In [2]:
```
!pip install pycaret

import pandas as pd
import pycaret
import seaborn as sns
import missingno as msno
import numpy as np
from pycaret.classification import *
sns.set()
sns.set_context("paper")
pd.set_option('display.max_colwidth', None)
import matplotlib.pyplot as plt
```

```
The system cannot find the path specified.
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
Cell In[2], line 3
      1 get_ipython().system('pip install pycaret -q > /dev/null 2>&1')
----> 3 import pandas as pd
      4 import pycaret
      5 import seaborn as sns

File ~\AppData\Local\Programs\Python\Python311\Lib\site-packages\pandas\__init__.py:22
     19 del _hard_dependencies, _dependency, _missing_dependencies
     21 # numpy compat
---> 22 from pandas.compat import is_numpy_dev as _is_numpy_dev  # pyright: ignore # no
qa:F401
     24 try:
     25     from pandas._libs import hashtable as _hashtable, lib as _lib, tslib as _ts
lib

File ~\AppData\Local\Programs\Python\Python311\Lib\site-packages\pandas\compat\__init_
_.py:18
     15 from typing import TYPE_CHECKING
     17 from pandas._typing import F
---> 18 from pandas.compat.numpy import (
     19     is_numpy_dev,
     20     np_version_under1p21,
     21 )
     22 from pandas.compat.pyarrow import (
     23     pa_version_under1p01,
     24     pa_version_under2p0,
   (...)
     31     pa_version_under9p0,
     32 )
     34 if TYPE_CHECKING:

File ~\AppData\Local\Programs\Python\Python311\Lib\site-packages\pandas\compat\numpy\__
init__.py:4
      1 """ support numpy compatibility across versions """
      2 import numpy as np
----> 4 from pandas.util.version import Version
      6 # numpy versioning
      7 _np_version = np.__version__

File ~\AppData\Local\Programs\Python\Python311\Lib\site-packages\pandas\util\__init__.p
y:2
      1 # pyright: reportUnusedImport = false
----> 2 from pandas.util._decorators import (  # noqa:F401
      3     Appender,
      4     Substitution,
      5     cache_readonly,
      6 )
      8 from pandas.core.util.hashing import (  # noqa:F401
      9     hash_array,
     10     hash_pandas_object,
     11 )
     14 def __getattr__(name):

File ~\AppData\Local\Programs\Python\Python311\Lib\site-packages\pandas\util\_decorator
s.py:14
      6 from typing import (
      7     Any,
      8     Callable,
      9     Mapping,
     10     cast,
     11 )
     12 import warnings
---> 14 from pandas._libs.properties import cache_readonly
     15 from pandas._typing import (
     16     F,
     17     T,
     18 )
     19 from pandas.util._exceptions import find_stack_level

File ~\AppData\Local\Programs\Python\Python311\Lib\site-packages\pandas\_libs\__init__.
py:13
      1 __all__ = [
      2     "NaT",
      3     "NaTType",
   (...)
      9     "Interval",
     10 ]
---> 13 from pandas._libs.interval import Interval
     14 from pandas._libs.tslibs import (
     15     NaT,
     16     NaTType,
   (...)
     21     iNaT,
     22 )

File ~\AppData\Local\Programs\Python\Python311\Lib\site-packages\pandas\_libs\interval.
pyx:1, in init pandas._libs.interval()

ValueError: numpy.dtype size changed, may indicate binary incompatibility. Expected 96
from C header, got 88 from PyObject
```

In [ ]:

```
```

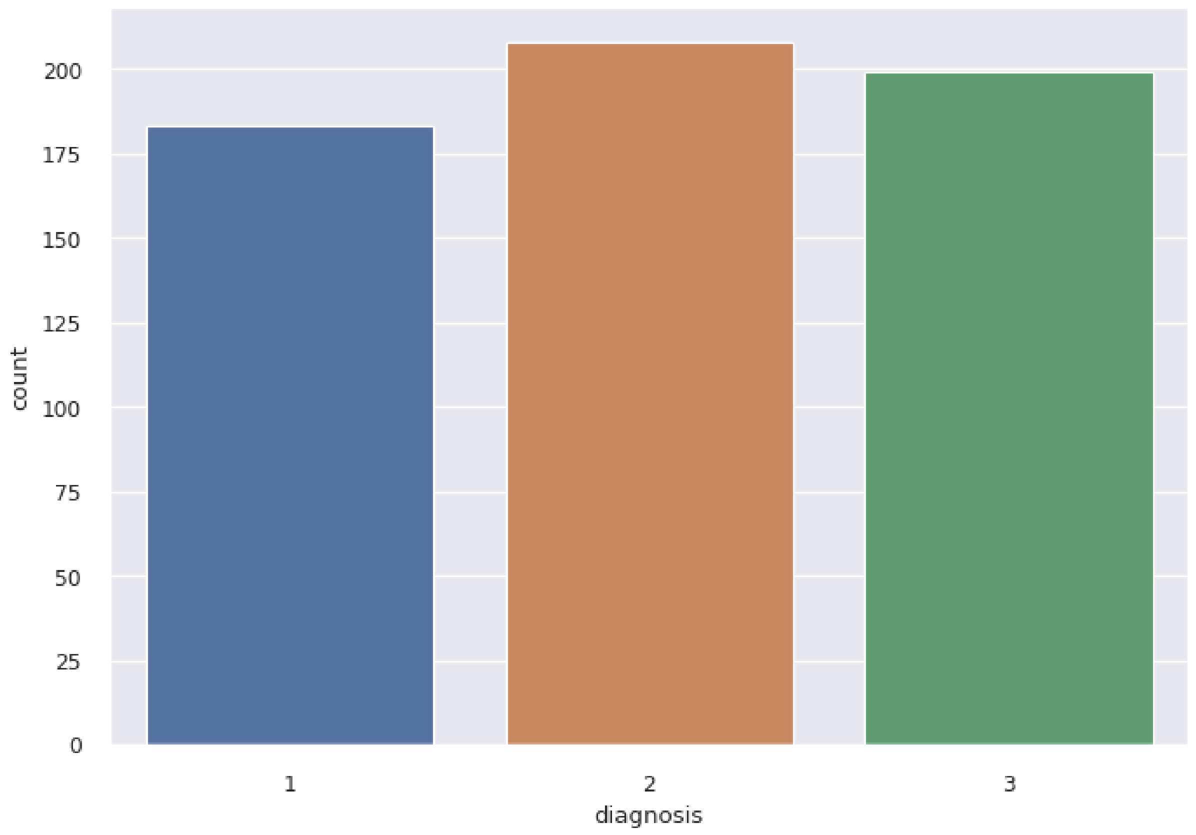
In [2]:

```
df = pd.read_csv('../input/urinary-biomarkers-for-pancreatic-cancer/Debernardi et al 202
print("The data has the shape: ",df.shape)
```

```
The data has the shape:  (590, 13)
```

In [3]:
```
sns.countplot(data = df, x = 'diagnosis')
```

Out[3]:
```
<AxesSubplot: xlabel='diagnosis', ylabel='count'>
```



In [4]:
```
df.sample(5).T
```

Out[4]:

sample_id	S143	S471	S33	S423	S409
patient_cohort	Cohort2	Cohort1	Cohort1	Cohort1	Cohort1
sample_origin	BPTB	LIV	BPTB	LIV	LIV
age	36	62	50	68	69
sex	F	F	M	M	F
diagnosis	1	3	1	3	3
stage	NaN	IIB	NaN	IIB	III
benign_sample_diagnosis	NaN	NaN	NaN	NaN	NaN
plasma_CA19_9	5.128234	318.0	3.53	91.0	556.0
creatinine	0.96135	1.36851	0.57681	2.30724	0.91611
LYVE1	0.019426	3.035614	0.535693	6.221869	7.494335
REG1B	47.254685	168.10784	17.93163	63.468804	77.32123
TFF1	19.42577	941.162229	139.494255	583.1935	1423.229437
REG1A	NaN	334.069	81.61	78.535	1232.933

In [5]:
```
df.describe()
```

Out[5]:

	age	diagnosis	plasma_CA19_9	creatinine	LYVE1	REG1B	TFF1	RE
count	590.000000	590.000000	350.000000	590.000000	590.000000	590.000000	590.000000	306.00
mean	59.079661	2.027119	654.002944	0.855383	3.063530	111.774090	597.868722	735.28
std	13.109520	0.804873	2430.317642	0.639028	3.438796	196.267110	1010.477245	1477.24
min	26.000000	1.000000	0.000000	0.056550	0.000129	0.001104	0.005293	0.00
25%	50.000000	1.000000	8.000000	0.373230	0.167179	10.757216	43.961000	80.69
50%	60.000000	2.000000	26.500000	0.723840	1.649862	34.303353	259.873974	208.53
75%	69.000000	3.000000	294.000000	1.139482	5.205037	122.741013	742.736000	649.00
max	89.000000	3.000000	31000.000000	4.116840	23.890323	1403.897600	13344.300000	13200.00

In [6]:
```
df.describe(include = 'object')
```

Out[6]:

	patient_cohort	sample_origin	sex	stage	benign_sample_diagnosis
count	590	590	590	199	208
unique	2	4	2	8	52
top	Cohort1	BPTB	F	III	Pancreatitis
freq	332	409	299	76	41

4/ Features

In [7]:
```
pd.read_csv('../input/urinary-biomarkers-for-pancreatic-cancer/Debernardi et al 2020 docu
```

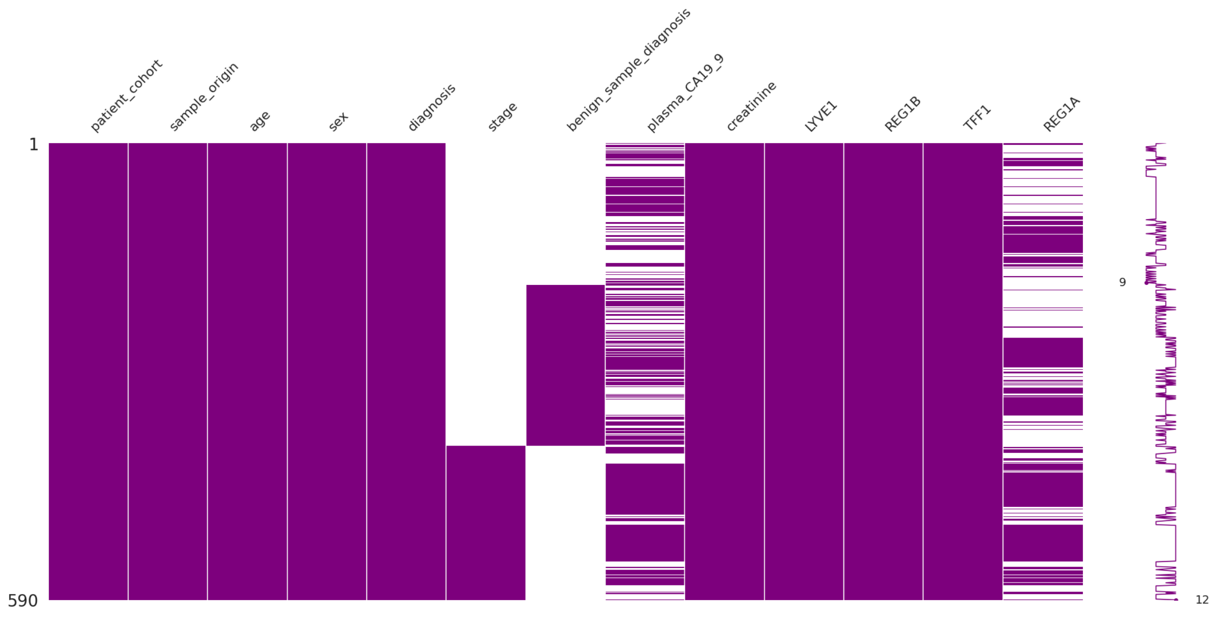
Out[7]:

Column name	Details
sample_id	Unique string identifying each subject
patient_cohort	Cohort 1, previously used samples; Cohort 2, newly added samples
sample_origin	BPTB: Barts Pancreas Tissue Bank, London, UK; ESP: Spanish National Cancer Research Centre, Madrid, Spain; LIV: Liverpool University, UK; UCL: University College London, UK
age	Age in years
sex	M = male, F = female
diagnosis	1 = control (no pancreatic disease), 2 = benign hepatobiliary disease (119 of which are chronic pancreatitis); 3 = Pancreatic ductal adenocarcinoma, i.e. pancreatic cancer
stage	For those with pancratic cancer, what stage was it? One of IA, IB, IIA, IIIB, III, IV
benign_sample_diagnosis	For those with a benign, non-cancerous diagnosis, what was the diagnosis?
plasma_CA19_9	Blood plasma levels of CA 19–9 monoclonal antibody that is often elevated in patients with pancreatic cancer. Only assessed in 350 patients (one goal of the study was to compare various CA 19-9 cutpoints from a blood sample to the model developed using urinary samples).
creatinine	Urinary biomarker of kidney function
LYVE1	Urinary levels of Lymphatic vessel endothelial hyaluronan receptor 1, a protein that may play a role in tumor metastasis
REG1B	Urinary levels of a protein that may be associated with pancreas regeneration.
TFF1	Urinary levels of Trefoil Factor 1, which may be related to regeneration and repair of the urinary tract
REG1A	Urinary levels of a protein that may be associated with pancreas regeneration. Only assessed in 306 patients (one goal of the study was to assess REG1B vs REG1A)

5/ Missing values

In [8]:
```
msno.matrix(df, color = (.5,0,.5))
```

Out[8]:
```
<AxesSubplot: >
```



Notice that large numbers of values for 'stage' and 'benign_sample_diagnosis' appear to be missing. Only diagnosis 2 values are present in the 'benign_sample_diagnosis' feature (as the name suggests) whereas only diagnosis 3 values are present in the 'stage' feature.

In [9]:
```
df[df['benign_sample_diagnosis'].isnull() == False].diagnosis.value_counts()
```

Out[9]:
```
2    208
Name: diagnosis, dtype: int64
```

In [10]:
```
df[df['stage'].isnull() == False].diagnosis.value_counts()
```

Out[10]:
```
3    199
Name: diagnosis, dtype: int64
```

These two features contain information **directly linked to the diagnosis target** and left in will **ruin** your model through **data leakage.** Many notebooks using this dataset make this mistake and achieve what seem to be highly accurate but ultimately unreliable models as a result.

In [11]:
```
df.isnull().sum()
```

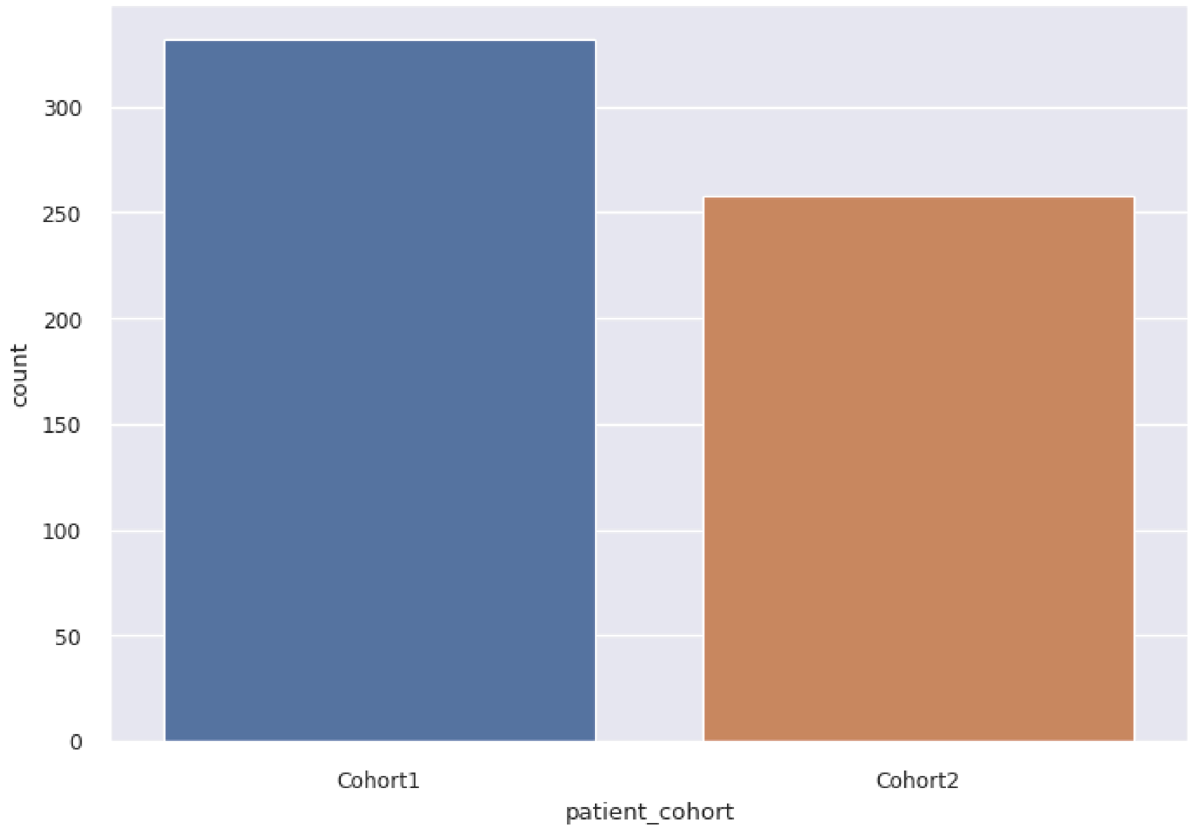
Out[11]:
```
patient_cohort             0
sample_origin              0
age                        0
sex                        0
diagnosis                  0
stage                    391
benign_sample_diagnosis  382
plasma_CA19_9            240
creatinine                 0
LYVE1                      0
REG1B                      0
TFF1                       0
REG1A                    284
dtype: int64
```

Also large numbers of values for 'plasma_CA19_9' and 'REG1A' are also missing, so we will need to choose a suitabel imputation strategy.

6/ Cohort

In [12]:
```
sns.countplot(x = df.patient_cohort)
```

Out[12]:
```
<AxesSubplot: xlabel='patient_cohort', ylabel='count'>
```



The two Cohorts consist of 'previously added samples' and 'newly added samples.' The Cohort feature is often left in models but should it be?

In [13]:
```
df.groupby('diagnosis')['patient_cohort'].value_counts(normalize = True)
```

Out[13]:
```
diagnosis  patient_cohort
1          Cohort2           0.557377
           Cohort1           0.442623
2          Cohort2           0.572115
           Cohort1           0.427885
3          Cohort1           0.814070
           Cohort2           0.185930
Name: patient_cohort, dtype: float64
```

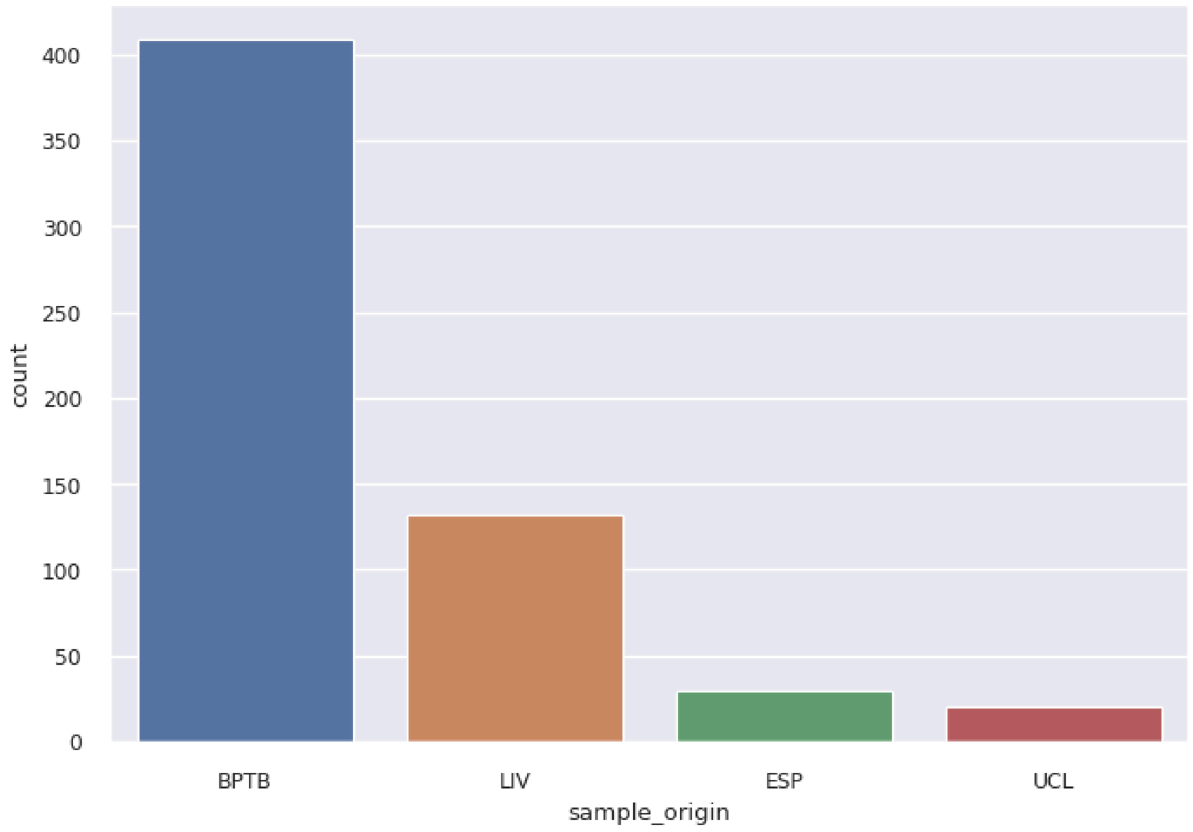
We can see from the above that 81% of patients diagnosed with cancer are in the Cohort1 group compared to only 19% in Cohort2. Any model using this feature would therefore assume that being in Cohort1 means that cancer is more likely and weight this feature accordingly,

However this feature should not be used because it will never appear in any future data and does not help us understand the impact of urinary biomarkers on diagnosis.

7/ Origin

In [14]:
```
sns.countplot(x = df.sample_origin)
```

Out[14]:
```
<AxesSubplot: xlabel='sample_origin', ylabel='count'>
```



Samples are drawn from four locations. Once again this feature is often used within models but perhaps should not be.

In [15]:
```
df.groupby('sample_origin')['diagnosis'].value_counts(normalize = True)
```

Out[15]:
```
sample_origin  diagnosis
BPTB           1            0.447433
               2            0.349633
               3            0.202934
ESP            3            0.793103
               2            0.206897
LIV            3            0.704545
               2            0.295455
UCL            2            1.000000
Name: diagnosis, dtype: float64
```

We can see above each sample origin site has different diagnosis proportions. It turns out that UCL samples contain only benign patient diagnoses, for example, whereas 70% of Liverpool's patients have cancer. Clearly if the model learned these weights it would not be at all helpful in determining the impact of urinary biomarkers.

8/ Useful features

Average levels of biomarker features are much higher amongst the cancer patients.

In [16]:
```
groups = df.groupby('diagnosis').mean()
groups.style.highlight_max()
```

Out[16]:

	age	plasma_CA19_9	creatinine	LYVE1	REG1B	TFF1	REG1A
diagnosis							
1	56.333333	8.749569	0.797633	1.212887	41.327901	169.024140	227.871886
2	54.701923	61.785741	0.847929	2.084612	64.174510	448.256897	547.458092
3	66.180905	1476.154733	0.916281	5.788567	226.308587	1148.611527	1138.323721

Some biomarkers reach their highest levels as the cancer progresses.

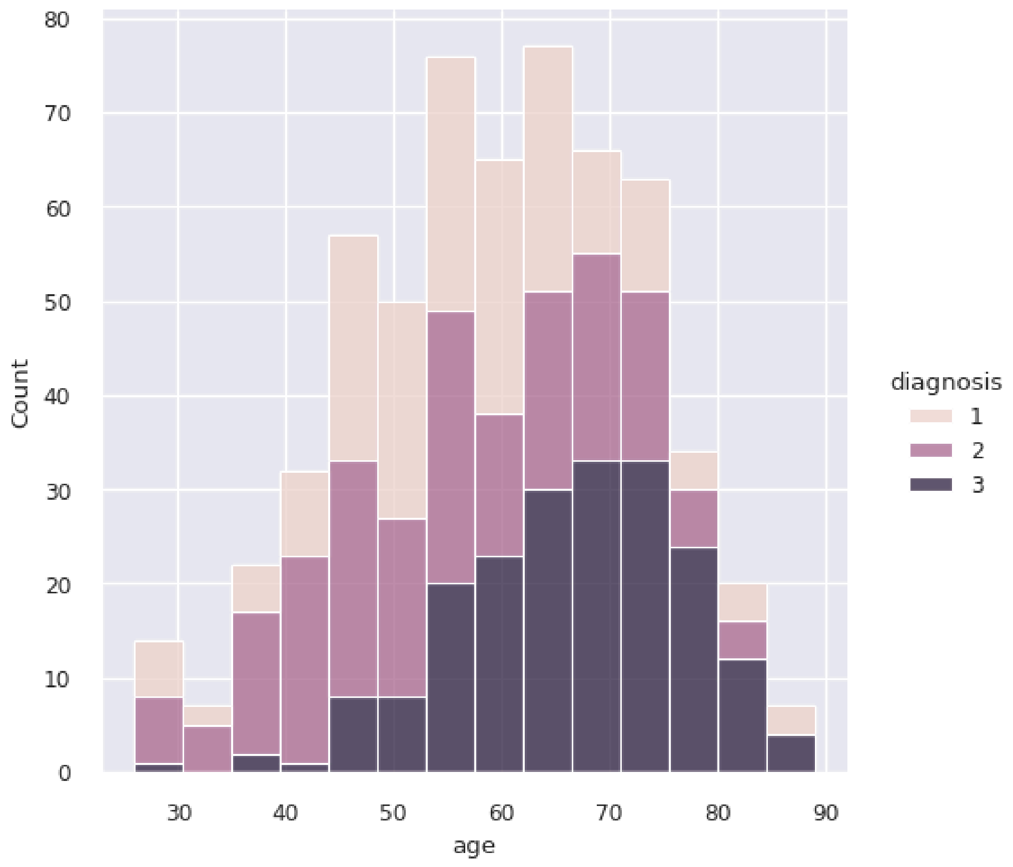
In [17]:
```
stage = df.groupby('stage').mean()
stage.drop(columns = 'diagnosis').style.highlight_max()
```

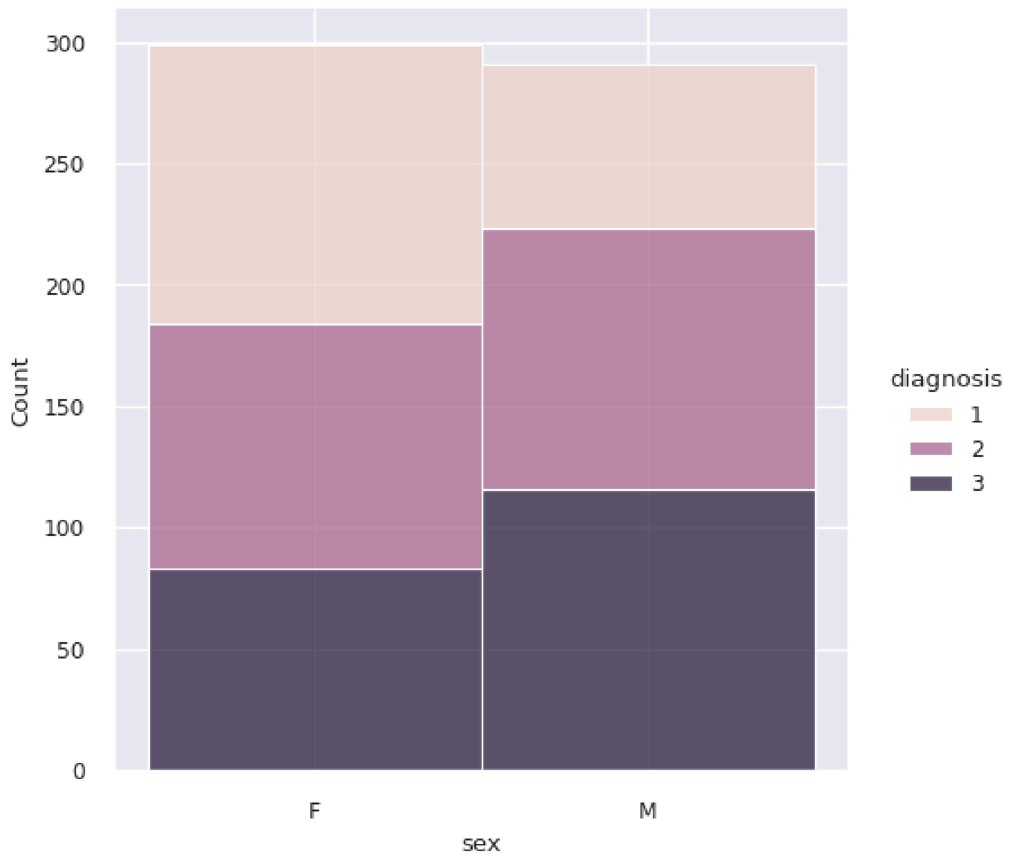
Out[17]:

	age	plasma_CA19_9	creatinine	LYVE1	REG1B	TFF1	REG1A
stage							
I	81.000000	nan	0.565500	12.017150	431.422530	874.099700	nan
IA	56.666667	10.666667	0.882180	2.030466	87.426656	330.596590	182.727500
IB	68.083333	1486.866667	0.615453	3.069541	128.816342	564.475333	1811.717200
II	65.714286	nan	1.016284	9.979902	503.062302	1467.856400	1929.561250
IIA	64.818182	592.909091	0.643642	3.113806	206.682191	1607.506765	636.385556
IIB	67.838235	1345.557833	0.782386	5.294798	199.195550	1068.569260	764.179700
III	63.789474	1662.508308	1.074896	6.296259	221.185408	1118.929278	1148.339125
IV	69.904762	3430.300000	1.078759	7.348032	316.456271	1632.152213	4132.146000

Pancreatic cancer likelihood increases with age and seems to affect men more than women.

In [18]:
```python
for feature in ['age','sex']:
    sns.displot(df,x= feature, hue="diagnosis", multiple='stack')
```





Several features have a strong correlation with diagnosis.

In [19]:
```
corr = df.corr().diagnosis.sort_values(ascending = False)
corr = corr.to_frame().drop(index = 'diagnosis')
corr.style.highlight_max()
```

Out[19]:

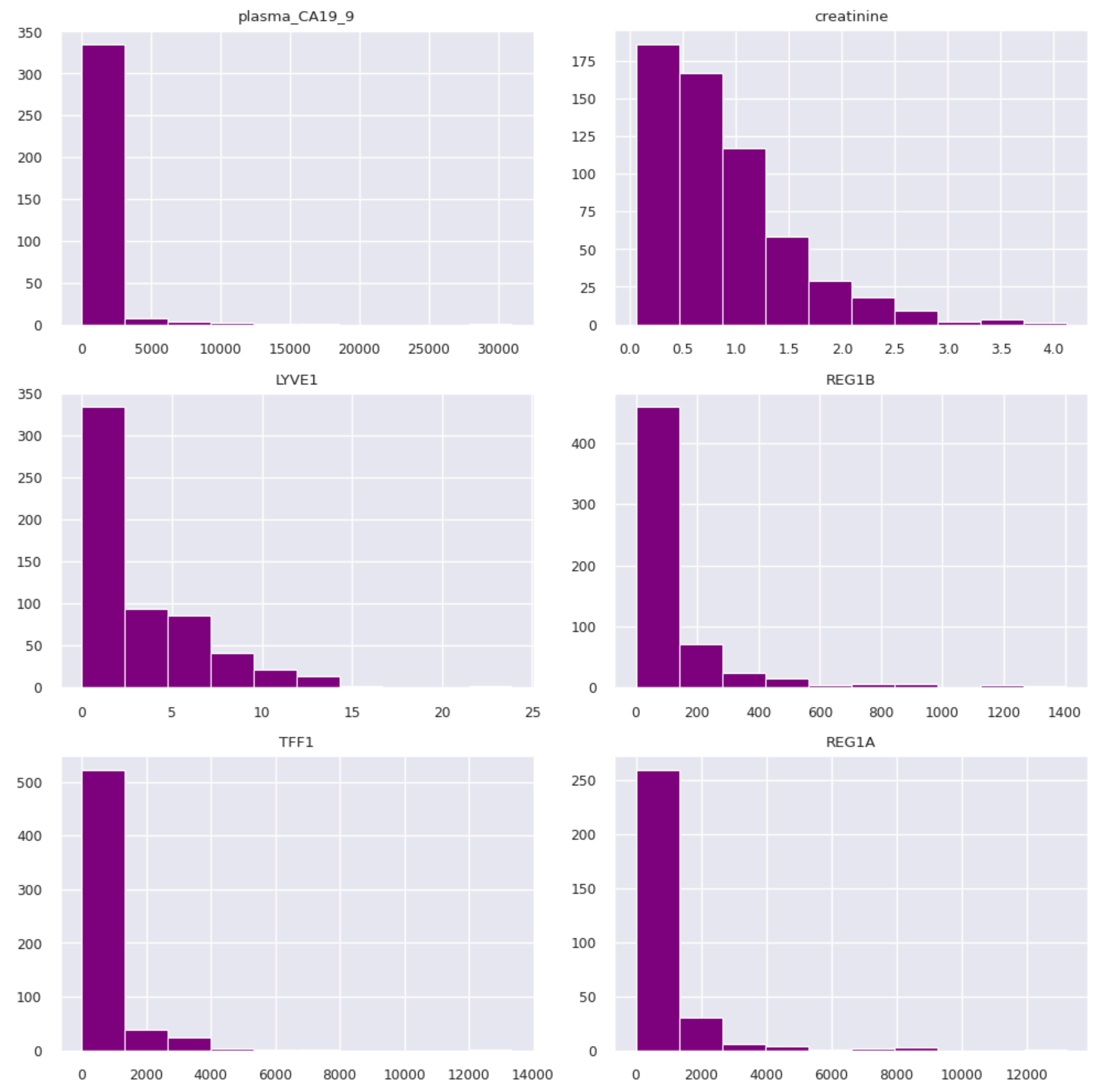
	diagnosis
LYVE1	0.540384
TFF1	0.392613
REG1B	0.383516
age	0.308251
plasma_CA19_9	0.263950
REG1A	0.260110
creatinine	0.074888

All the biomarker features seem to be right-skewed.

In [20]:
```
df.drop(columns = ['diagnosis','age']).skew().sort_values(ascending = False)
```

Out[20]:
```
plasma_CA19_9    8.018985
TFF1             5.158302
REG1A            4.469123
REG1B            3.333925
creatinine       1.466413
LYVE1            1.394014
dtype: float64
```

```
In [21]: df.drop(columns = ['diagnosis','age']).hist(figsize=(10,10), grid = True, color = 'purple
         plt.tight_layout()
```



9/ Classification

In this section we treat diagnosis as a multiclass problem, aiming to sort the patients into the three categories above.

```
In [22]: features_to_ignore = ['patient_cohort', 'sample_origin','stage','benign_sample_diagnosis
```

In [23]:
```
s = setup(df, target = 'diagnosis', experiment_name = 'pancreas', train_size = 0.8, sess
```

	Description	Value
0	Session id	71
1	Target	diagnosis
2	Target type	Multiclass
3	Target mapping	1: 0, 2: 1, 3: 2
4	Original data shape	(590, 13)
5	Transformed data shape	(590, 9)
6	Transformed train set shape	(472, 9)
7	Transformed test set shape	(118, 9)
8	Ignore features	4
9	Numeric features	7
10	Categorical features	1
11	Rows with missing values	100.0%
12	Preprocess	True
13	Imputation type	simple
14	Numeric imputation	median
15	Categorical imputation	mode
16	Maximum one-hot encoding	25
17	Encoding method	None
18	Normalize	True
19	Normalize method	zscore
20	Fold Generator	StratifiedKFold
21	Fold Number	10
22	CPU Jobs	-1
23	Use GPU	False
24	Log Experiment	False
25	Experiment Name	pancreas
26	USI	ade5

In [24]:
```
best = compare_models(n_select = 5,sort = 'Accuracy')
```

	Model	Accuracy	AUC	Recall	Prec.	F1	Kappa	MCC	TT (Sec)
gbc	Gradient Boosting Classifier	0.7477	0.0000	0.7477	0.7521	0.7466	0.6211	0.6238	0.2670
xgboost	Extreme Gradient Boosting	0.7414	0.8815	0.7414	0.7459	0.7400	0.6118	0.6148	0.1350
catboost	CatBoost Classifier	0.7413	0.8869	0.7413	0.7483	0.7414	0.6115	0.6140	2.7880
rf	Random Forest Classifier	0.7138	0.8751	0.7138	0.7155	0.7111	0.5705	0.5734	0.1420
et	Extra Trees Classifier	0.7137	0.8582	0.7137	0.7203	0.7127	0.5701	0.5735	0.1180
lightgbm	Light Gradient Boosting Machine	0.7074	0.8753	0.7074	0.7138	0.7057	0.5608	0.5645	0.3390
ada	Ada Boost Classifier	0.6290	0.0000	0.6290	0.6486	0.6232	0.4413	0.4513	0.0890
dt	Decision Tree Classifier	0.6273	0.7194	0.6273	0.6358	0.6253	0.4401	0.4446	0.0420
lr	Logistic Regression	0.6098	0.0000	0.6098	0.6245	0.6095	0.4166	0.4220	0.4080
svm	SVM - Linear Kernel	0.5613	0.0000	0.5613	0.5721	0.5399	0.3424	0.3535	0.0400
lda	Linear Discriminant Analysis	0.5569	0.0000	0.5569	0.5696	0.5592	0.3359	0.3380	0.0360
ridge	Ridge Classifier	0.5548	0.0000	0.5548	0.5538	0.5497	0.3334	0.3366	0.0360
knn	K Neighbors Classifier	0.5445	0.7424	0.5445	0.5630	0.5427	0.3181	0.3240	0.0470
qda	Quadratic Discriminant Analysis	0.5167	0.0000	0.5167	0.5430	0.4802	0.2846	0.3172	0.0360
nb	Naive Bayes	0.4977	0.7298	0.4977	0.5171	0.4553	0.2572	0.2913	0.0400
dummy	Dummy Classifier	0.3517	0.5000	0.3517	0.1238	0.1831	0.0000	0.0000	0.0930

```
Processing:   0%|           | 0/73 [00:00<?, ?it/s]
```

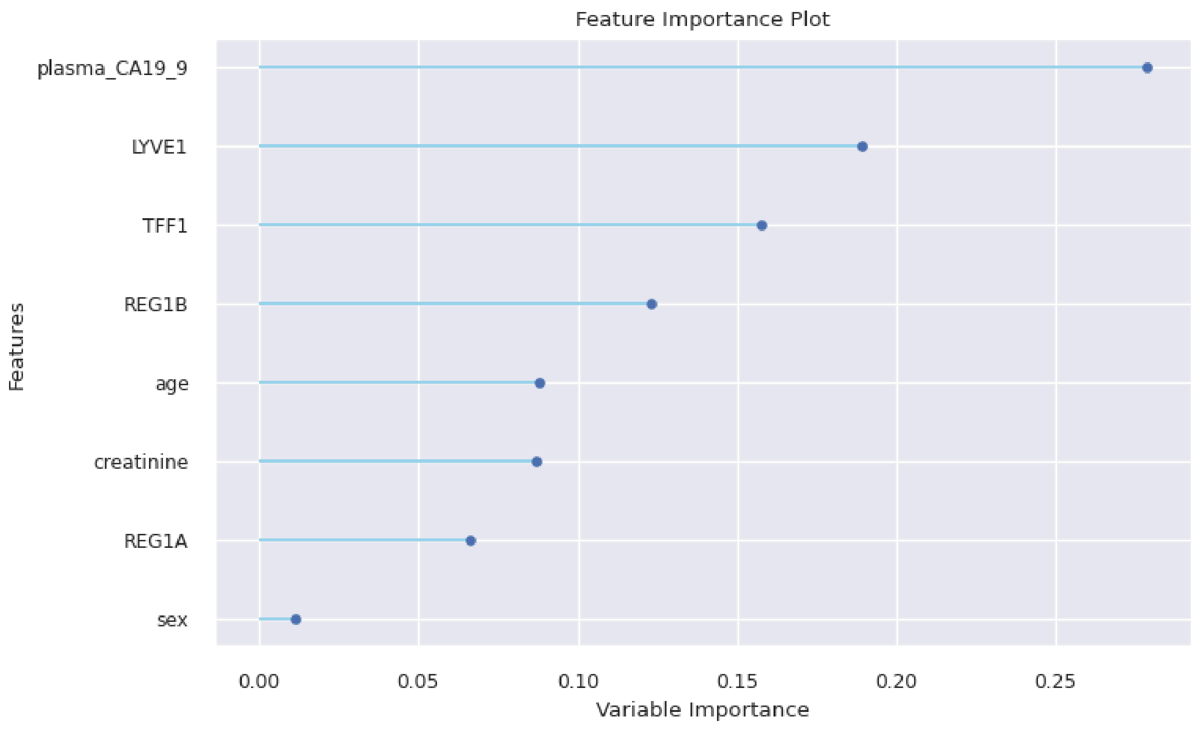
In [25]:
```
tuned = tune_model(best[0])
```

	Accuracy	AUC	Recall	Prec.	F1	Kappa	MCC
Fold							
0	0.7917	0.0000	0.7917	0.7911	0.7862	0.6865	0.6906
1	0.7917	0.0000	0.7917	0.7903	0.7893	0.6865	0.6878
2	0.7234	0.0000	0.7234	0.7272	0.7248	0.5852	0.5856
3	0.7021	0.0000	0.7021	0.6996	0.6960	0.5521	0.5555
4	0.7021	0.0000	0.7021	0.7281	0.7070	0.5524	0.5597
5	0.7021	0.0000	0.7021	0.7171	0.7051	0.5539	0.5573
6	0.7447	0.0000	0.7447	0.7406	0.7382	0.6179	0.6217
7	0.7447	0.0000	0.7447	0.7489	0.7463	0.6155	0.6160
8	0.8085	0.0000	0.8085	0.8130	0.8102	0.7117	0.7121
9	0.8298	0.0000	0.8298	0.8338	0.8278	0.7451	0.7486
Mean	0.7541	0.0000	0.7541	0.7590	0.7531	0.6307	0.6335
Std	0.0455	0.0000	0.0455	0.0427	0.0447	0.0682	0.0676

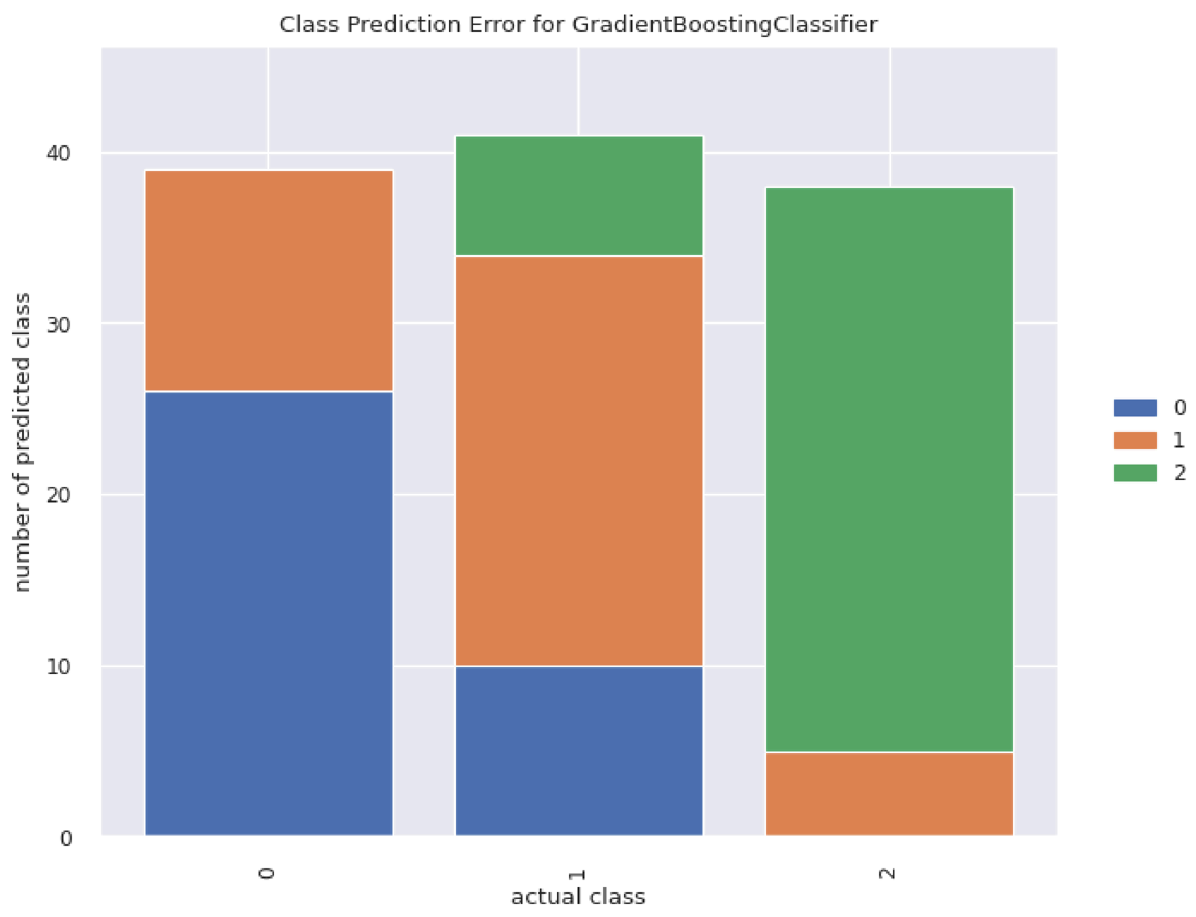
```
Processing:   0%|           | 0/7 [00:00<?, ?it/s]

Fitting 10 folds for each of 10 candidates, totalling 100 fits
```

10/ Model understanding

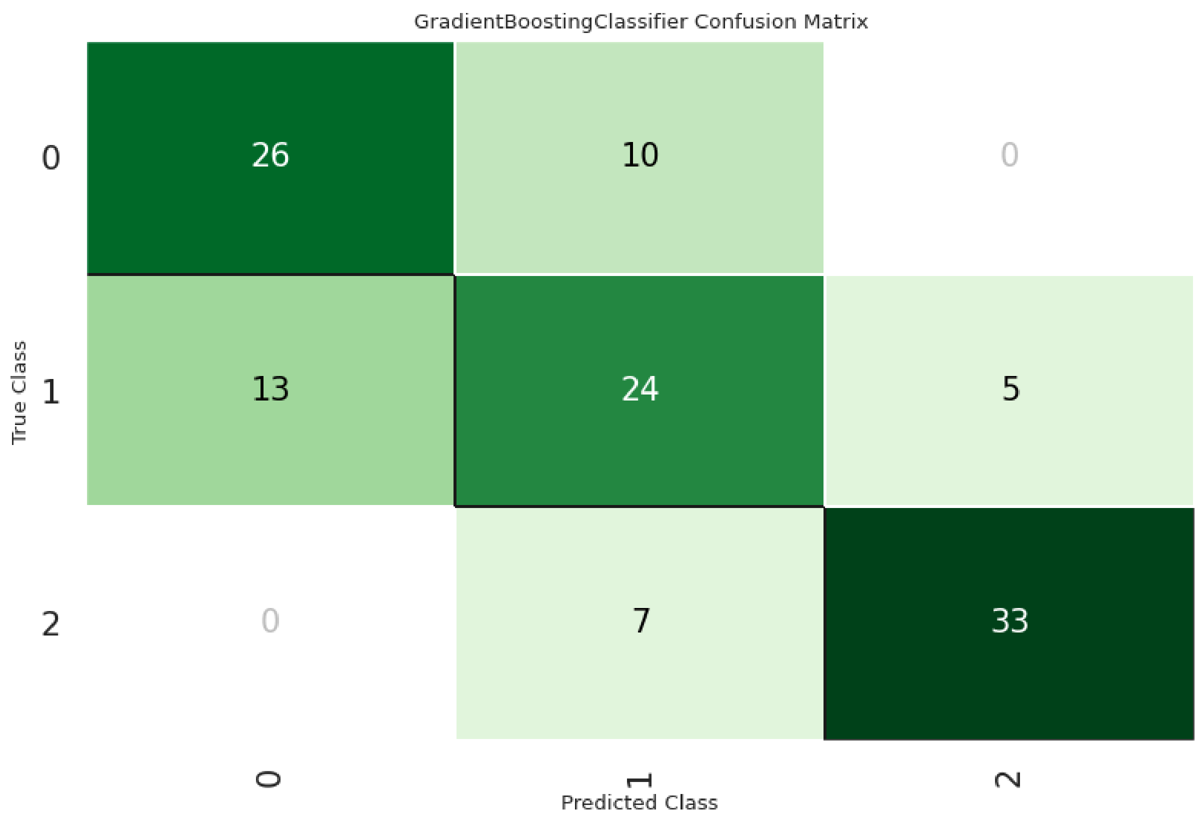
In [26]:
```
plot_model(tuned, plot = 'feature')
```



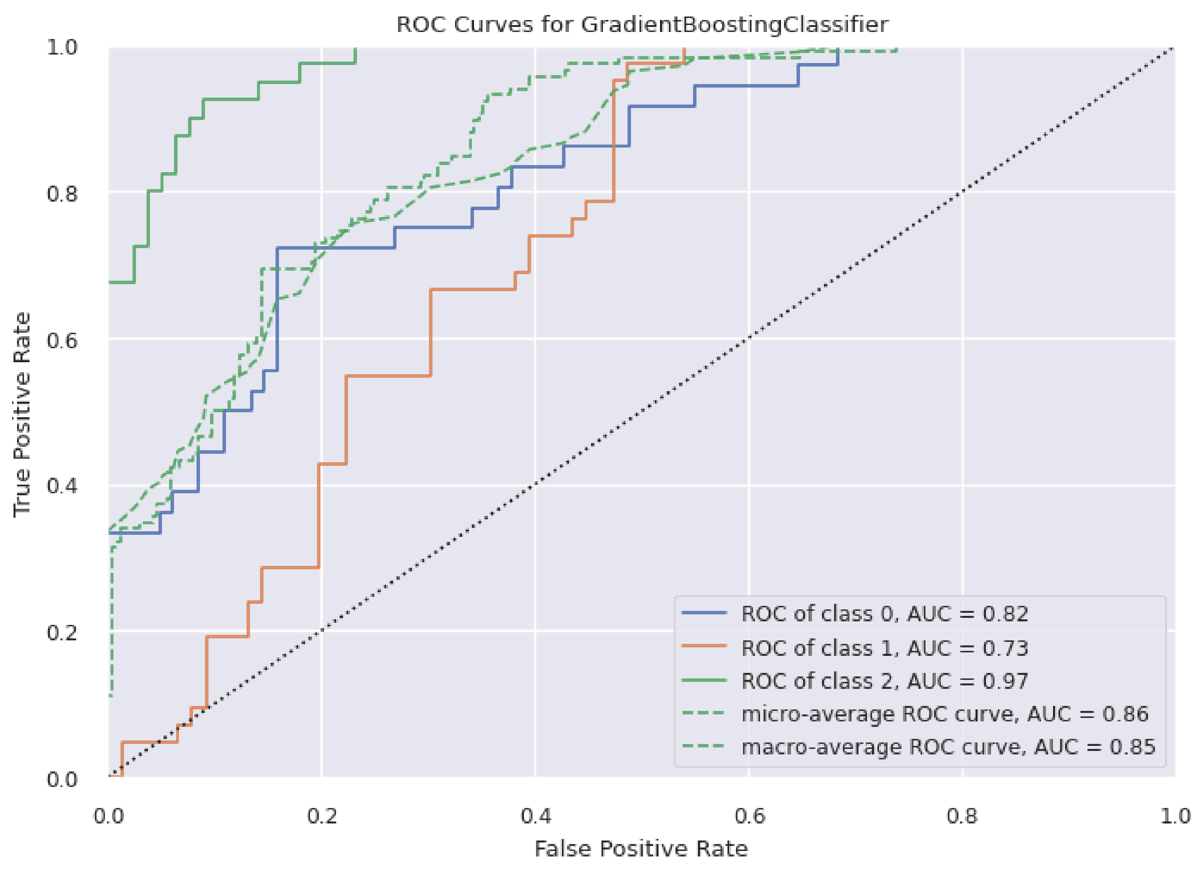
```
In [27]: plot_model(tuned, plot = 'error')
```



```
In [28]: plot_model(tuned, plot = 'confusion_matrix')
```

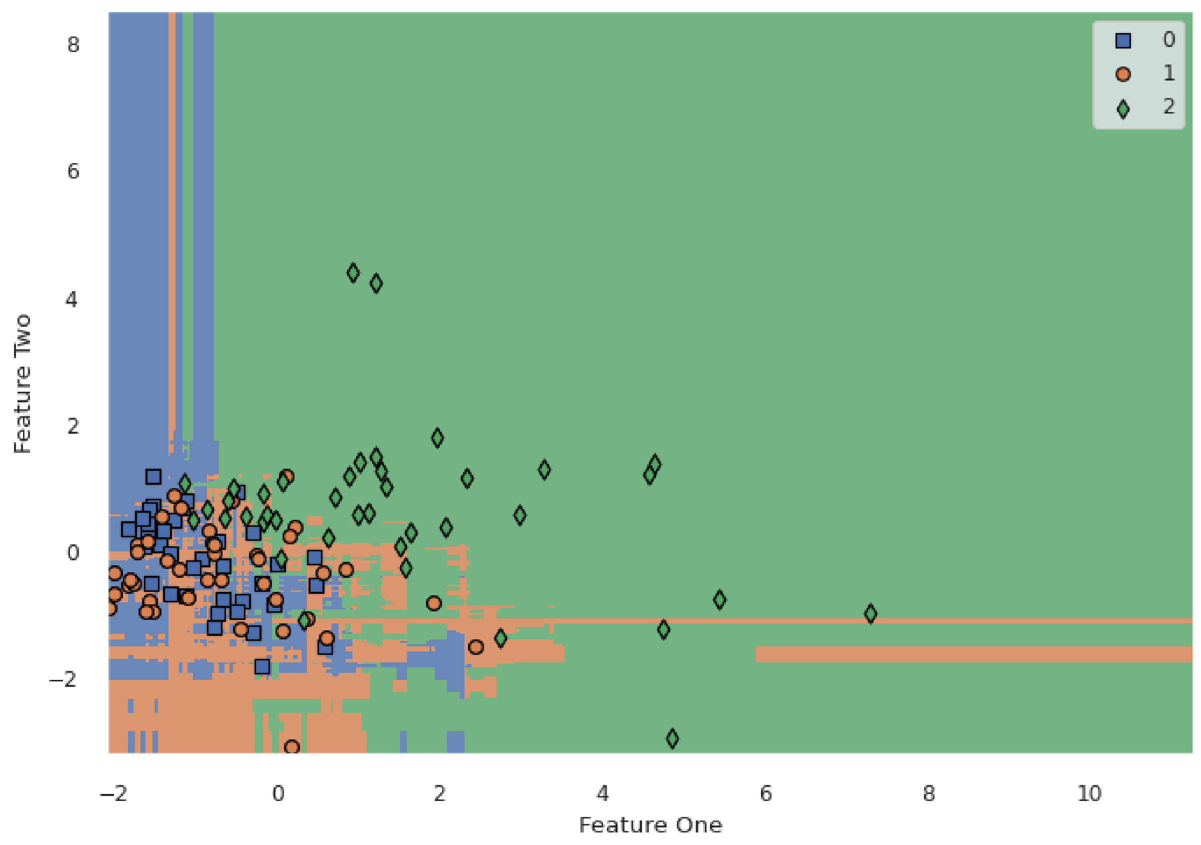


In [29]:
```python
plot_model(tuned, plot = 'auc')
```



```
The model appears to be very good at distinguishing class 2 (cancer) from the classes.
```

In [30]:
```
plot_model(tuned, plot = 'boundary')
```



In [31]:
```
preds = predict_model(tuned)
```

	Model	Accuracy	AUC	Recall	Prec.	F1	Kappa	MCC
0	Gradient Boosting Classifier	0.7034	0.8412	0.7034	0.7061	0.7042	0.5549	0.5553

11/ Finalise model

We finalise the model by training on the whole dataset.

In [32]:
```
final = finalize_model(tuned)
save_model(final, 'pancreas_pipeline')
preds = predict_model(final)
```

```
Transformation Pipeline and Model Successfully Saved
```

	Model	Accuracy	AUC	Recall	Prec.	F1	Kappa	MCC
0	Gradient Boosting Classifier	0.9153	0.9770	0.9153	0.9175	0.9160	0.8727	0.8731

In [33]:
```
tuned
```

Out[33]:
```
GradientBoostingClassifier(ccp_alpha=0.0, criterion='friedman_mse', init=None,
                           learning_rate=0.05, loss='log_loss', max_depth=6,
                           max_features='log2', max_leaf_nodes=None,
                           min_impurity_decrease=0.0005, min_samples_leaf=3,
                           min_samples_split=10, min_weight_fraction_leaf=0.0,
                           n_estimators=80, n_iter_no_change=None,
                           random_state=71, subsample=0.9, tol=0.0001,
                           validation_fraction=0.1, verbose=0,
                           warm_start=False)
```

In a Jupyter environment, please rerun this cell to show the HTML representation or trust the notebook.
On GitHub, the HTML representation is unable to render, please try loading this page with nbviewer.org.

12/ Conclusion

Several other notebooks using this dataset report accuracy values greater than 85%. In all cases they have done so by utilising features which lead to data leakage ('stage' and 'benign_sample_diagnosis') or features which may not be available in a future generalisable model ('cohort' and 'origin'). It would be great to see an accuracy score exceeding the one achieved here.