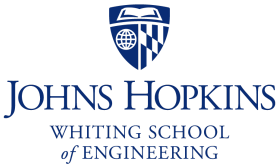
Preprocessing Datasets for Machine Learning



Introduction

In practice, the data acquired for real world problems are often incomplete, noisy, and inconsistent. A few percentage of non-clean data points may affect the final performance by a few percentage drop. If a few steps of preprocessing were taken in the right direction, then better results would be easily achievable. A good data preprocessing is a necessary step for good machine learning performance, and it is widely accepted that preprocessing takes the bulk of the overall machine learning effort.

In addition to data "cleaning", certain algorithms require data features properties in certain ways, such as **normalized** and **standardized** to make the method work better. For example clustering approaches by distance measures require data features to be normalized. The following procedures are common steps in preprocessing:

- Data formatting, cleaning
- Discretization, one-hot encoding
- Data integration and transformation
- Data reduction

Data Formatting and Cleaning

Machine learning frameworks, such as `pandas`, `scikit-learn`, `Weka`, expect dataset files to be in certain formats to be able to process them. The Comma Separated Values **CSV** is one of the most common file formats. Such as, the file `breast_cancer_raw.csv` and first 4 rows,

"age"	"menopause"	"tumor-size"	"inv-nodes"	"node-caps"	"deg-malig"	"breast"	"breast-quad"	"irradiat"	"recurr
44	"premeno"	21	2	"no"	2	"right"	"left_up"	"no"	"no-recurrer events"
46	"premeno"	22	3	"yes"	3	"right"	"left_up"	"no"	"recurre events"
46	"premeno"	22	3	"yes"	3	"right"	"left_up"	"no"	"recurre events"

When examining datasets sometimes we see the files might contain artifacts:

- single quotes in double quotes, i.e. `"Cote d'Azor"` or reversed? e.g. `'Cote d'Azor'`
- single quotes to differentiate between strings and values. i.e. `'1'` or `1`
- use of semicolon instead of commas e.g. `1;50;red;` in a row

In addition to the data formats artifacts, we might also see:

- duplicates of data lines (why is this undesired?)
- missing values (marked as `'?'` in Weka or `'NaN'` in pandas for numerical variables)
- incorrect entries (e.g. clerical errors)

Note that framework programs such as Weka learners are mature and strong enough to work with these problems without necessitating us cleaning them by a preprocessing stage. However, if we do the preprocessing ourselves, then we always increase the **quality of the dataset** and this helps the following stages of machine learning pipeline.

Worked Example

Consider the breast cancer dataset file located at the module page. Load it with `pandas` library and check for (1.) duplicates, (2.) missing values, (3.) incorrect entries. In the following cells, for each problem that the dataset has, a correction is provided once the situation is determined.

In [1]:
```
# Following avoids a warning for KMeans
%env OMP_NUM_THREADS=2

# Standard libraries we always include
%matplotlib inline
import matplotlib.pyplot as plt
plt.rcParams["figure.dpi"] = 72
from IPython.display import display
import numpy as np
import pandas as pd
import seaborn as sns; sns.set(style="ticks", color_codes=True)

# Locate and load the data file
df = pd.read_csv('../../../EP_datasets/breast_cancer_raw.csv')
print(f'#rows={len(df)} #columns={len(df.columns)}')

# Print some info and plots to get a feeling about the dataset
print(df.dtypes)
```

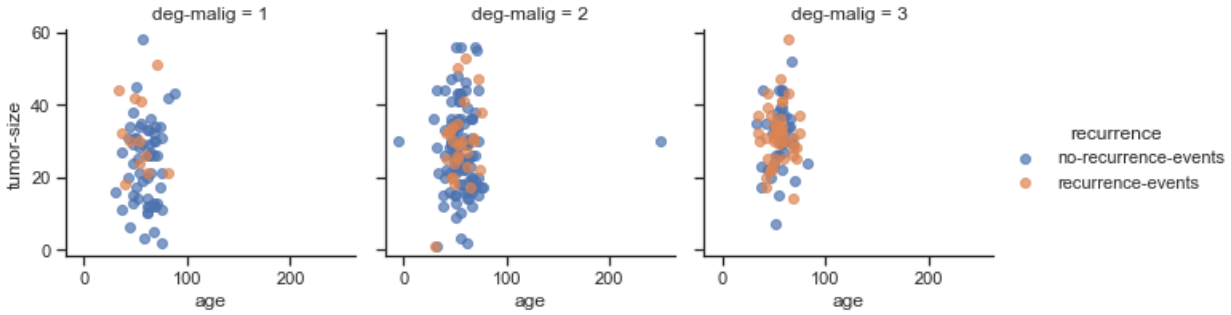
```
env: OMP_NUM_THREADS=2
#rows=298 #columns=10
age             float64
menopause        object
tumor-size      float64
inv-nodes       float64
node-caps        object
deg-malig         int64
breast           object
breast-quad      object
irradiat         object
recurrence       object
dtype: object
```

In [2]:
```
df.head()
```

Out[2]:

	age	menopause	tumor-size	inv-nodes	node-caps	deg-malig	breast	breast-quad	irradiat	recurrence
0	44.0	premeno	21.0	2.0	no	2	right	left_up	no	no-recurrence-events
1	46.0	premeno	22.0	3.0	yes	3	right	left_up	no	recurrence-events
2	46.0	premeno	22.0	3.0	yes	3	right	left_up	no	recurrence-events
3	46.0	premeno	22.0	3.0	yes	3	right	left_up	no	recurrence-events
4	46.0	premeno	22.0	3.0	yes	3	right	left_up	no	recurrence-events

In [3]:
```
# Make sure use a '_variable' name to avoid shadowing variable names in other c
def plot_bc(_df, xyscale=None):  # xyscale to use on the plots
    g = sns.FacetGrid(_df, col='deg-malig', hue='recurrence')
    g.fig.set_dpi(72)
    g.map(plt.scatter, 'age', 'tumor-size', alpha=.7)
    g.add_legend()
    if xyscale is not None:
        plt.xlim(xyscale[0], xyscale[1])
        plt.ylim(xyscale[0], xyscale[1])
    plt.show()

plot_bc(df)
```



Observe: In the second plot what is that data point at age 250?? ...Hmmm.

Duplicates

Let's check duplicate values in our dataset.

In [4]:
```
# Check for duplicates, this adds a new column to the dataset
df["is_duplicate"]= df.duplicated()

# Note that when using f-strings, the internal quote character must be differer
print(f"#total= {len(df)}")
print(f"#duplicated= {len(df[df['is_duplicate']==True])}")
```

```
#total= 298
#duplicated= 5
```

In [5]:
```
# Print rows which have True in column 'is_duplicate'
df[df['is_duplicate']==True]
```

Out[5]:

	age	menopause	tumor-size	inv-nodes	node-caps	deg-malig	breast	breast-quad	irradiat	recurrence	is_du
2	46.0	premeno	22.0	3.0	yes	3	right	left_up	no	recurrence-events	
3	46.0	premeno	22.0	3.0	yes	3	right	left_up	no	recurrence-events	
4	46.0	premeno	22.0	3.0	yes	3	right	left_up	no	recurrence-events	
12	61.0	premeno	29.0	5.0	no	2	right	left_up	yes	no-recurrence-events	
13	61.0	premeno	29.0	5.0	no	2	right	left_up	yes	no-recurrence-events	

In [6]:
```
# Drop the duplicate rows using index - best way to drop in pandas
index_to_drop = df[df['is_duplicate']==True].index
df.drop(index_to_drop, inplace=True)

# Remove the duplicate marker column
df.drop(columns='is_duplicate', inplace=True)
print(f'#total= {len(df)}')
```

```
#total= 293
```

Observe: Total number of rows (data points) reduced to 293

Missing Values

Let's impute missing values. If we do not handle missing values, then very often the ML algorithms will handle them internally.

The safest and most common approach: Use **mean** (or equally acceptable **median**) for numerical values; and **mode** for nominal values to **impute** missing values. Note that a

variable is the entire feature or column of data.

Mean: $\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$

Median: $\tilde{x} = \frac{x[|x|/2] + x[|x|/2+1]}{2}$

Mode: $\hat{x} = \underset{x}{\mathbf{argmax}} f(x)$

Mean vs Mode

- Mean is the **average value** of the feature, mode is the **most frequent level** in the feature
- Mean is proper for numerical, mode is proper for nominal features
  - e.g. Mode might end up being 1 in a large column of real numbers when all levels are expressed for just once
- Mode is not sensitive to noise or outliers
- Mean value might not exist in the column, mode value is the most frequent level

In [7]:
```
# Do we have NaN in our dataset?
df.isnull().any()
```

Out[7]:
```
age             True
menopause      False
tumor-size      True
inv-nodes       True
node-caps      False
deg-malig      False
breast         False
breast-quad    False
irradiat       False
recurrence     False
dtype: bool
```

In [8]:
```
# We do have NaN - three numerical variables - check first cell, it says float
display(df[df['age'].isnull()])
display(df[df['tumor-size'].isnull()])
display(df[df['inv-nodes'].isnull()])
```

	age	menopause	tumor-size	inv-nodes	node-caps	deg-malig	breast	breast-quad	irradiat	recurrence
25	NaN	ge40	34.0	1.0	no	1	right	central	no	no-recurrence-events
26	NaN	ge40	28.0	1.0	no	2	right	left_up	no	no-recurrence-events

	age	menopause	tumor-size	inv-nodes	node-caps	deg-malig	breast	breast-quad	irradiat	recurrence
27	52.0	premeno	NaN	3.0	no	2	left	left_low	yes	recurrence-events
28	37.0	premeno	NaN	2.0	no	3	left	central	no	no-recurrence-events

	age	menopause	tumor-size	inv-nodes	node-caps	deg-malig	breast	breast-quad	irradiat	recurrence
29	62.0	premeno	10.0	NaN	no	1	right	left_up	no	no-recurrence-events

In [9]:
```
# Mean values of numerical columns
means = {c:df[c].mean() for c in df.columns if df[c].dtype != object}

print(f"mean-age= {means['age']}")
print(f"mean-tumor-size= {means['tumor-size']}")
print(f"mean-inv-nodes= {means['inv-nodes']}")

# Impute
df['age'] = df['age'].fillna(means['age'])
df['tumor-size'] = df['tumor-size'].fillna(means['tumor-size'])
df['inv-nodes'] = df['inv-nodes'].fillna(means['inv-nodes'])

# Check with the previous cell results
display(df.loc[[24,25,26,27,28]])
```

```
mean-age= 56.261168384879724
mean-tumor-size= 28.343642611683848
mean-inv-nodes= 3.5753424657534247
```

	age	menopause	tumor-size	inv-nodes	node-caps	deg-malig	breast	breast-quad	irradiat	recurren
24	62.000000	premeno	10.000000	6.0	no	1	right	left_up	no	recurren eve
25	56.261168	ge40	34.000000	1.0	no	1	right	central	no	recurren eve
26	56.261168	ge40	28.000000	1.0	no	2	right	left_up	no	recurren eve
27	52.000000	premeno	28.343643	3.0	no	2	left	left_low	yes	recurren eve
28	37.000000	premeno	28.343643	2.0	no	3	left	central	no	recurren eve

Missing Nominal Values

Finding missing values in nominal variables is more tricky. First let's look at the nominal variables and then see what kind of unique values these nominal variables take. i.e. this is the **level** of the nominal variable drawn from a finite alphabet. Unless a numerical type (`int64` , `float64` , etc.) `df.dtype` will correspond to an **object** which is a `object` class after being read into a `DataFrame` from a CSV file.

It is generally accepted to impute the **mode** of the feature when a level missing. Such as `no` for the missing `node-caps` levels as in below.

In [10]:
```
# What are the column types?
df.dtypes
```

Out[10]:
```
age             float64
menopause        object
tumor-size      float64
inv-nodes       float64
node-caps        object
deg-malig         int64
breast           object
breast-quad      object
irradiat         object
recurrence       object
dtype: object
```

In [11]:
```
# Check unique levels and see any marker is used for a missing level
for col in df.columns:
    if df[col].dtype == object:
        print(col, df[col].unique())
```

```
menopause ['premeno' 'ge40' 'lt40']
node-caps ['no' 'yes' '?']
breast ['right' 'left']
breast-quad ['left_up' 'central' 'left_low' 'right_up' 'right_low' '?']
irradiat ['no' 'yes']
recurrence ['no-recurrence-events' 'recurrence-events']
```

The variables `node-caps` and `breast-quad` has `'?'` levels which need to be **imputed** with values to help the preprocessing.

In [12]:
```
# Check the next feature
display(df['node-caps'].value_counts())

print('mode-node-caps', df['node-caps'].value_counts().index[0])
```

```
no     227
yes     56
?       10
Name: node-caps, dtype: int64
mode-node-caps no
```

In [13]:
```
# Check the next feature
display(df['breast-quad'].value_counts())

print('mode-breast-quad', df['breast-quad'].value_counts().index[0])
```

```
left_low     111
left_up       99
right_up      33
right_low     26
central       23
?              1
Name: breast-quad, dtype: int64
mode-breast-quad left_low
```

In [14]:
```
# Replace '?' with mode - value/level with highest frequency in the feature
df['node-caps'] = df['node-caps'].replace({'?':'no'})
df['breast-quad'] = df['breast-quad'].replace({'?':'left_low'})
```

In [15]:
```
# Again, check unique levels and see any marker is used or left out for a missi
for col in df.columns:
    if df[col].dtype == object:
        print (col, df[col].unique())
```

```
menopause ['premeno' 'ge40' 'lt40']
node-caps ['no' 'yes']
breast ['right' 'left']
breast-quad ['left_up' 'central' 'left_low' 'right_up' 'right_low']
irradiat ['no' 'yes']
recurrence ['no-recurrence-events' 'recurrence-events']
```

Incorrect Entries

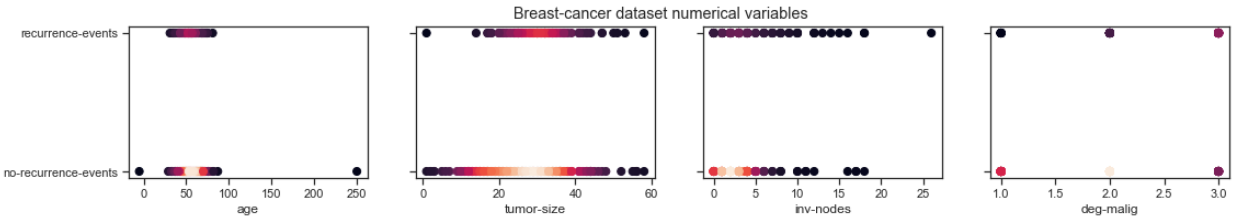
Remember the age value `250` from previous cells?

Finding out incorrect entries is more difficult than the previous steps as incorrect entries truly depend on the data column and **domain knowledge**. For this step we will look at the plots of numerical columns and figure out possible incorrect entries, such as outliers. Also, subject-matter experts (SME) would help greatly in real-world projects about incorrect entries.

Note it may not be easy (or possible at all) to correct the incorrect entries and sometimes the best is dropping that data point.

In [16]:
```
# Let's use kernel density estimation to color the density
from scipy.stats import gaussian_kde

# We will reuse this plotting function later
def plot_bc_numericals(_df):
    fig, axs = plt.subplots(1, 4, figsize=(18, 2.5), sharey=True, dpi=72)
    y = _df['recurrence'].astype('category').cat.codes.ravel()
    xy = np.vstack([_df['age'],y]); z = gaussian_kde(xy)(xy)
    axs[0].scatter(_df['age'], _df['recurrence'], c=z, s=50, edgecolor=None)
    axs[0].set_xlabel('age')
    xy = np.vstack([_df['tumor-size'],y]); z = gaussian_kde(xy)(xy)
    axs[1].scatter(_df['tumor-size'], _df['recurrence'], c=z, s=50, edgecolor=N
    axs[1].set_xlabel('tumor-size')
    xy = np.vstack([_df['inv-nodes'],y]); z = gaussian_kde(xy)(xy)
    axs[2].scatter(_df['inv-nodes'], _df['recurrence'], c=z, s=50, edgecolor=No
    axs[2].set_xlabel('inv-nodes')
    xy = np.vstack([_df['deg-malig'],y]); z = gaussian_kde(xy)(xy)
```

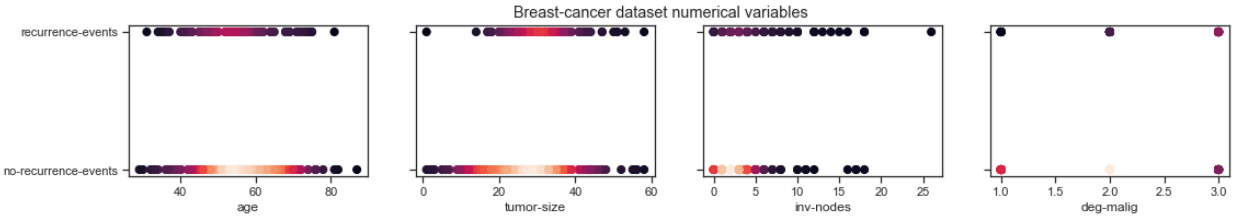
```
    axs[3].scatter(_df['deg-malig'], _df['recurrence'], c=z, s=50, edgecolor=No
    axs[3].set_xlabel('deg-malig')
    fig.suptitle('Breast-cancer dataset numerical variables')
    plt.show()

plot_bc_numericals(df)
```



In [17]:
```
# Remove that line with the incorrect age=250 and age=-5
dftemp = df.copy()  # use a temporary DataFrame
display(dftemp[dftemp['age']==250])
index_to_drop = dftemp[dftemp['age']==250].index
dftemp.drop(index_to_drop, inplace=True)
index_to_drop = dftemp[dftemp['age']==-5].index
dftemp.drop(index_to_drop, inplace=True)

# Check results
print(f'#total= {len(dftemp)}')
plot_bc_numericals(dftemp)
```

	age	menopause	tumor-size	inv-nodes	node-caps	deg-malig	breast	breast-quad	irradiat	recurrence
10	250.0	premeno	30.0	3.0	no	2	left	right_low	yes	no-recurrence-events

```
#total= 291
```



In [18]:
```
# Let's reset the indices to the dataframe after dropping a few rows
dftemp = dftemp.reset_index(drop=True)
```

Question: What if we don't reset the index?

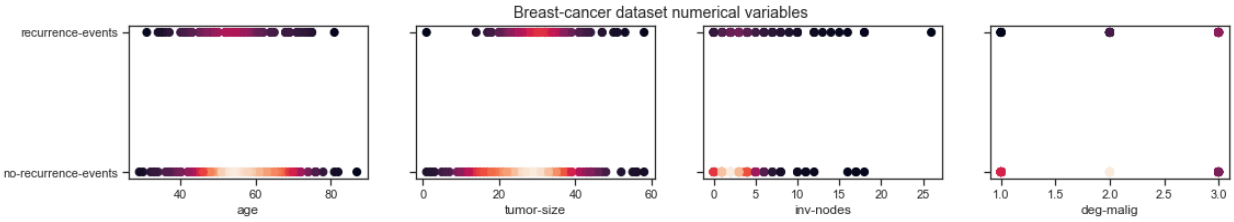
Alternative Data Manipulation

- Use of `apply` method via passing a `lambda`
- Use age as an integer variable, possibly using integer for all 'age' values

In [19]:
```
# Replace anomalous ages with mean when age is less than 0 or greater than 120
mean_age = int(df['age'].mean())
df['age'] = df['age'].apply(lambda x: mean_age if x<0 or x>120 else x)
```

```
# Check results
print(f'#total= {len(df)}')
plot_bc_numericals(df)
```

```
#total= 293
```



Cleaning Complete

Compare the previous two cells to see the effect of removing the incorrect age entry.

At this point we are ready to apply a few learners to our data such as the Random Forest classifier.

Discretization

Discretization is the process where a numerical variable is mapped to some levels by binning. This step is a big research/engineering area in machine learning. Recall that an example was provided in the past modules where the target (dependent) variable was discretized into three levels.

For our purposes, in this step, we will do the post-discretization, and apply one hot encoding to a nominal/discretized variable. Note that the variable might be a nominal variable naturally, such as the `'breast'` variable which takes values from the alphabet {`'left'`, `'right'`}.

Generally we keep the dependent variable as integer even if the cardinality is more than 2.

Now, we would like to continue preparing (preprocess) the dataset further to meet the requirements of the classifier that we would like to use - Random Forest classifier from `scikit-learn` library. This classifier works only on numerical data, thus we will convert the nominal variables into one hot encoded numerical variables, as explained in previous modules.

In [20]:
```
# pandas get_dummies function is the one-hot-encoder
def encode_onehot(_df, _f):
    _df2 = pd.get_dummies(_df[_f], prefix='', prefix_sep='').groupby(level=0, a
    _df3 = pd.concat([_df, _df2], axis=1)
    _df3 = _df3.drop([_f], axis=1)
    return _df3

# Print nominal variables
```

```
for f in list(df.columns.values):
    if df[f].dtype == object:
        print(f)
```

```
menopause
node-caps
breast
breast-quad
irradiat
recurrence
```

Question: Will we one-hot-encode the dependent variable `'recurrence'`?

In [21]:
```
# Display the original
display(df['menopause'][:10])

# Apply the onehot-encoding method
df_o = encode_onehot(df, 'menopause')

# Check the onehot-encoded version of this feature
cols = []
for f in list(df_o.columns.values):
    if 'menopause' in f:
        cols += [f]
```

```
0     premeno
1     premeno
5        ge40
6        ge40
7     premeno
8     premeno
9     premeno
10    premeno
11    premeno
14       ge40
Name: menopause, dtype: object
```

In [22]:
```
# Display the onehot-encoded
display(df_o[cols][:10])
```

	menopause - ge40	menopause - lt40	menopause - premeno
0	0	0	1
1	0	0	1
5	1	0	0
6	1	0	0
7	0	0	1
8	0	0	1
9	0	0	1
10	0	0	1
11	0	0	1
14	1	0	0

In [23]:
```
# Apply the rest of the nominal features too
df_o = encode_onehot(df_o, 'node-caps')
df_o = encode_onehot(df_o, 'breast')
df_o = encode_onehot(df_o, 'breast-quad')
df_o = encode_onehot(df_o, 'irradiat')
```

In [24]:
```
# Let's check how many features we have
print(f'before={len(df.columns)}, after={len(df_o.columns)}')
```

```
before=10, after=19
```

In [25]:
```
df_o.head()
```

Out[25]:

	age	tumor-size	inv-nodes	deg-malig	recurrence	menopause - ge40	menopause - lt40	menopause - premeno	node-caps - no	node-caps - yes
0	44.0	21.0	2.0	2	no-recurrence-events	0	0	1	1	0
1	46.0	22.0	3.0	3	recurrence-events	0	0	1	0	1
5	56.0	19.0	4.0	1	no-recurrence-events	1	0	0	1	0
6	58.0	41.0	0.0	2	recurrence-events	1	0	0	1	0
7	53.0	36.0	0.0	3	no-recurrence-events	0	0	1	0	1

Evaluation

Next, let's classify the preprocessed dataset using the following strategies:

1. 80% random train-test split
2. Leave-one-out
3. 10-fold cross validation
4. Stratified 10-fold cross validation

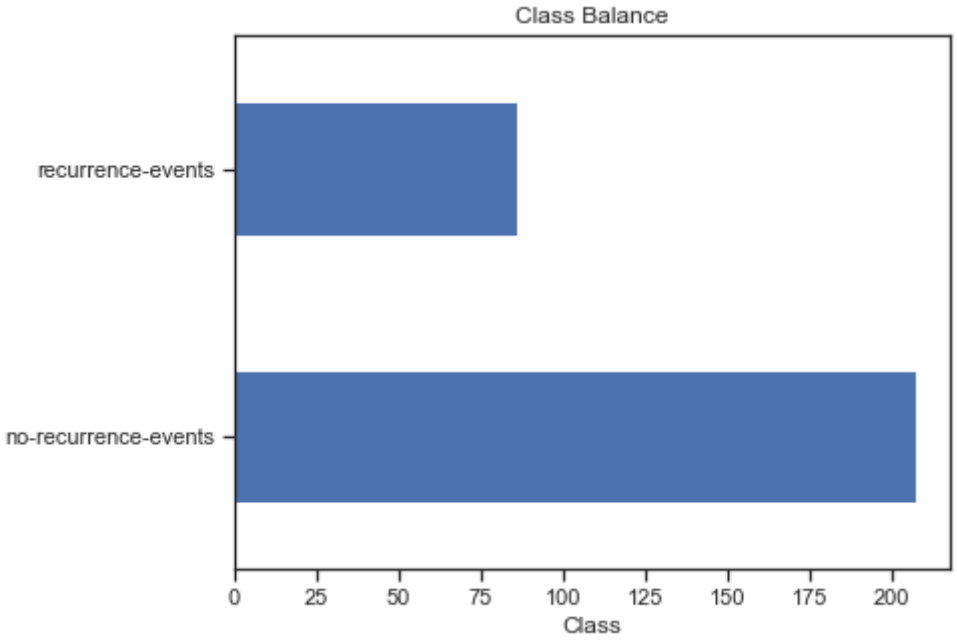
Note that the target variable is binary, predicting when the cancer is recurred, or the cancer did not recur. Clearly this dataset has ground truth captured from the data source, or in other words, dataset is pre-labeled, or carry the ground truth. Thus, we will employ **supervised learning**.

Important: Do not forget to remove the target (predicted, dependent) variable from `X`. Remember the `Dataframe` we are working already has the target variable, and we will move it to `y` vector.

In [26]:
```
# Show that the dependent variable is unbalanced
display(df['recurrence'].value_counts())
```

```
df['recurrence'].value_counts().plot(kind='barh', xlabel='Class', title='Class

# The semicolon above causes hiding the result of the last expression in the Ce
```

```
no-recurrence-events    207
recurrence-events        86
Name: recurrence, dtype: int64
```



In [27]:
```
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score, f1_score
from sklearn.model_selection import KFold, StratifiedKFold, train_test_split

# Converting from class labels integers
# df_o['recurrence'] = df_o['recurrence'].replace({'recurrence-events':1, 'no-r

# We will reuse the classifier function below
def rf_train_test(_X_tr, _X_ts, _y_tr, _y_ts):
    # Create a new random forest classifier, with working 4 parallel cores
    rf = RandomForestClassifier(n_estimators=200, max_depth=5, random_state=0,
    # Train on training data
    rf.fit(_X_tr, _y_tr)
    # Test on training data
    y_pred = rf.predict(_X_ts)
    # Return more proper evaluation metric
    # return f1_score(_y_ts, y_pred, pos_label='recurrence-events', zero_divisi
    # Return accuracy
    return accuracy_score(_y_ts, y_pred)
```

In [28]:
```
# Prepare the input X matrix and target y vector
X = df_o.loc[:, df_o.columns != 'recurrence'].values
y = df_o.loc[:, df_o.columns == 'recurrence'].values.ravel()
```

In [29]:
```
# Sanity check
print(y[:10])
```

```
['no-recurrence-events' 'recurrence-events' 'no-recurrence-events'
 'recurrence-events' 'no-recurrence-events' 'recurrence-events'
 'no-recurrence-events' 'no-recurrence-events' 'no-recurrence-events'
 'no-recurrence-events']
```

80% Random Train-test Split Evaluation

In [30]:
```
# 80% split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20, rando
rf_train_test(X_train, X_test, y_train, y_test)
```

Out[30]:
```
0.7966101694915254
```

Question: What will be the performance (i.e., accuracy) when we run the above cell again? Will you see any variations?

In [31]:
```
# Run 10 times
for i in range(10):
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20, r
    print(rf_train_test(X_train, X_test, y_train, y_test))
```

```
0.7966101694915254
0.7796610169491526
0.7966101694915254
0.7627118644067796
0.6610169491525424
0.7627118644067796
0.7457627118644068
0.7288135593220338
0.7627118644067796
0.7457627118644068
```

Important: As the training and testing partition changes, the performance follows respectively.

Question: How can we measure the performance so that we can be sure of reporting it right?

In [32]:
```
%%time

# Run 100 times and collect statistics
Accuracies = []
for _ in range(100):
    X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.20, r
    Accuracies += [rf_train_test(X_train, X_test, y_train, y_test)]

print(f'80% train-test split accuracy is {np.mean(Accuracies):.3f} {chr(177)}{r
```

```
80% train-test split accuracy is 0.797 ±0.0000
CPU times: total: 22.3 s
Wall time: 20.6 s
```

Leave-one-out Evaluation

Leave-one-out evaluation keeps a single data point and label for test and uses all except for the test vector for training. Then, the evaluation process repeats this for each of the remaining data points, having a total number of N accuracies.
The `sklearn` API says `train` and `test` require a 2D `X` and 1D `y` even when there is only one data point. Below code generates the test vectors properly.

This evaluation is helpful when data is scarce such as in the Bioinformatics and Medical fields.

In [33]:
```
%%time

# Leave one out testing - this takes relatively longer
N = X.shape[0]
Accuracies = []
for i in range (0,N):
    # Keep the 2D vector for the single test data point X
    X_test = X[i].reshape(1, -1)
    X_train = np.delete(np.array(X, copy=True), i, axis=0)

    # Keep the 1D vector for the single test label y
    y_test = [y[i]]
    y_train = np.delete(np.array(y, copy=True), i, axis=0)
    Accuracies += [rf_train_test(X_train, X_test, y_train, y_test)]

# Sanity
print(f'Leave-one-out accuracy N= {N}, #accuracies= {len(Accuracies)}')

# Score
print(f'Leave-one-out accuracy is {np.mean(Accuracies):.3f} {chr(177)}{np.std(A
```

```
Leave-one-out accuracy N= 293, #accuracies= 293
Leave-one-out accuracy is 0.737 ±0.4402
CPU times: total: 1min 7s
Wall time: 1min 1s
```

10-fold Cross Validation Evaluation

In [34]:
```
%%time

# 10-fold cross validation
Accuracies = []
kfold = KFold(n_splits=10,shuffle=False)
for train_index, test_index in kfold.split(X, y):
    acc = rf_train_test(X[train_index], X[test_index], y[train_index], y[test_i
    Accuracies += [acc]

print(f'10-fold cross validation accuracy is {np.mean(Accuracies):.3f} {chr(177
```

```
10-fold cross validation accuracy is 0.747 ±0.0595
CPU times: total: 2.3 s
Wall time: 2.12 s
```

Stratified 10-fold Cross Validation Evaluation

In [35]:
```
%%time

def eval_classifier(_X, _y, _niter):
    accs = []
    for i in range(_niter):
        kf = StratifiedKFold(n_splits=10,shuffle=True,random_state=i)
        for tr_ix, ts_ix in kf.split(_X, _y):
            accuracy = rf_train_test(_X[tr_ix], _X[ts_ix], _y[tr_ix], _y[ts_ix]
            accs += [accuracy]

    print(f'Stratified 10-fold CV acc={np.mean(accs):.3f} {chr(177)}{np.std(acc

eval_classifier(X, y, 1)
eval_classifier(X, y, 10)
```

```
Stratified 10-fold CV acc=0.734 ±0.0734 with 1 iterations
Stratified 10-fold CV acc=0.738 ±0.0656 with 10 iterations
CPU times: total: 26.4 s
Wall time: 23.5 s
```

Note the above performance results for discussion in the following cells.

Question: What are the differences between these four evaluation methods?

Data Transformation

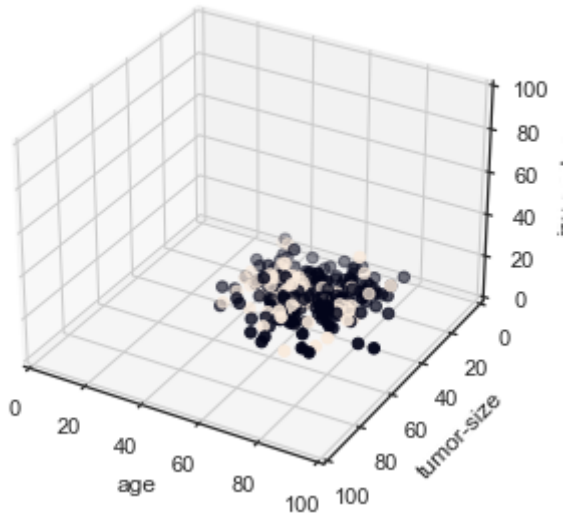
Now that we preprocessed and used the data for classification we can move to other interesting problems.

Imagine, we did not have the ground truth, so that a supervised learning was not possible. A natural approach in this case is clustering the data to see if there are some patterns or models we can come up with that explains the cancer behavior. We will attempt answering questions like *"Is there a direct relation between menopause and cancer?"*

First, let's draw some plots where the x, y and z-dimensions are `'age'`, `'tumor-size'`, `'inv-nodes'` and color is `'recurrence'`.

In [36]:
```
from mpl_toolkits.mplot3d import Axes3D

# Deep copy original dataframe
df2 = df.copy()

# Convert every feature to numbers
df2['recurrence'] = df['recurrence'].astype("category").cat.codes

df2['menopause'] = df['menopause'].astype("category").cat.codes.astype('float')
df2['node-caps'] = df['node-caps'].astype("category").cat.codes.astype('float')
df2['breast'] = df['breast'].astype("category").cat.codes.astype('float')
df2['breast-quad'] = df['breast-quad'].astype("category").cat.codes.astype('flo
df2['irradiat'] = df['irradiat'].astype("category").cat.codes.astype('float')

df2['deg-malig'] = df['deg-malig'].astype('float')
```

```
def draw3d(_df, _mn, _mx):
    fig = plt.figure(dpi=72)
    ax = fig.add_subplot(111, projection='3d')
    ax.set_xlim3d(_mn, _mx)
    ax.set_ylim3d(_mn, _mx)
    ax.set_zlim3d(_mn, _mx)
    ax.set_ylim(ax.get_ylim()[::-1])
    ax.scatter(_df['age'], _df['tumor-size'], _df['inv-nodes'], c=_df['recurrer
    ax.set_xlabel('age'); ax.set_ylabel('tumor-size'); ax.set_zlabel('inv-nodes

draw3d(df2, 0, 100)
```



Question: Do the dimensions `'age'`, `'tumor-size'`, `'inv-nodes'` look fine in the above 3D plot?

Answer: The features are clumped and not nicely occupy $[0 - 100]$ range, i.e. we are not seeing a spherical cluster shape.

Let's cluster the cancer data, without using the ground truth. We have to convert the nominal variables to numerical by using the category codes like we applied to `'recurrence'` variable.

Important: Make sure every variable is of the same type, e.g. `float32`.

Important: Note that the values `'recurrence'` took { `0`, `1` }, and by looking at the 3d plot above, can we easily find out which values (`0` or `1`) corresponds to `'recurrence-events'` levels?

In [37]:
```
from sklearn.cluster import KMeans

def kmeans(_X, _y, niter):  # do it niter times to collect statistics
    accuracies = []
    for _ in range(niter):
        # We know that there are two levels in target variable - thus n_cluster
        km = KMeans(n_clusters=2, random_state=0, n_init=10)
        clusters = km.fit_predict(_X)
        accuracies += [accuracy_score(_y, clusters)]
```

```
    return np.mean(accuracies)

X = df2.loc[:, df2.columns != 'recurrence'].values
y = df2.loc[:, df2.columns == 'recurrence'].values.ravel()

print(f'Clustering error= {kmeans(X, y, 100):.3f}')
```

```
Clustering error= 0.529
```

Above performance is not very good as the error is almost equivalent to random choice, which would be $\frac{1}{2}$ since we have 2 classes.

Normalization and Standardization

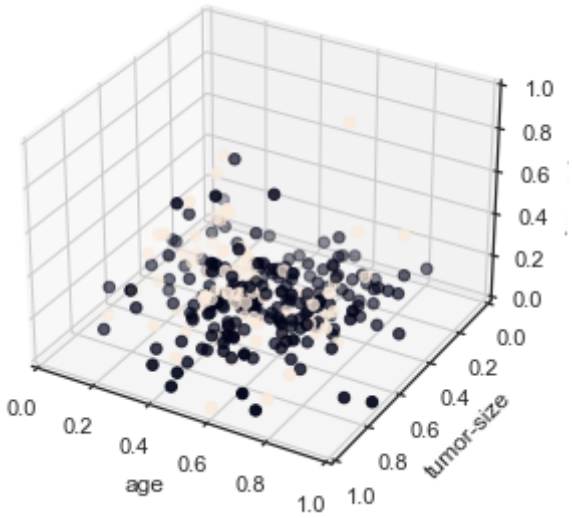
Mapping the values of a column to $[0, 1]$ range is normalization: $\frac{x_i - \min(x)}{\max(x) - \min(x)}$

Standardization is mapping the values to a 0-mean 1-standard-deviation distribution: $\frac{x_i - \text{mean}(x)}{\text{stdev}(x)}$

Normalization makes the **optimization surface** more **spherical**, which helps the optimizer using each feature with equal importance. This is especially important and helping for **distance** based methods, such as neural networks, SVM, etc. Note that some probabilistic methods are Naive Bayes, decision trees, etc.

Let's try two scalers from `sklearn.preprocessing` 1.Normalization `MinMaxScaler()`, 2. Standardization `scale()`

In [38]:
```
from sklearn import preprocessing

min_max_scaler = preprocessing.MinMaxScaler()
df2[['age', 'tumor-size', 'inv-nodes']] = min_max_scaler.fit_transform(df2[['ag

draw3d(df2, 0, 1)
```



By normalizing the values through expansion and contraction to $[0, 1]$ we achieve the **distance** between the data points are in the same "range" or unit. Thus, the distance metrics like Euclidean distance will weigh each **dimension** or feature **equally**.

Example: Imagine a dataset which has speed in miles $[0, 100]$ and time traveled in seconds $[0, 43200]$ (12 hours max). A proper approach would be mapping both features into $[0, 1]$ scale to treat the feature space spherically. For actual feature values an inverse transformation can be used to map back to the original units (for example to be presented to user).

A distance metric d in M dimensions (`Dataframe` has M number of columns) such as Euclidean $d_{ik} = \sqrt{\sum_{j=0}^{M}(x_{ij} - x_{kj})^2}$

As an example, clustering algorithms use some form of distance metric such as Euclidean distance between pairs of data points.

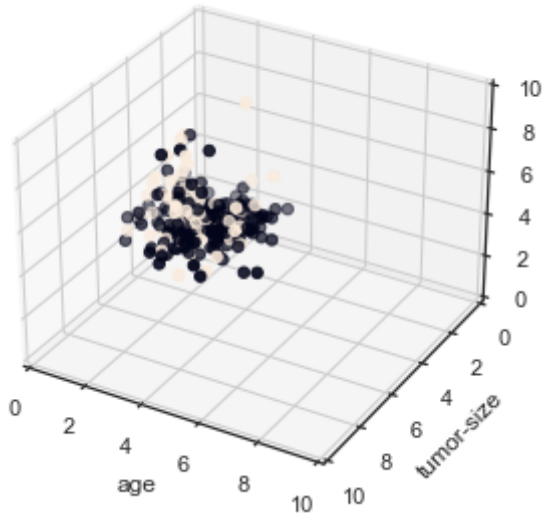
As can be seen from above example, normalization of variables is a necessary step for clustering.

In [39]:
```
df2[['deg-malig', 'breast-quad']] = min_max_scaler.fit_transform(df2[['deg-mali

X = df2.loc[:, df2.columns != 'recurrence'].values
y = df2.loc[:, df2.columns == 'recurrence'].values.ravel()

print(f'Clustering error= {kmeans(X, y, 100):.3f}')
```

```
Clustering error= 0.491
```

And now standardization.

In [40]:
```
df2[['age', 'tumor-size', 'inv-nodes']] = preprocessing.scale(df2[['age', 'tumo

draw3d(df2, 0, 10)
```



In [41]:
```
df2.head()
```

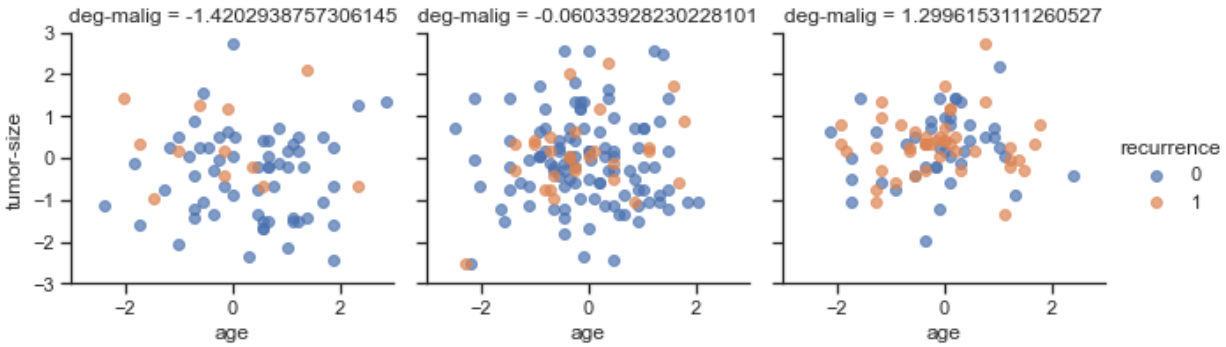
Out[41]:

	age	menopause	tumor-size	inv-nodes	node-caps	deg-malig	breast	breast-quad	irradiat	recurr
0	-1.089465	2.0	-0.679846	-0.425865	0.0	0.5	1.0	0.50	0.0	
1	-0.904923	2.0	-0.587270	-0.155533	1.0	1.0	1.0	0.50	0.0	
5	0.017786	0.0	-0.864999	0.114798	0.0	0.0	1.0	0.00	0.0	
6	0.202328	0.0	1.171677	-0.966529	0.0	0.5	0.0	0.25	0.0	
7	-0.259027	2.0	0.708796	-0.966529	1.0	1.0	1.0	0.25	1.0	

In [42]:
```
df2[['deg-malig', 'breast-quad']] = preprocessing.scale(df2[['deg-malig', 'brea

X = df2.loc[:, df2.columns != 'recurrence'].values
y = df2.loc[:, df2.columns == 'recurrence'].values.ravel()

print(f'Clustering error= {kmeans(X, y, 100):.3f}')
```

```
Clustering error= 0.488
```

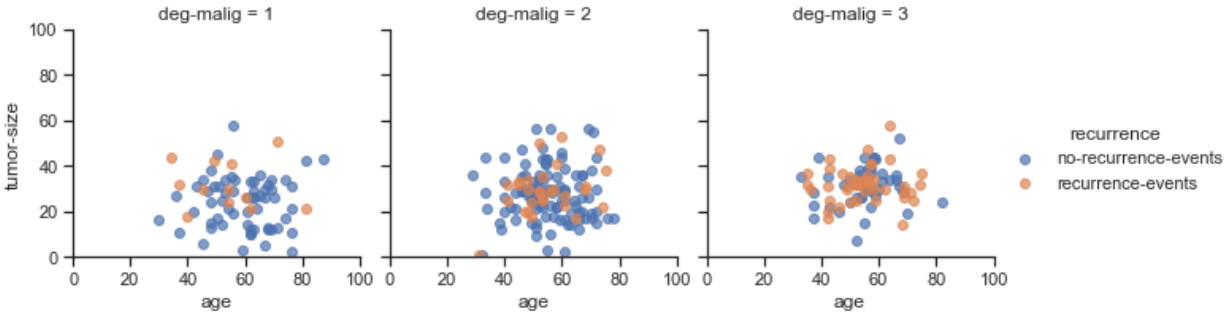
In [43]:
```
# Scaled
plot_bc(df2, xyscale=[-3,3])
```



Question: Do you see any difference/improvement on the variables compared to the first set of plots in cell 1, repeated below?

Answer: Shapes are same but axis scales are different.

In [44]:
```
# Original
plot_bc(df, xyscale=[0,100])
```



Note that after variable transformation, variables become more spherical or Gaussian like, but then the levels or data points do not correspond to any meaningful value in the domain knowledge that the dataset originally belonged to. For example `'deg-malig'` had three levels {1, 2, 3} which probably meant something to the doctors dealing with cancer patients. However, depending on the dataset, such transformations make a difference, albeit a few percentage improvement on the performance.

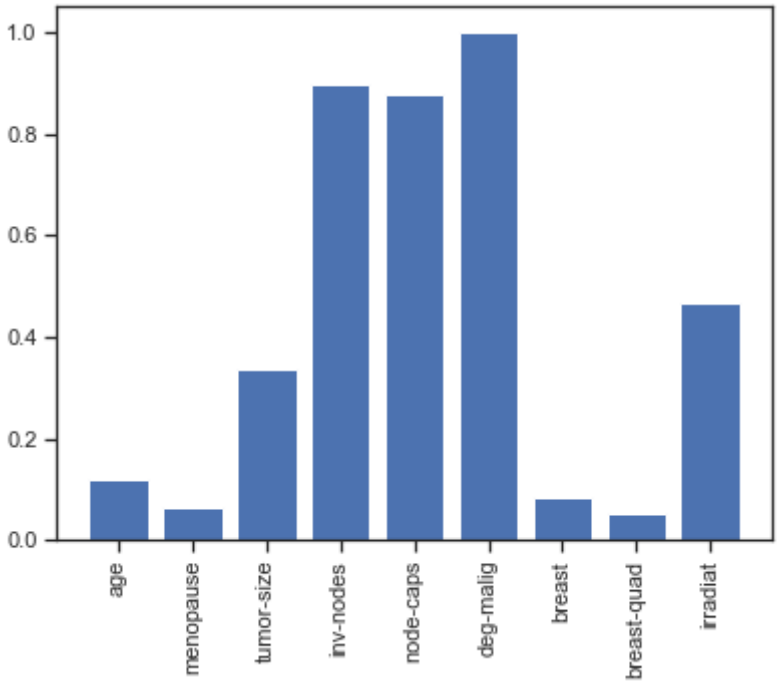
Data Reduction

Reducing the data helps in a few ways:

- Faster method run-time, such as training
- More generalized models, decreases overfitting
- Simpler models that make more sense to the domain expert or subject-matter expert (SME)
- In some cases better accuracy performance - not necessarily always happens

Feature ranking and **feature selection** is a common stage that is executed after cleaning and preprocessing the data. In the following cells we will examine the variable rankings by **Univariate Feature Selection**.

In [45]:
```
from sklearn.feature_selection import SelectPercentile, f_classif


selector = SelectPercentile(f_classif, percentile=10)
# Fit the data
selector.fit(X, y)
scores = -np.log10(selector.pvalues_)
scores /= scores.max()

# Display
cols = list(df2.loc[:, df2.columns != 'recurrence'].columns.values)
y_pos = np.arange(len(cols))
plt.bar(y_pos, scores)
plt.xticks(y_pos, cols, rotation=90)
plt.show()
```



Question: Can we drop `'age'`, `'menopause'`, `'breast'`, `'breast-quad'` variables and redo the classification evaluation without a performance loss?

In [46]:
```
df3 = df2.copy()
df3.drop(columns='age', inplace=True)
df3.drop(columns='menopause', inplace=True)
df3.drop(columns='breast', inplace=True)
df3.drop(columns='breast-quad', inplace=True)

X = df3.loc[:, df3.columns != 'recurrence'].values
y = df3.loc[:, df3.columns == 'recurrence'].values.ravel()
```

In [47]:
```
eval_classifier(X, y, 10)
```

```
Stratified 10-fold CV acc=0.755 ±0.0610 with 10 iterations
```

Wow! The performance accuracy did not drop. And we have less data columns now.

Note that we had standardized the data in the previous steps. Let's go back to the original dataset just after the cleaning was completed.

In [48]:
```
df4 = df_o.copy()
df4.drop(columns='age', inplace=True)

# 'menopause' was onehot-encoded
for col in df4.columns.values:
    if 'menopause' in col:
        df4.drop(columns=col, inplace=True)

# 'breast' was onehot-encoded
for col in df4.columns.values:
    if 'breast' in col:
        df4.drop(columns=col, inplace=True)

# 'breast-quad' was onehot-encoded
```

```
for col in df4.columns.values:
    if 'breast-quad' in col:
        df4.drop(columns=col, inplace=True)

X = df4.loc[:, df4.columns != 'recurrence'].values
y = df4.loc[:, df4.columns == 'recurrence'].values.ravel()
```

In [49]:
```
eval_classifier(X, y, 10)
```

```
Stratified 10-fold CV acc=0.755 ±0.0584 with 10 iterations
```

In [50]:
```
X = df_o.loc[:, df_o.columns.isin(['deg-malig', 'inv-nodes', 'node-caps - yes',
X.shape
```

Out[50]:
```
(293, 4)
```

In [51]:
```
eval_classifier(X, y, 10)
```

```
Stratified 10-fold CV acc=0.758 ±0.0633 with 10 iterations
```

More success! The performance accuracy increased! Or did we bias it?

Harder Question: Do you accept the performance increase as a valid increase? Or would you attribute it to the variance of error?

Question: What is the most important take-away in this effort?

References

1. Raschka, Sebastian. Python Machine Learning Ed. 3. Packt Publishing, 2019.

Exercises

Exercise 1. Change the cross validation from 10 folds to 3 folds and report its evaluation performance. Do you think 3-fold CV is better than 10-fold CV?

Exercise 2. Use only one feature/column in your classifier model to predict cancer. Report the best 10-fold CV performance.

Exercise 3. Use only `'age'` feature in your classifier model to predict cancer. Report the best 10-fold CV performance.

Exercise 4. Change the `accuracy_score` to `f1_score` and repeat previous exercises. Report findings.

In [52]:
```
%%html
<style>
    table {margin-left: 0 !important;}
```

```
</style>
<!-- Display markdown tables left oriented in this notebook. -->
```
