E"]
plt.figure(figsize=(10, 10))
plt.xlim(digits_pca[:, 0].min(), digits_pca[:, 0].max())
plt.ylim(digits_pca[:, 1].min(), digits_pca[:, 1].max())
for i in range(len(digits.data)):
    # actually plot the digits as text instead of using scatter
    plt.text(digits_pca[i, 0], digits_pca[i, 1], str(digits.target[i]),
             color = colors[digits.target[i]],
             fontdict={'weight': 'bold', 'size': 9})
plt.xlabel("First principal component")
plt.ylabel("Second principal component")
```

Out[29]: Text(0,0.5,'Second principal component')

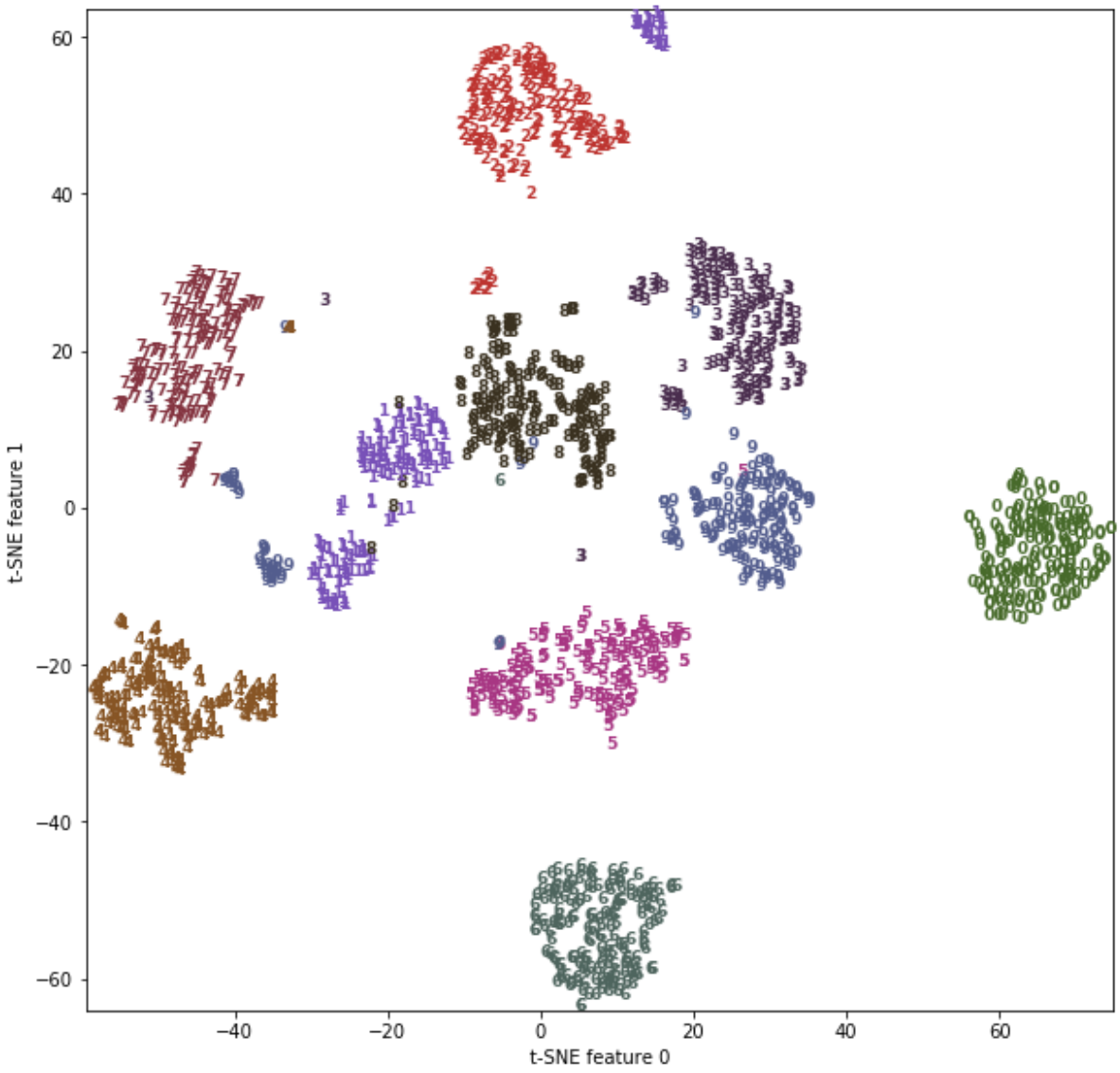


Prin t-SNE se obtin trasaturi mult mai bine diferentiate:

In [30]:
```
# sursa: https://github.com/amueller/introduction_to_ml_with_python/blob/master/03-unsupervised-learning.ipynb
from sklearn.manifold import TSNE
tsne = TSNE(random_state=42)
# use fit_transform instead of fit, as TSNE has no transform method
digits_tsne = tsne.fit_transform(digits.data)
```

In [31]:
```
# sursa: https://github.com/amueller/introduction_to_ml_with_python/blob/master/03-unsupervised-learning.ipynb
plt.figure(figsize=(10, 10))
plt.xlim(digits_tsne[:, 0].min(), digits_tsne[:, 0].max() + 1)
plt.ylim(digits_tsne[:, 1].min(), digits_tsne[:, 1].max() + 1)
for i in range(len(digits.data)):
    # actually plot the digits as text instead of using scatter
    plt.text(digits_tsne[i, 0], digits_tsne[i, 1], str(digits.target[i]),
             color = colors[digits.target[i]],
             fontdict={'weight': 'bold', 'size': 9})
plt.xlabel("t-SNE feature 0")
plt.ylabel("t-SNE feature 1")
```

Out[31]: Text(0,0.5,'t-SNE feature 1')



7.2. Clustering-ul

Clusteringul vizeaza obtinerea de partitii ale setului initial de date. Intre elementele care apartin aceluiasi cluster se considera ca exista relatii de similaritate mai mari decat intre elemente care apartin unor clustere diferite. De exemplu, se doreste impartirea unor imagini cu oameni, in grupuri cu similaritate interna; nu se cunoaste nimic despre indentitatea persoanelor din poze sau metadate.

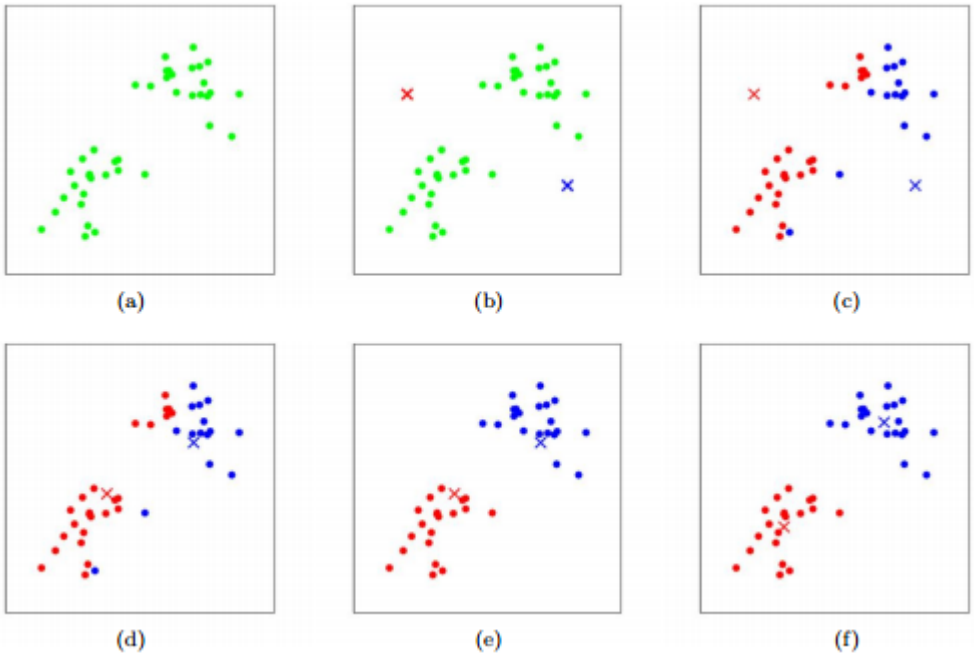
7.2.1 K-means

K-means este cel mai popular algoritm de clustering. El incearca sa grupeze datele in k clustere. Fiecare cluster este definit printr-un centru de greutate (centroid), ale carui coordonate sunt mediile aritmetice ale coordonatelor punctelor care apartin de acelasi cluster. Un punct din setul de instruire sau de testare este asociat cu cel mai apropiat centroid.

Bibliografie:

1. K-means, Stanford CS 221 (http://stanford.edu/~cpiech/cs221/handouts/kmeans.html)
2. K-means and Hierarchical Clustering, Tutorial Slides by Andrew Moore (https://www.autonlab.org/tutorials/kmeans.html)
3. Curs Sisteme computationale inteligente (https://github.com/lmsasu/cursuri/blob/master/SistemeComputationaleInteligente/SistemeComputationaleInte sectiunea 8.4

Ideea de baza este de a determina prin pasi succesivi o pozitionare a centroizilor, precum si o impartire a setului initial de instruire in subseturi (posibil, desi arareori, vide) asociate fiecarui centroid.



Sursa: ref [1] de mai sus.

In [32]:
```
from sklearn.datasets import make_blobs
from sklearn.cluster import KMeans
```

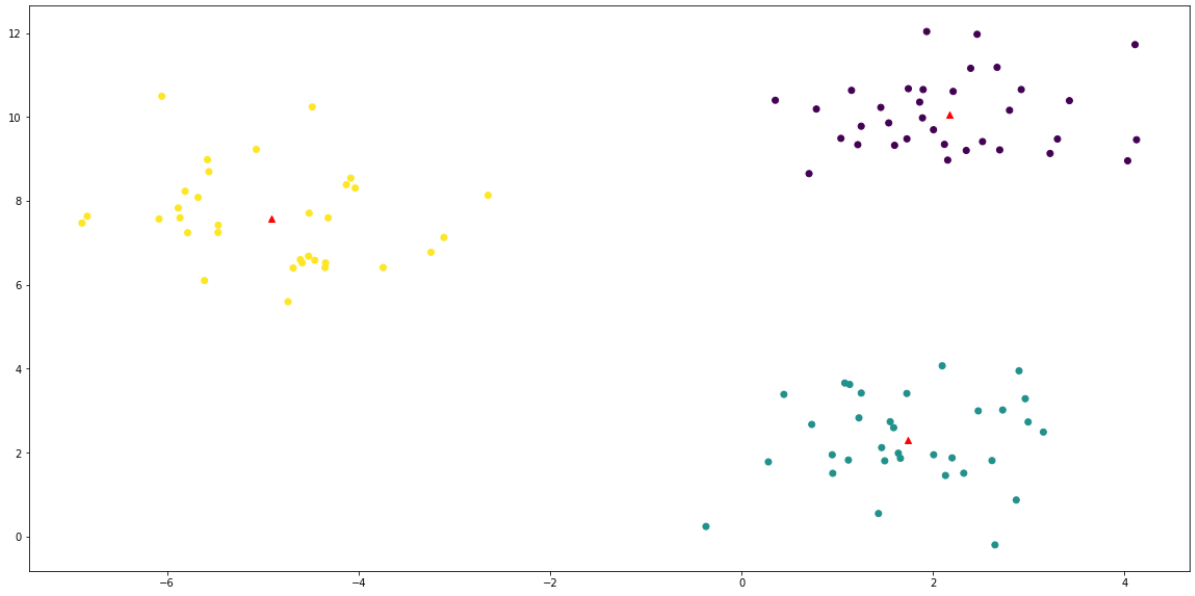
In [33]:
```
X, y = make_blobs()
X.shape
```

Out[33]:
```
(100, 2)
```

In [34]:
```
plt.figure(figsize=(20, 10))
plt.scatter(X[:, 0], X[:, 1], c=y)

kmeans = KMeans(n_clusters=3)
kmeans.fit(X)
centroids = kmeans.cluster_centers_
plt.scatter(centroids[:, 0], centroids[:, 1], marker='^', c='red')
```

Out[34]:
```
<matplotlib.collections.PathCollection at 0xc6df278>
```



Urmatoarele situatii sunt defavorabile pentru algoritmul k-means:

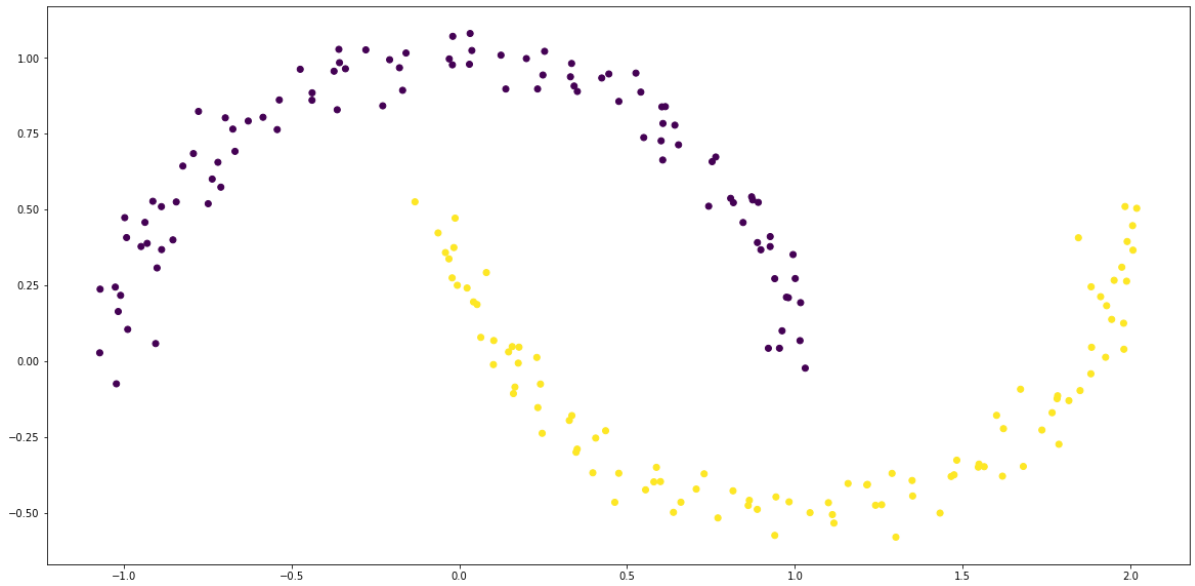
1. numar de clustere necunoscut apriori
2. cazul in care datele nu au forma aproximativ globulara si de diametre egale
3. densitati de distributie diferite in clustere
4. alegere neinspirata a pozitiilor centroizilor; pot rezulta centroizi care partitioneaza un grup de puncte; pot rezulta centroizi orfani = fara puncte asociate
5. nu trateaza bine situatiile in care clusterele nu sunt sferice.

Pentru aceasta ultima situatie dam exemplul de mai jos:

In [35]:
```
from sklearn.datasets import make_moons
X, y = make_moons(n_samples=200, noise=0.05, random_state=0)
```

In [36]:
```
plt.figure(figsize=(20, 10))
plt.scatter(X[:, 0], X[:, 1], c=y)
```

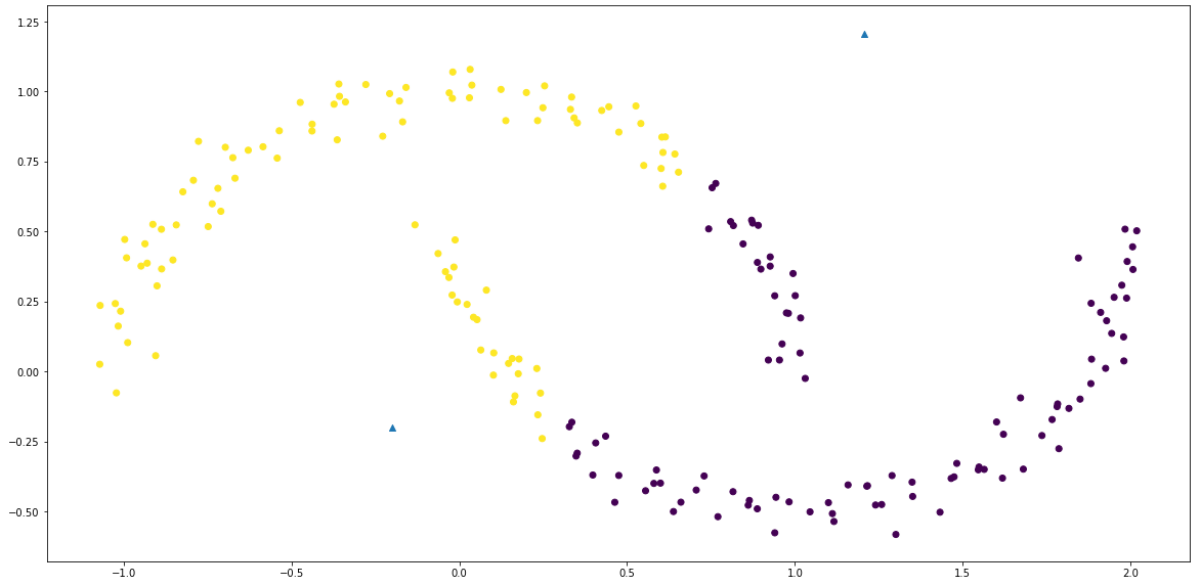
Out[36]: <matplotlib.collections.PathCollection at 0xc747978>



In [37]:
```
kmeans = KMeans(n_clusters=2)
kmeans.fit(X)
y_pred = kmeans.predict(X)

plt.figure(figsize=(20, 10))
plt.scatter(X[:, 0], X[:, 1], c=y_pred)
plt.scatter(kmeans.cluster_centers_[:, 0], kmeans.cluster_centers_[:, 0], mark
er='^')
```

Out[37]: <matplotlib.collections.PathCollection at 0xdfb5390>



Pentru situatia in care determinarea apartenentei de clustere este data de densitatea de repartitie, mai degraba decat de distanta (cum e cazul de mai sus), sunt recomandati algoritmi precum DBSCAN.

Ideea algoritmului DBSCAN este de a determina clustere ce acopera regiuni dense de date; clusterele sunt separate de regiuni cu densitate mica. DBSCAN nu necesita precizarea apriori a numarului de clustere (cu toate ca are alti hiperparametri ce trebuie specificati); in plus, poate eticheta unele date ca fiind zgomot, adica neafiliate niciunui cluster.

Bibliografie:

1. A Density-Based Algorithm for Discovering Clusters in Large Spatial Databases with Noise (https://www.aaai.org/Papers/KDD/1996/KDD96-037.pdf)

In [38]:
```
from sklearn.cluster import DBSCAN
```

In [39]:
```
dbscan = DBSCAN()#valoarea implicita pentru eps e 0.5
clusters = dbscan.fit_predict(X)
clusters
```

Out[39]:
```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], dtype=int64)
```

Rezulattul de mai sus arata ca se obtine un singur cluster. Prin modificarea valorilor hiperparametrilor eps si min_samples se obtin rezultate complet diferite:

In [40]:
```
dbscan = DBSCAN(eps=0.25, )
clusters = dbscan.fit_predict(X)
clusters
```

Out[40]:
```
array([0, 1, 1, 0, 1, 1, 0, 1, 0, 1, 0, 1, 1, 1, 0, 0, 0, 1, 0, 0, 1, 1, 0,
       1, 0, 1, 1, 1, 1, 0, 0, 0, 1, 1, 0, 1, 1, 0, 0, 1, 1, 0, 0, 1, 1, 0,
       0, 0, 1, 1, 0, 1, 1, 0, 1, 0, 0, 1, 0, 0, 1, 0, 1, 0, 1, 0, 0, 1, 0,
       0, 1, 0, 1, 1, 1, 0, 1, 0, 0, 1, 1, 0, 1, 1, 1, 0, 0, 0, 1, 1, 0, 0,
       1, 0, 1, 1, 1, 1, 0, 1, 1, 1, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0,
       1, 0, 1, 1, 0, 0, 0, 1, 0, 1, 0, 0, 1, 1, 1, 0, 0, 0, 1, 1, 1, 1, 0,
       1, 0, 1, 1, 0, 0, 0, 0, 1, 1, 0, 1, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 1,
       1, 0, 1, 1, 1, 0, 1, 1, 1, 0, 0, 0, 0, 1, 1, 1, 0, 0, 0, 1, 0, 1, 1,
       1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 1, 1, 0, 1], dtype=int64)
```

In [41]:
```
plt.figure(figsize=(20, 10))
plt.scatter(X[:, 0], X[:, 1], c=clusters)
# plt.scatter(kmeans.cluster_centers_[:, 0], kmeans.cluster_centers_[:, 0], ma
rker='^')
```

Out[41]: <matplotlib.collections.PathCollection at 0xc652b70>