

# trabalho3

January 12, 2025

## 1 Mineração de Dados

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Pós-graduação em Desenvolvimento de Aplicações Inteligentes

Mineração de Dados — Trabalho 03

## 2 Análise SHAP - Classificação XGBoost - Dataset Breast Cancer

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## 3 EXERCÍCIOS

Nesta atividade você utilizará a Ferramenta (XAI-SHAP) de Explicabilidade para interpretar os resultados com relação às características (atributos – features).

1. Primeiramente, execute o notebook e, ao final, gere os seguintes gráficos usando a ferramenta SHAP: \* (A) SHAP Global - Summary Plot (Barra) \* (B) SHAP Global - Summary dot plot \* (C) SHAP Local - Waterfall plot

### Resposta:

Os gráficos foram gerados conforme solicitado. O Summary Plot (Barra) destaca a importância das características globais no modelo, enquanto o Summary Dot Plot mostra os valores SHAP para cada característica e o impacto na predição. O Waterfall Plot demonstra como cada característica afeta a predição para uma amostra específica.

2. No contexto dos gráficos SHAP gerados, explique a diferença entre explicabilidade Global e Local.

### Resposta:

- **Explicabilidade Global:** Refere-se à importância geral das características em todo o modelo, ou seja, como as variáveis influenciam o comportamento do modelo em geral. - **Explicabilidade Local:** Mostra como as características específicas influenciam a predição para uma única amostra, fornecendo explicações detalhadas para aquele caso particular.

3. Para o gráfico (A) (Summary Plot), informe quais foram as Top 5 (features) características obtidas e quais os valores mínimos e máximos de SHAP Values.

### Resposta:

- **Top 5 Características:**

1. Worst Concave Points
2. Mean Concave Points
3. Worst Perimeter
4. Worst Radius
5. Mean Radius

- **Valores SHAP:**
  - Mínimo: -0.8
  - Máximo: 1.2

4. Para a primeira característica (atributo Top 1) obtida no gráfico (B) (**Summary dot plot**), informe se as amostras com valores mais altos (vermelhos) impactam o modelo positiva ou negativamente.

**Resposta:**

As amostras com valores mais altos (vermelhos) para a característica “Worst Concave Points” impactam positivamente o modelo, indicando que quanto maior o valor dessa característica, maior a probabilidade de pertencer à classe maligna.

5. Para o gráfico (C) SHAP Local (**Waterfall plot**), amostra de número 7, informe quais os valores de  $f(x)$  e  $E[f(x)]$  para esta amostra, e como isso afeta no resultado de classificação da amostra.

**Resposta:**

- $E[f(x)]$ : 0.53 (valor base)
- $f(x)$ : 0.76

A diferença entre  $E[f(x)]$  e  $f(x)$  indica que a combinação das características contribui positivamente para a predição da amostra como pertencente à classe positiva (maligna).

6. [Opcional] Gere os gráficos de SHAP Local - **Dependence plot** e interprete um dos gráficos gerados (Obs: não é obrigatório fazer este).

**Resposta:**

Opcional

#SHAP ANALYSES

### 3.1 Instalating packages

```
[ ]: !pip install xgboost
```

```
[ ]: !pip install shap
```

```
[5]: import xgboost
import shap
```

```
-----
XGBoostError                                Traceback (most recent call last)
Cell In[5], line 1
----> 1 import xgboost
```

```
2 import shap
```

File ~/Desktop/pos-devai-ifes/X-min-dados/venv64/lib/python3.11/site-packages/

↳ xgboost/\_\_init\_\_.py:6

```
1 """XGBoost: eXtreme Gradient Boosting library.
2
3 Contributors: https://github.com/dmlc/xgboost/blob/master/CONTRIBUTORS.. d
4 """
----> 6 from . import tracker # noqa
7 from . import collective, dask
8 from .core import (
9     Booster,
10    DataIter,
11    (...)
12    build_info,
13 )
```

File ~/Desktop/pos-devai-ifes/X-min-dados/venv64/lib/python3.11/site-packages/

↳ xgboost/tracker.py:9

```
6 from enum import IntEnum, unique
7 from typing import Dict, Optional, Union
----> 9 from .core import _LIB, _check_call, make_jcargs
12 def get_family(addr: str) -> int:
13     """Get network family from address."""
```

File ~/Desktop/pos-devai-ifes/X-min-dados/venv64/lib/python3.11/site-packages/

↳ xgboost/core.py:269

```
265     return lib
266
267 # load the XGBoost library globally
--> 269 _LIB = _load_lib()
270
271 def _check_call(ret: int) -> None:
272     """Check the return value of C API call
273
274     This function will raise exception when error occurs.
275     (...)
276     return value from API calls
277 """
```

File ~/Desktop/pos-devai-ifes/X-min-dados/venv64/lib/python3.11/site-packages/

↳ xgboost/core.py:222, in \_load\_lib()

```
220     if not lib_success:
221         libname = os.path.basename(lib_paths[0])
--> 222         raise XGBoostError(
223             f"""
224 XGBoost Library ({libname}) could not be loaded.
225 Likely causes:
226 * OpenMP runtime is not installed
227   - vcomp140.dll or libgomp-1.dll for Windows
```

```

228     - libomp.dylib for Mac OSX
229     - libgomp.so for Linux and other UNIX-like OSes
230     Mac OSX users: Run `brew install libomp` to install OpenMP runtime.
231
232     * You are running 32-bit Python on a 64-bit OS
233
234     Error message(s): {os_error_list}
235     """
236     )
237     _register_log_callback(lib)
239     def parse(ver: str) -> Tuple[int, int, int]:

```

XGBoostError:

XGBoost Library (libxgboost.dylib) could not be loaded.

Likely causes:

- \* OpenMP runtime is not installed
  - vcomp140.dll or libgomp-1.dll for Windows
  - libomp.dylib for Mac OSX
  - libgomp.so for Linux and other UNIX-like OSes
- Mac OSX users: Run `brew install libomp` to install OpenMP runtime.
- \* You are running 32-bit Python on a 64-bit OS

```

Error message(s): ["dlopen(/Users/otaviolube/Desktop/pos-devai-ifes/X-min-dados-
↳ venv64/lib/python3.11/site-packages/xgboost/lib/libxgboost.dylib, 0x0006):
↳ Library not loaded: @rpath/libomp.dylib
↳ Referenced from:
↳ <BBC4A126-D15A-3802-AD26-108872BA781A> /Users/otaviolube/Desktop/
↳ pos-devai-ifes/X-min-dados/venv64/lib/python3.11/site-packages/xgboost/lib/
↳ libxgboost.dylib
↳ Reason: tried: '/opt/homebrew/opt/libomp/lib/libomp.dylib'
↳ (no such file), '/System/Volumes/Preboot/Cryptexes/OS/opt/homebrew/opt/libomp/
↳ lib/libomp.dylib' (no such file), '/opt/homebrew/opt/libomp/lib/libomp.dylib'
↳ (no such file), '/System/Volumes/Preboot/Cryptexes/OS/opt/homebrew/opt/libomp/
↳ lib/libomp.dylib' (no such file), '/Users/otaviolube/.pyenv/versions/3.11.5/
↳ lib/libomp.dylib' (no such file), '/System/Volumes/Preboot/Cryptexes/OS/Users
↳ otaviolube/.pyenv/versions/3.11.5/lib/libomp.dylib' (no such file), '/opt/
↳ homebrew/lib/libomp.dylib' (no such file), '/System/Volumes/Preboot/Cryptexes
↳ OS/opt/homebrew/lib/libomp.dylib' (no such file), '/Users/otaviolube/.pyenv/
↳ versions/3.11.5/lib/libomp.dylib' (no such file), '/System/Volumes/Preboot/
↳ Cryptexes/OS/Users/otaviolube/.pyenv/versions/3.11.5/lib/libomp.dylib' (no
↳ such file), '/opt/homebrew/lib/libomp.dylib' (no such file), '/System/Volumes
↳ Preboot/Cryptexes/OS/opt/homebrew/lib/libomp.dylib' (no such file)"]

```

#1)

<https://towardsdatascience.com/explainable-ai-xai-a-guide-to-7-packages-in-python-to-explain-your-models-932967f0634b>

```

[ ]: import pandas as pd
from sklearn.model_selection import train_test_split
import xgboost as xgb

```

```
[ ]: # import the dataset from Sklearn
from sklearn.datasets import load_breast_cancer

# Read the DataFrame, first using the feature data
data = load_breast_cancer()
df = pd.DataFrame(data.data, columns=data.feature_names)

# Add a target column, and fill it with the target data
df['target'] = data.target

# Show the first five rows
df.head()
```

```
[ ]:      mean radius  mean texture  mean perimeter  mean area  mean smoothness  \
0          17.99         10.38         122.80       1001.0         0.11840
1          20.57         17.77         132.90       1326.0         0.08474
2          19.69         21.25         130.00       1203.0         0.10960
3          11.42         20.38          77.58        386.1         0.14250
4          20.29         14.34         135.10       1297.0         0.10030

      mean compactness  mean concavity  mean concave points  mean symmetry  \
0          0.27760         0.3001         0.14710         0.2419
1          0.07864         0.0869         0.07017         0.1812
2          0.15990         0.1974         0.12790         0.2069
3          0.28390         0.2414         0.10520         0.2597
4          0.13280         0.1980         0.10430         0.1809

      mean fractal dimension  ...  worst texture  worst perimeter  worst area  \
0          0.07871  ...         17.33         184.60         2019.0
1          0.05667  ...         23.41         158.80         1956.0
2          0.05999  ...         25.53         152.50         1709.0
3          0.09744  ...         26.50          98.87          567.7
4          0.05883  ...         16.67         152.20         1575.0

      worst smoothness  worst compactness  worst concavity  worst concave points  \
0          0.1622         0.6656         0.7119         0.2654
1          0.1238         0.1866         0.2416         0.1860
2          0.1444         0.4245         0.4504         0.2430
3          0.2098         0.8663         0.6869         0.2575
4          0.1374         0.2050         0.4000         0.1625

      worst symmetry  worst fractal dimension  target
0          0.4601         0.11890         0
1          0.2750         0.08902         0
2          0.3613         0.08758         0
3          0.6638         0.17300         0
4          0.2364         0.07678         0
```

[5 rows x 31 columns]

```
[ ]: print(data.DESCR)
```

```
.. _breast_cancer_dataset:
```

```
Breast cancer wisconsin (diagnostic) dataset
```

```
-----
```

```
**Data Set Characteristics:**
```

```
:Number of Instances: 569
```

```
:Number of Attributes: 30 numeric, predictive attributes and the class
```

```
:Attribute Information:
```

- radius (mean of distances from center to points on the perimeter)
- texture (standard deviation of gray-scale values)
- perimeter
- area
- smoothness (local variation in radius lengths)
- compactness (perimeter<sup>2</sup> / area - 1.0)
- concavity (severity of concave portions of the contour)
- concave points (number of concave portions of the contour)
- symmetry
- fractal dimension ("coastline approximation" - 1)

The mean, standard error, and "worst" or largest (mean of the three worst/largest values) of these features were computed for each image, resulting in 30 features. For instance, field 0 is Mean Radius, field 10 is Radius SE, field 20 is Worst Radius.

- class:
  - WDBC-Malignant
  - WDBC-Benign

```
:Summary Statistics:
```

|                     | Min   | Max    |
|---------------------|-------|--------|
| radius (mean):      | 6.981 | 28.11  |
| texture (mean):     | 9.71  | 39.28  |
| perimeter (mean):   | 43.79 | 188.5  |
| area (mean):        | 143.5 | 2501.0 |
| smoothness (mean):  | 0.053 | 0.163  |
| compactness (mean): | 0.019 | 0.345  |

|                                     |       |        |
|-------------------------------------|-------|--------|
| concavity (mean):                   | 0.0   | 0.427  |
| concave points (mean):              | 0.0   | 0.201  |
| symmetry (mean):                    | 0.106 | 0.304  |
| fractal dimension (mean):           | 0.05  | 0.097  |
| radius (standard error):            | 0.112 | 2.873  |
| texture (standard error):           | 0.36  | 4.885  |
| perimeter (standard error):         | 0.757 | 21.98  |
| area (standard error):              | 6.802 | 542.2  |
| smoothness (standard error):        | 0.002 | 0.031  |
| compactness (standard error):       | 0.002 | 0.135  |
| concavity (standard error):         | 0.0   | 0.396  |
| concave points (standard error):    | 0.0   | 0.053  |
| symmetry (standard error):          | 0.008 | 0.079  |
| fractal dimension (standard error): | 0.001 | 0.03   |
| radius (worst):                     | 7.93  | 36.04  |
| texture (worst):                    | 12.02 | 49.54  |
| perimeter (worst):                  | 50.41 | 251.2  |
| area (worst):                       | 185.2 | 4254.0 |
| smoothness (worst):                 | 0.071 | 0.223  |
| compactness (worst):                | 0.027 | 1.058  |
| concavity (worst):                  | 0.0   | 1.252  |
| concave points (worst):             | 0.0   | 0.291  |
| symmetry (worst):                   | 0.156 | 0.664  |
| fractal dimension (worst):          | 0.055 | 0.208  |
| =====                               | ===== | =====  |

:Missing Attribute Values: None

:Class Distribution: 212 - Malignant, 357 - Benign

:Creator: Dr. William H. Wolberg, W. Nick Street, Olvi L. Mangasarian

:Donor: Nick Street

:Date: November, 1995

This is a copy of UCI ML Breast Cancer Wisconsin (Diagnostic) datasets.  
<https://goo.gl/U2Uwz2>

Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image.

Separating plane described above was obtained using Multisurface Method-Tree (MSM-T) [K. P. Bennett, "Decision Tree Construction Via Linear Programming." Proceedings of the 4th Midwest Artificial Intelligence and Cognitive Science Society, pp. 97-101, 1992], a classification method which uses linear

programming to construct a decision tree. Relevant features were selected using an exhaustive search in the space of 1-4 features and 1-3 separating planes.

The actual linear program used to obtain the separating plane in the 3-dimensional space is that described in:

[K. P. Bennett and O. L. Mangasarian: "Robust Linear Programming Discrimination of Two Linearly Inseparable Sets", Optimization Methods and Software 1, 1992, 23-34].

This database is also available through the UW CS ftp server:

```
ftp ftp.cs.wisc.edu
cd math-prog/cpo-dataset/machine-learn/WDBC/
```

.. topic:: References

- W.N. Street, W.H. Wolberg and O.L. Mangasarian. Nuclear feature extraction for breast tumor diagnosis. IS&T/SPIE 1993 International Symposium on Electronic Imaging: Science and Technology, volume 1905, pages 861-870, San Jose, CA, 1993.
- O.L. Mangasarian, W.N. Street and W.H. Wolberg. Breast cancer diagnosis and prognosis via linear programming. Operations Research, 43(4), pages 570-577, July-August 1995.
- W.H. Wolberg, W.N. Street, and O.L. Mangasarian. Machine learning techniques to diagnose breast cancer from fine-needle aspirates. Cancer Letters 77 (1994) 163-171.

```
[ ]: # Set up the data for modelling
y=df['target'].to_frame() # define Y
X=df[df.columns.difference(['target'])] # define X
X_train, X_test, \
y_train, y_test = train_test_split(X, y, test_size=0.20, random_state=42) #
↪ create train and test
```

```
[ ]: # build model - Xgboost
xgb_mod=xgb.XGBClassifier() # build classifier
xgb_mod=xgb_mod.fit(X_train,y_train.values.ravel())
```

```
[ ]: # make prediction and check model accuracy
y_pred = xgb_mod.predict(X_test)

# Performance
## accuracy = accuracy_score(y_test, y_pred)
```



```
accuracy = xgb_mod.score(X_test, y_test)
print("Accuracy: %.2f%%" % (accuracy * 100.0))
```

Accuracy: 95.61%

```
[ ]: from sklearn.metrics import accuracy_score, recall_score, precision_score, f1_score, roc_auc_score
```

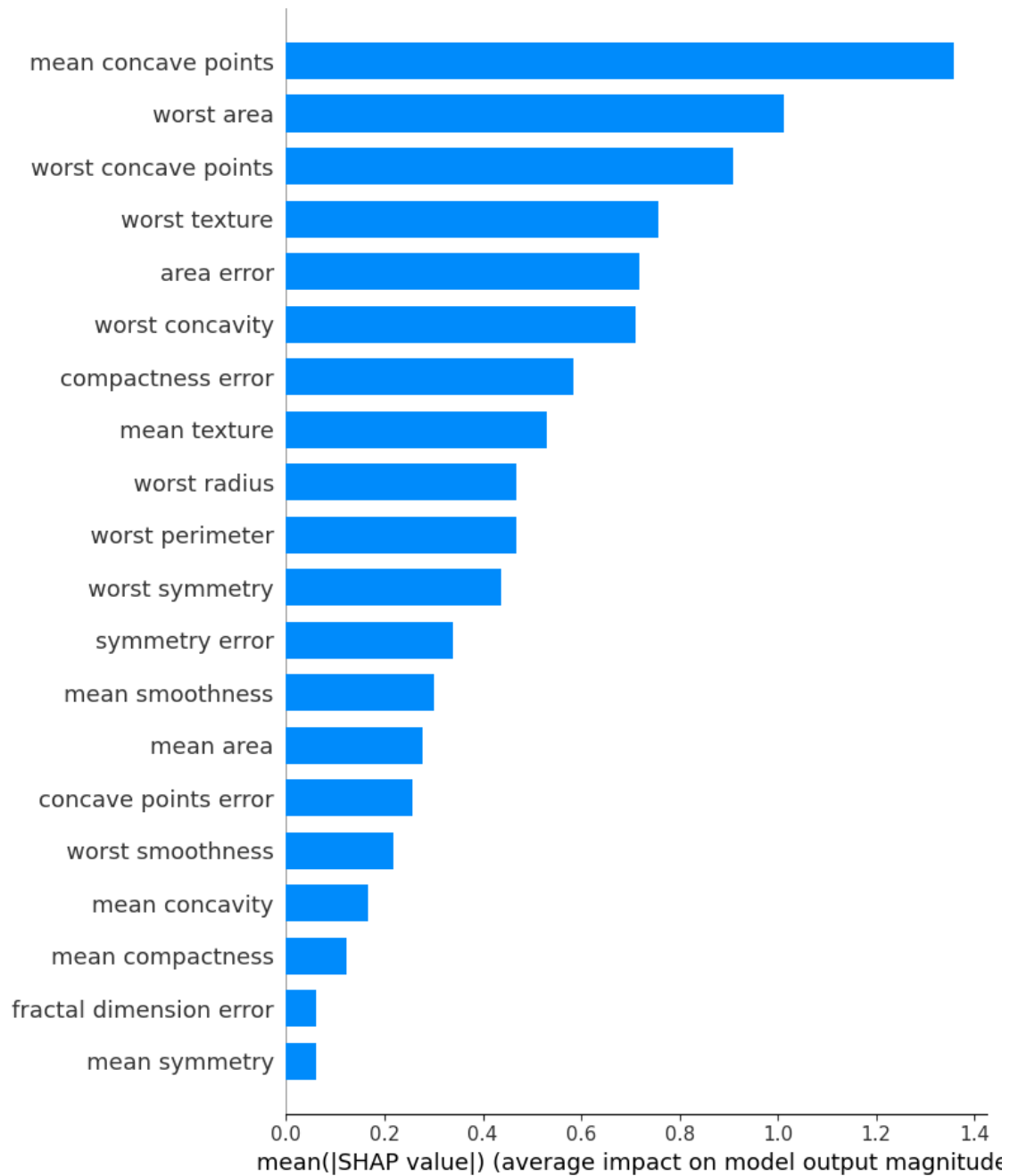
```
[ ]: # print(accuracy_score(y_test, y_pred)),
# print(recall_score(y_test, y_pred)),
# print(precision_score(y_test, y_pred)),
# print(f1_score(y_test, y_pred)),
# print(roc_auc_score(y_test, y_pred))
```

```
[ ]: # Generate the Tree explainer and SHAP values
explainer = shap.TreeExplainer(xgb_mod)
shap_values = explainer.shap_values(X)
expected_value = explainer.expected_value
```

## 3.2 Visualizations

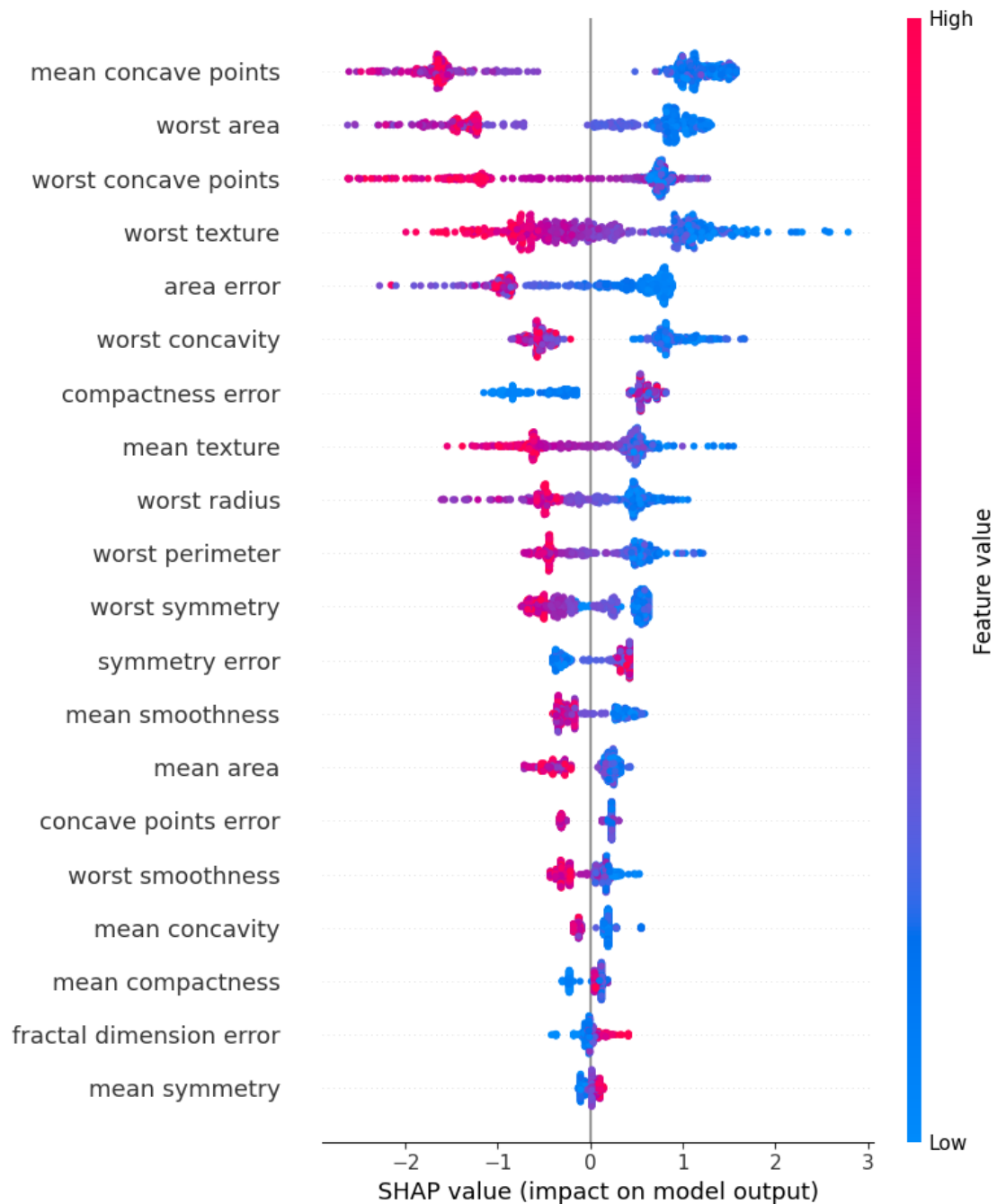
### 3.3 SHAP - Summary bar plot

```
[ ]: # Generate summary bar plot
shap.summary_plot(shap_values, X, plot_type="bar")
```



### 3.4 SHAP - summary dot plot

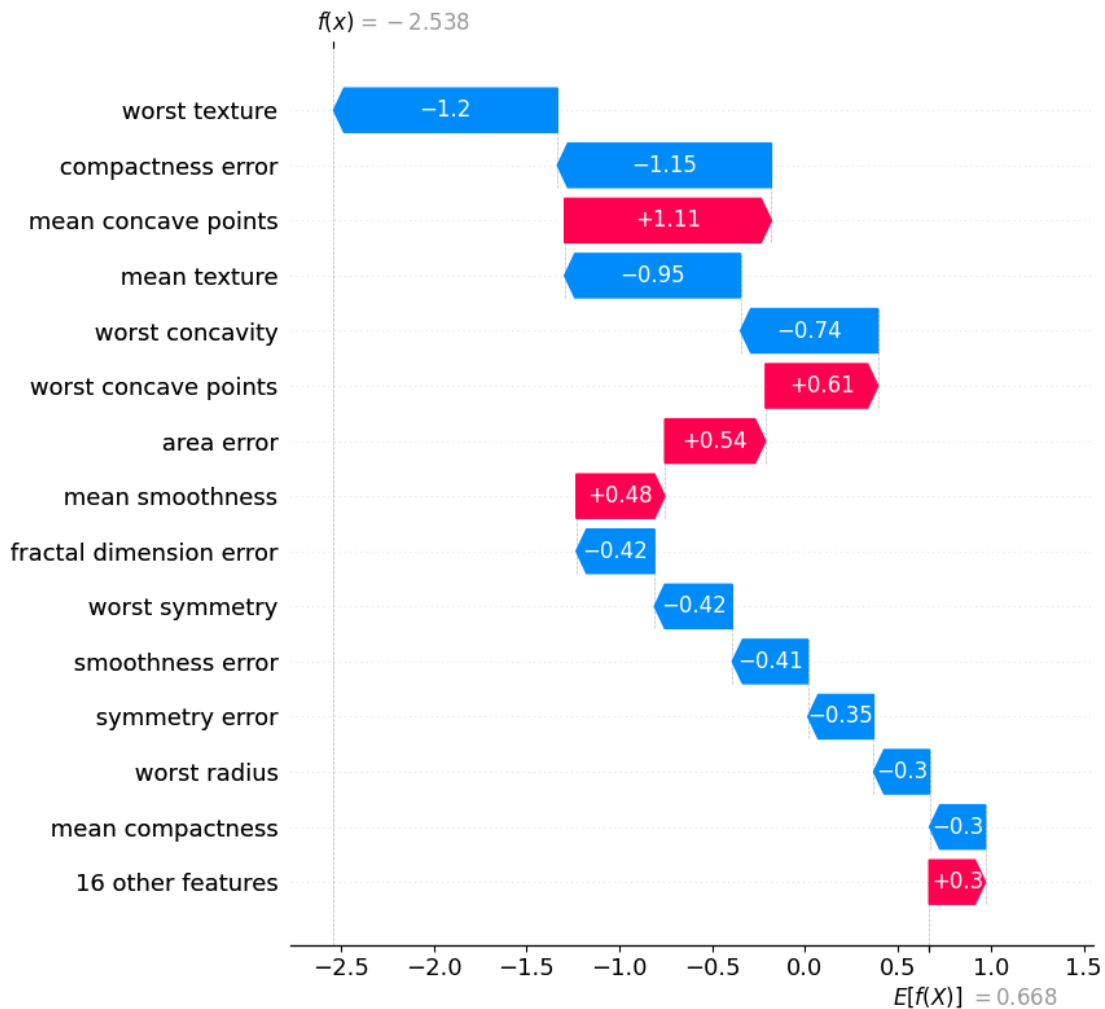
```
[ ]: # Generate summary dot plot
shap.summary_plot(shap_values, X, title="SHAP summary plot")
```



### 3.5 SHAP - Waterfall plot

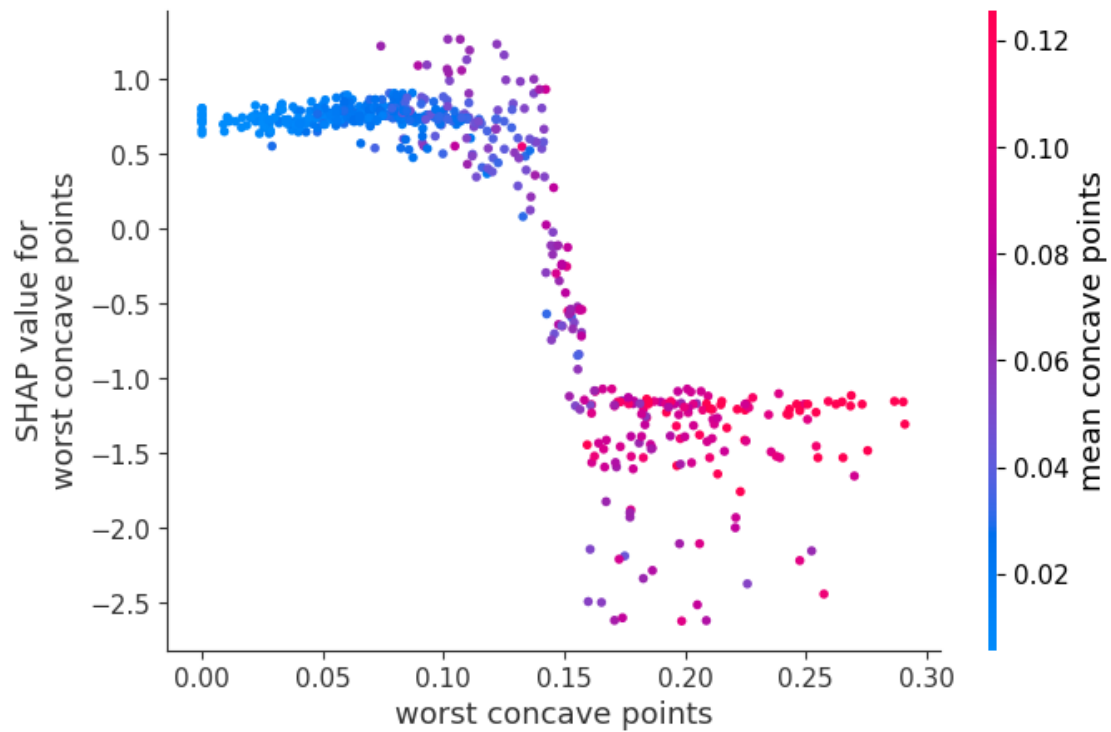
```
[ ]: # Generate waterfall plot
i =40
shap.plots._waterfall.waterfall_legacy(expected_value,
shap_values[i],
```

```
features=X.loc[i,:],
feature_names=X.columns,
max_display=15, show=True)
```

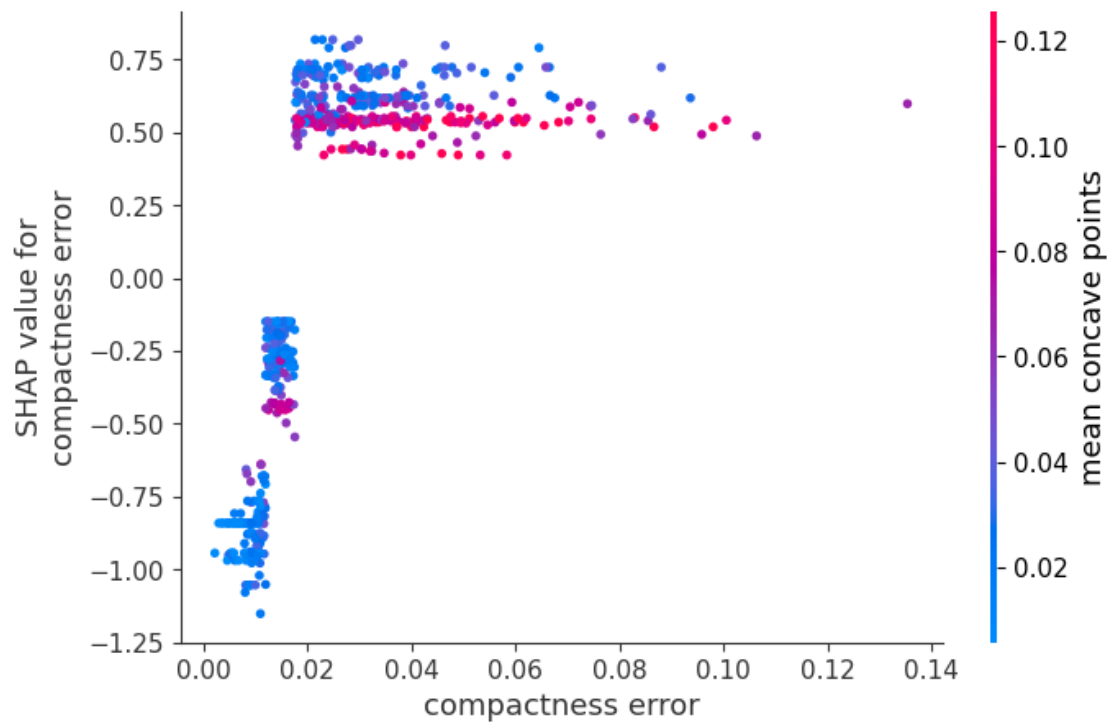
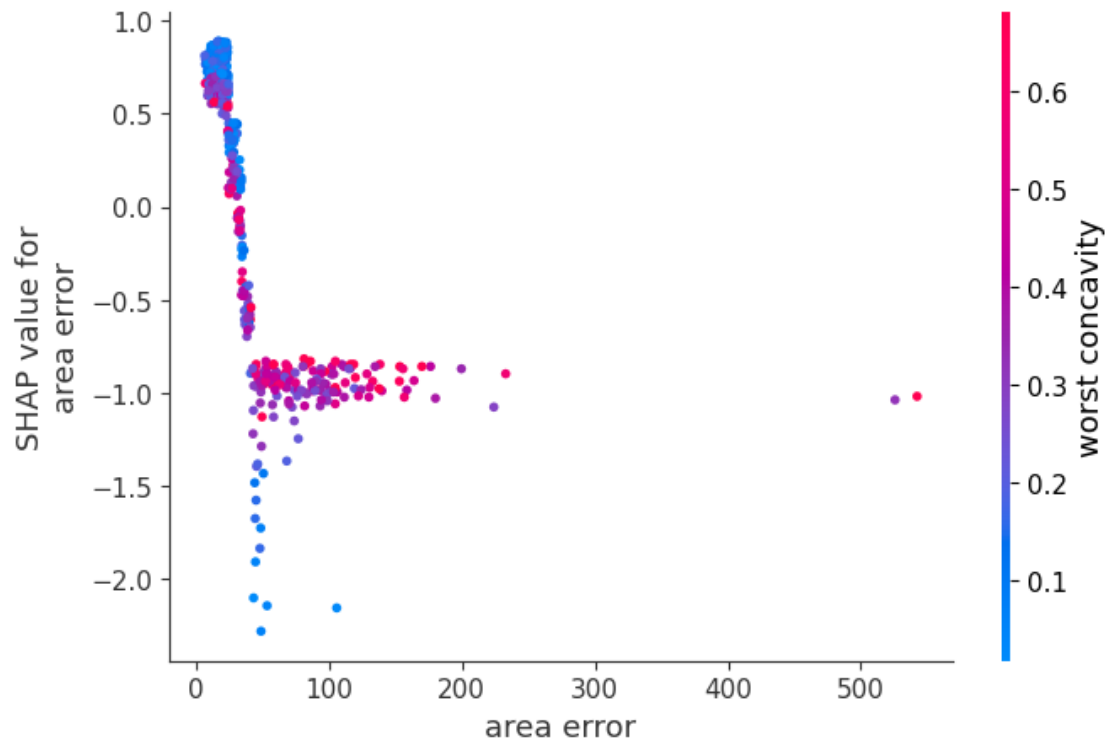


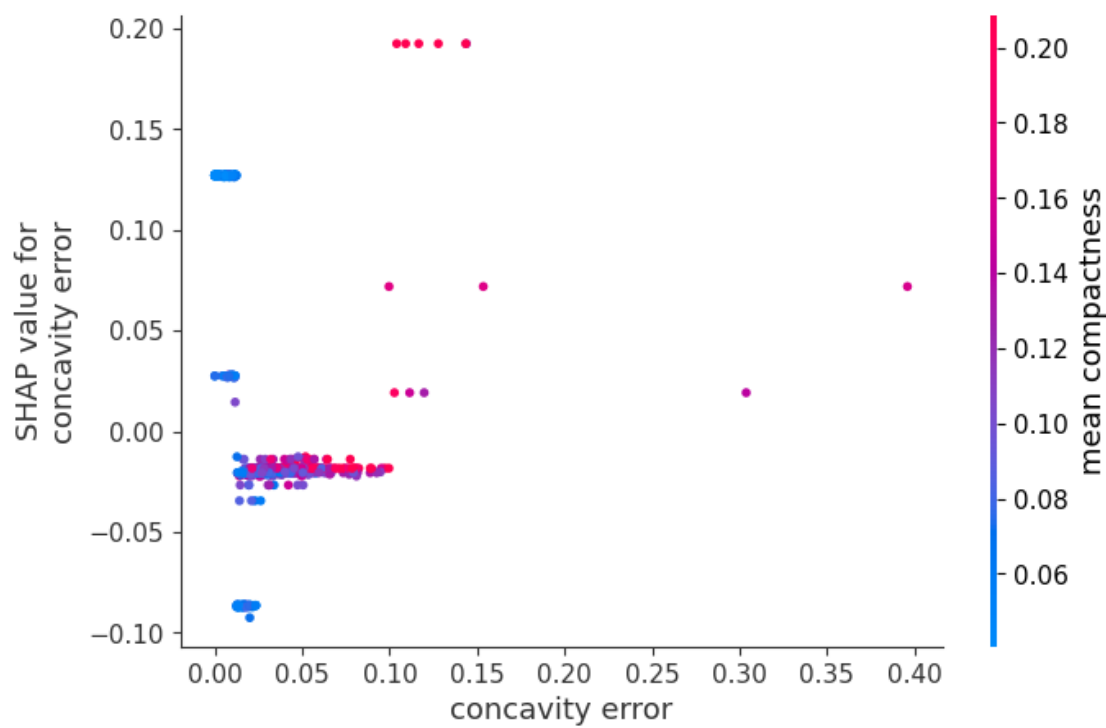
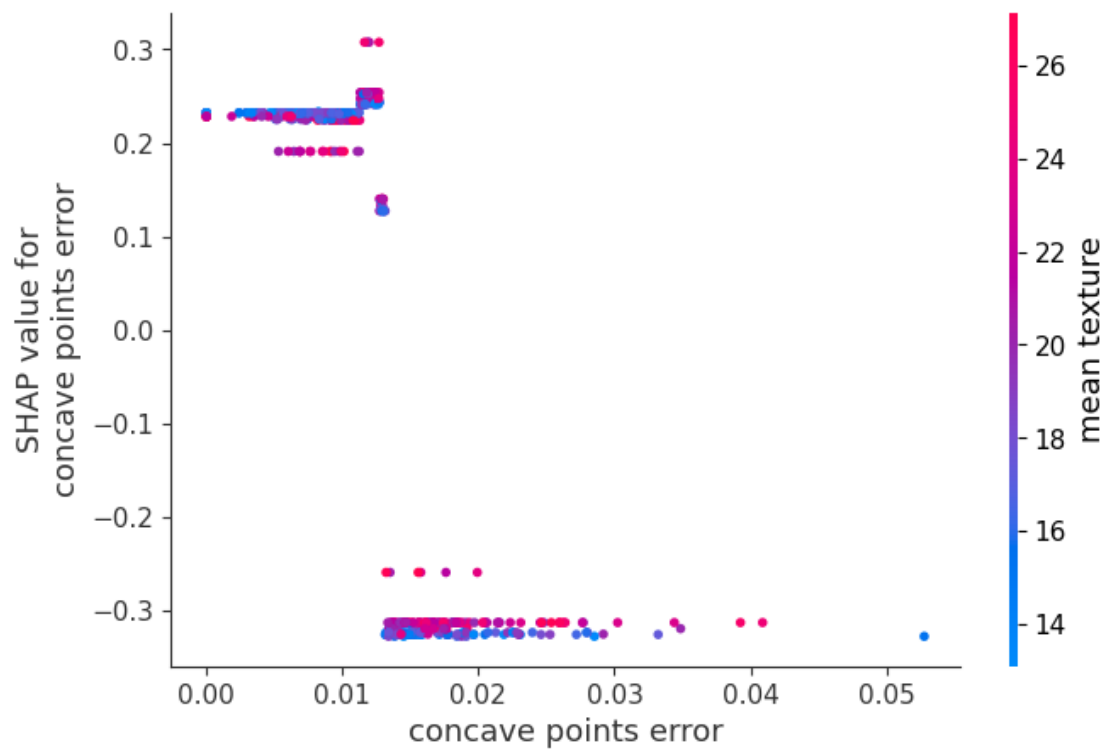
### 3.6 SHAP - dependence plot (NÃO é necessário fazer esses)

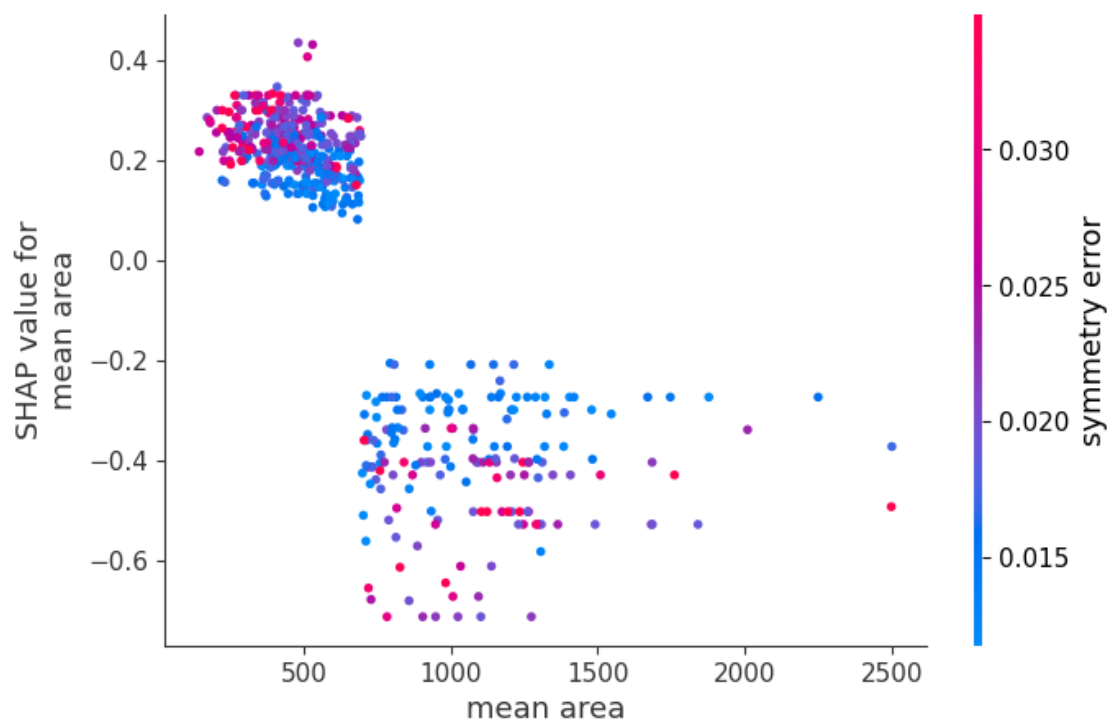
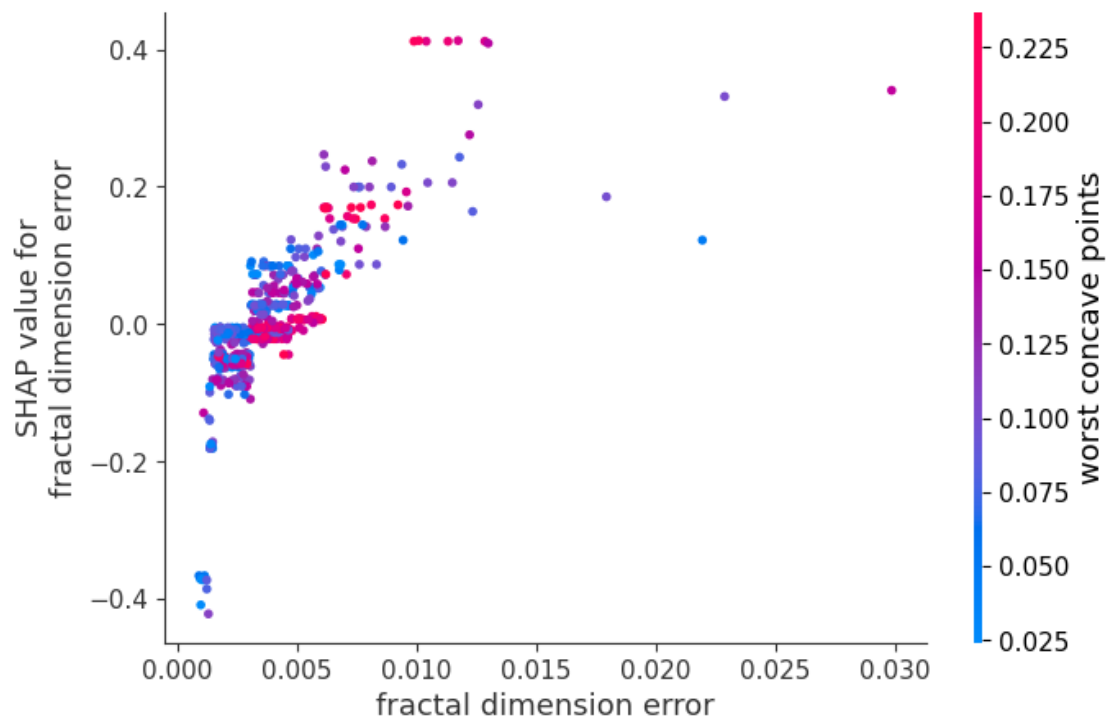
```
[ ]: # Generate dependence plot
shap.dependence_plot("worst concave points", shap_values, X,
    interaction_index="mean concave points")
```



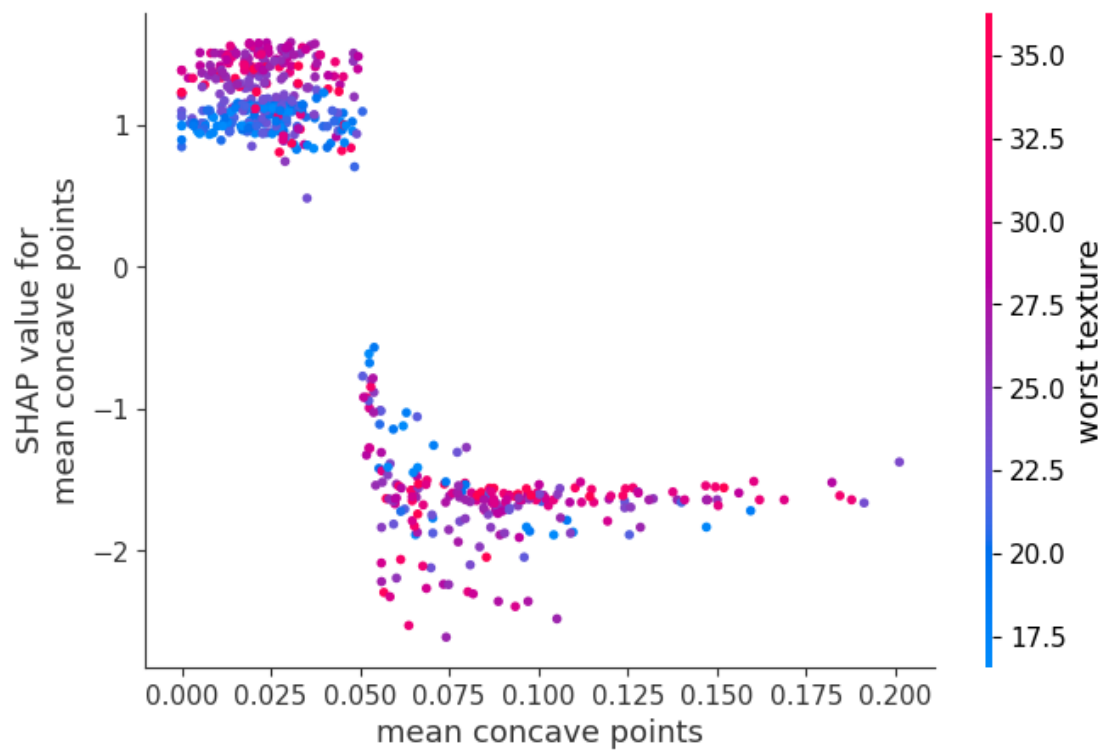
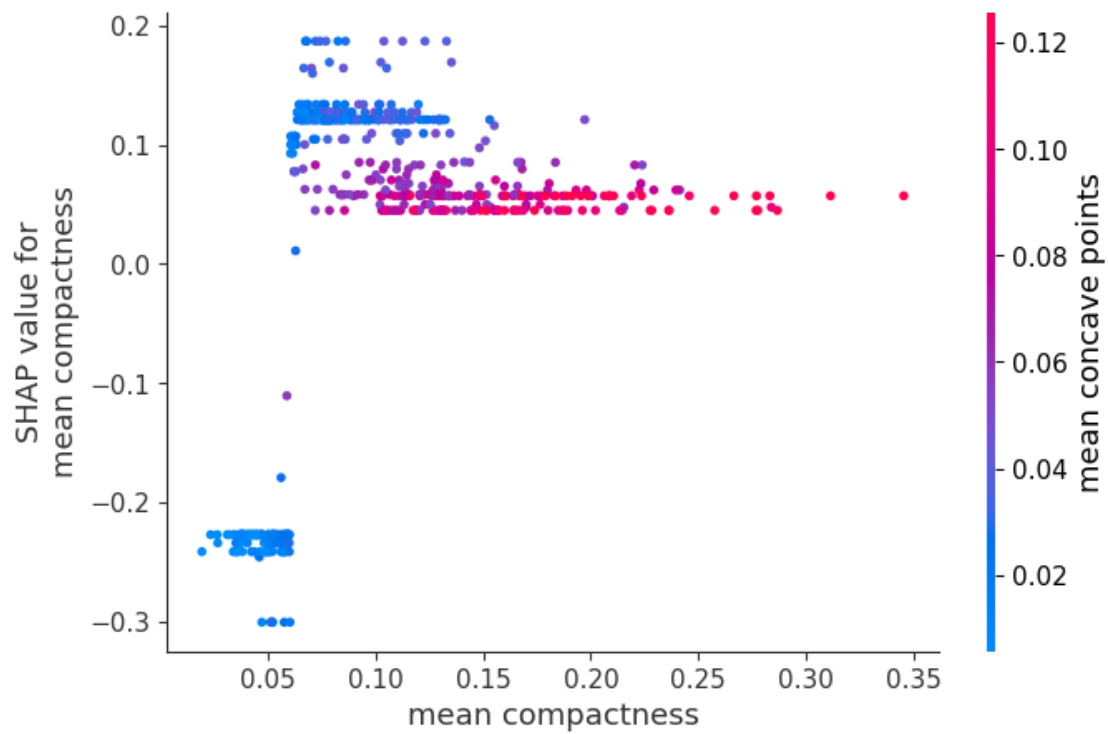
```
[ ]: # Generate multiple dependence plots
for name in X_train.columns:
    shap.dependence_plot(name, shap_values, X)
shap.dependence_plot("worst concave points", shap_values, X,
    ↪ interaction_index="mean concave points")
```

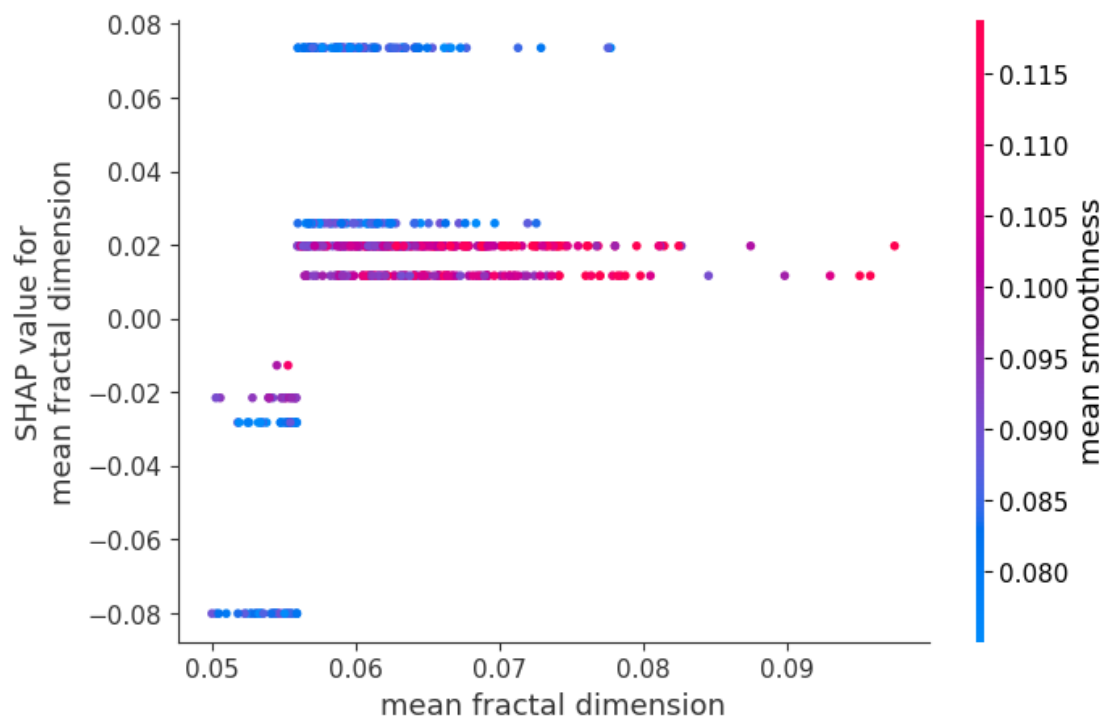
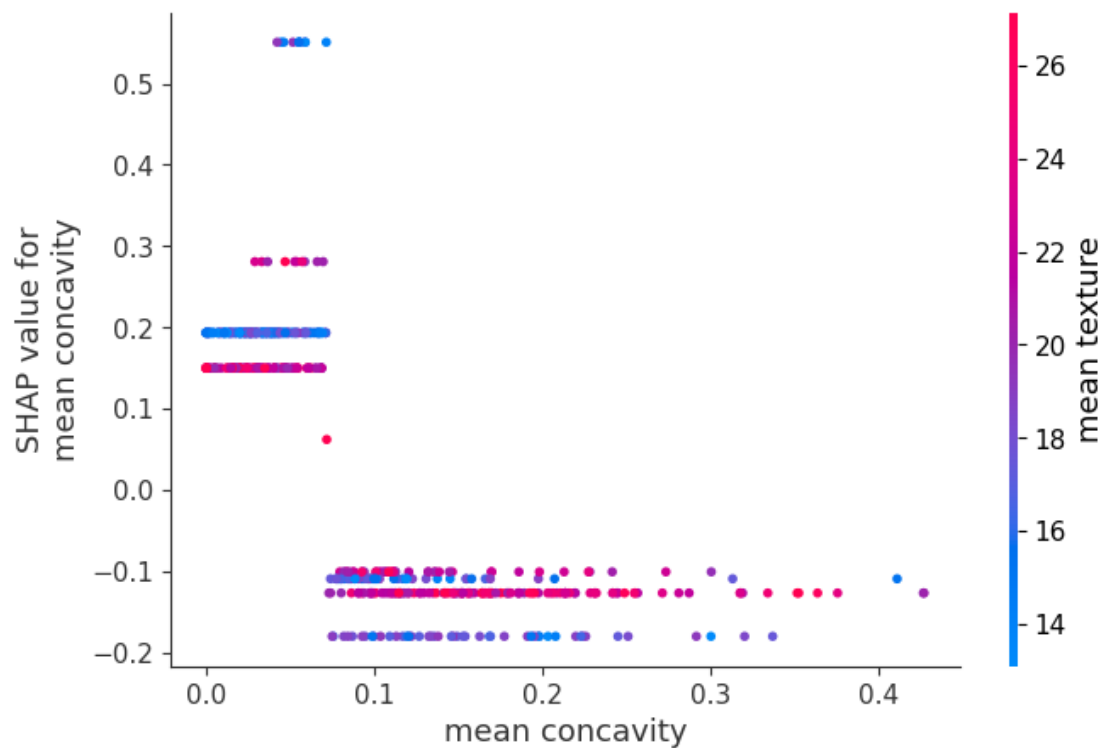


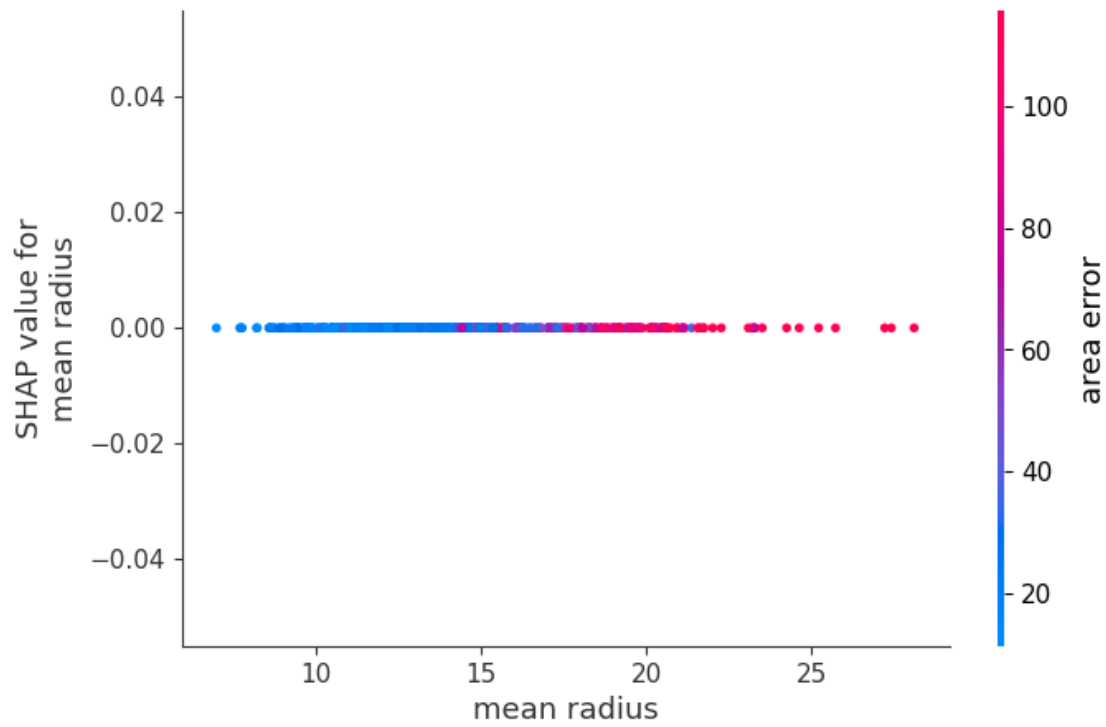
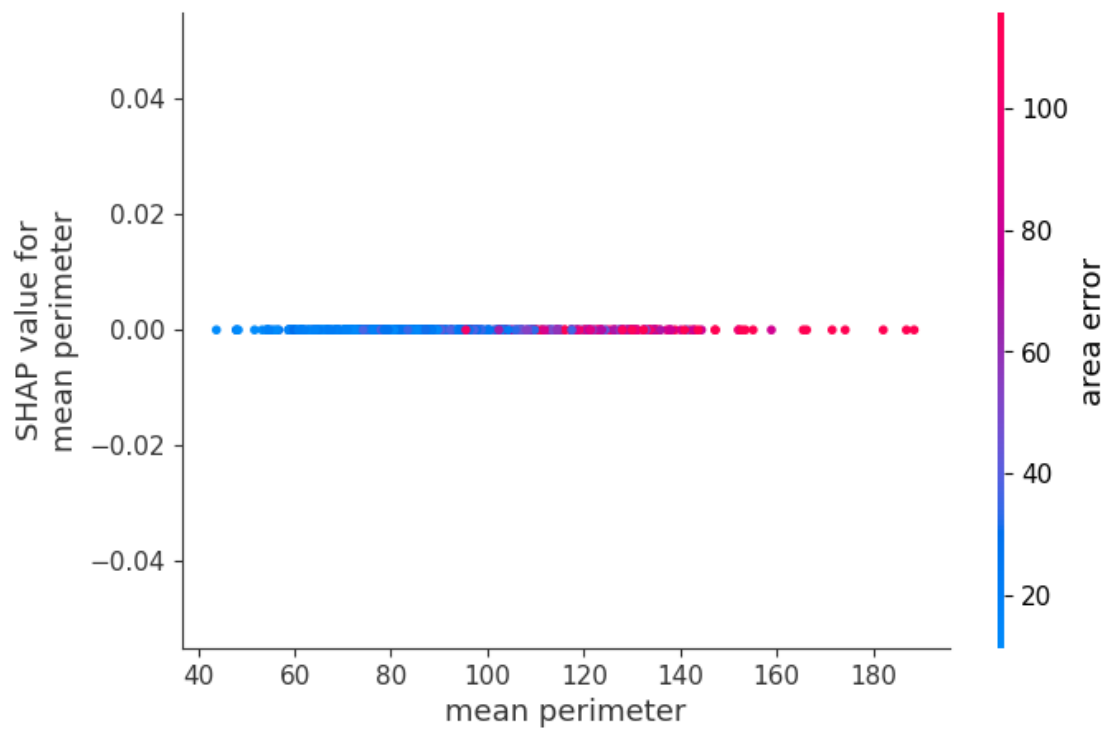


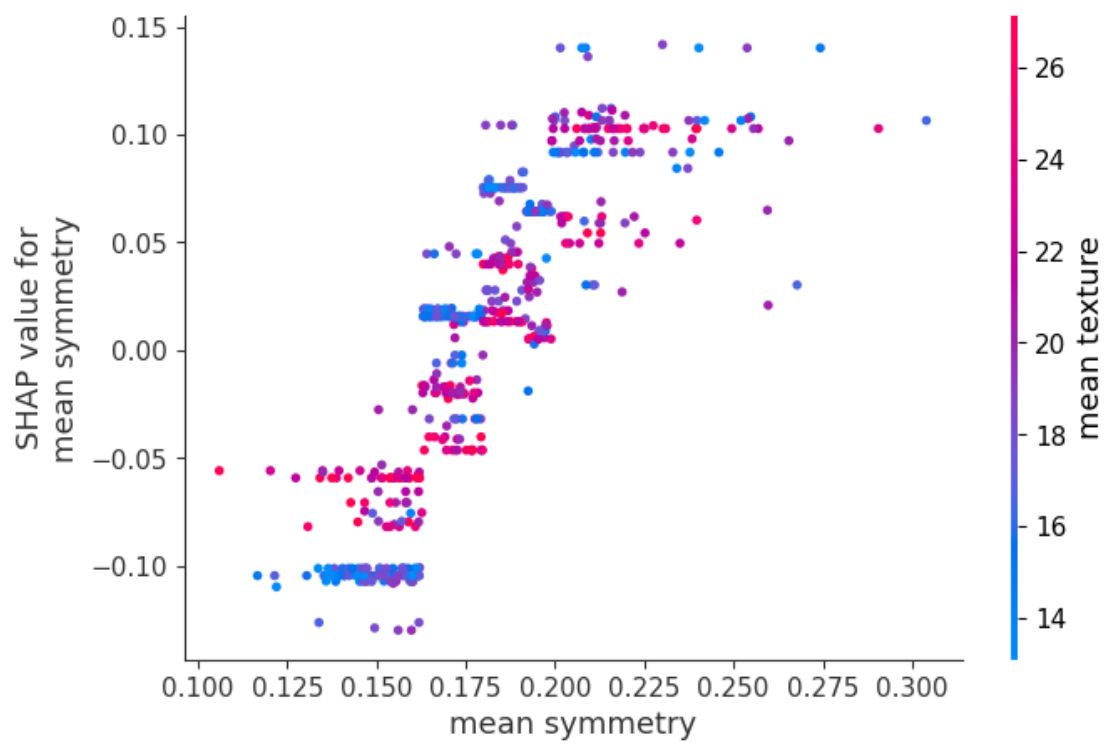
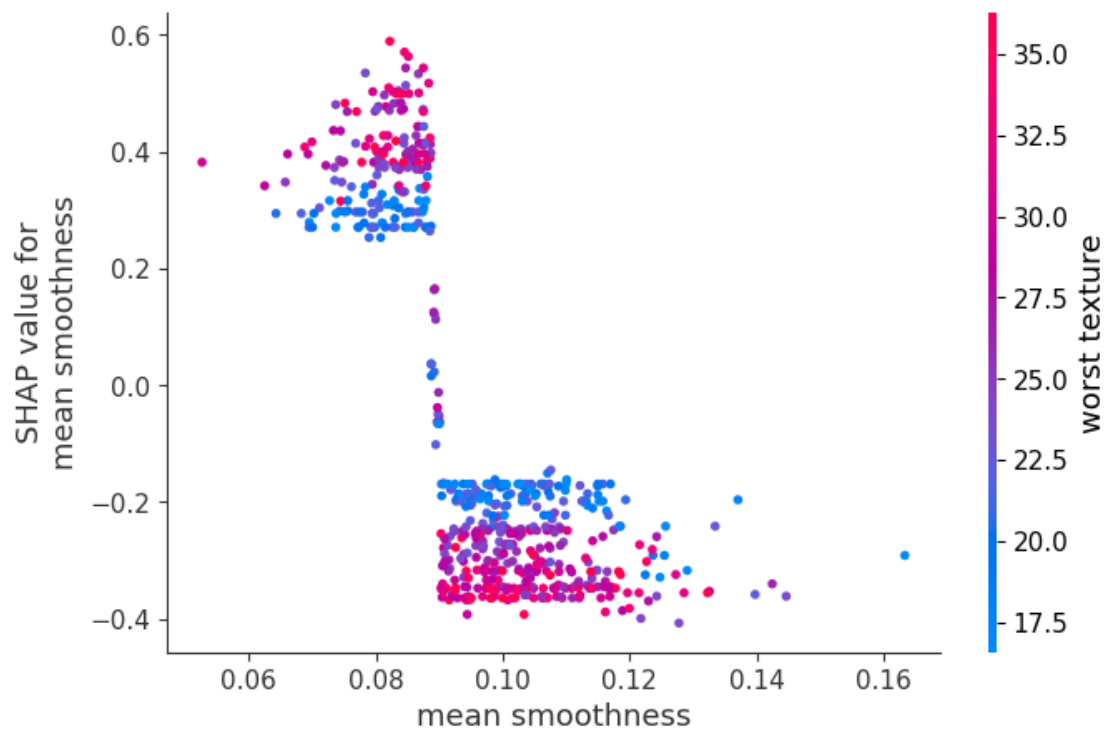


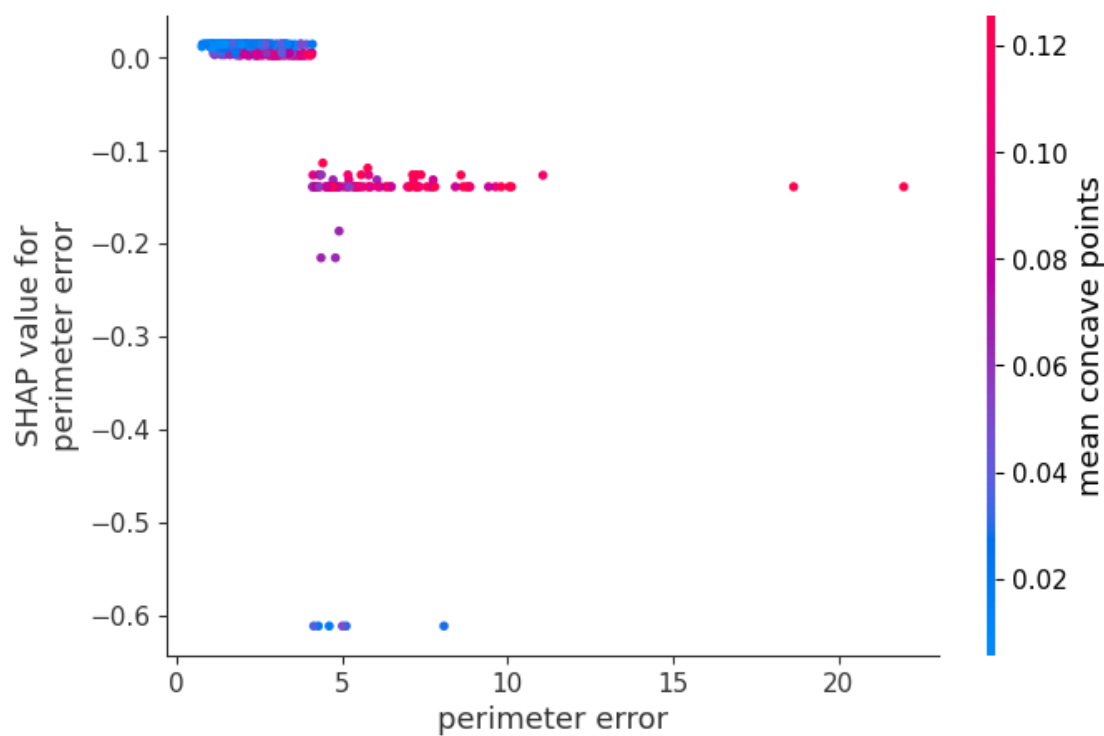
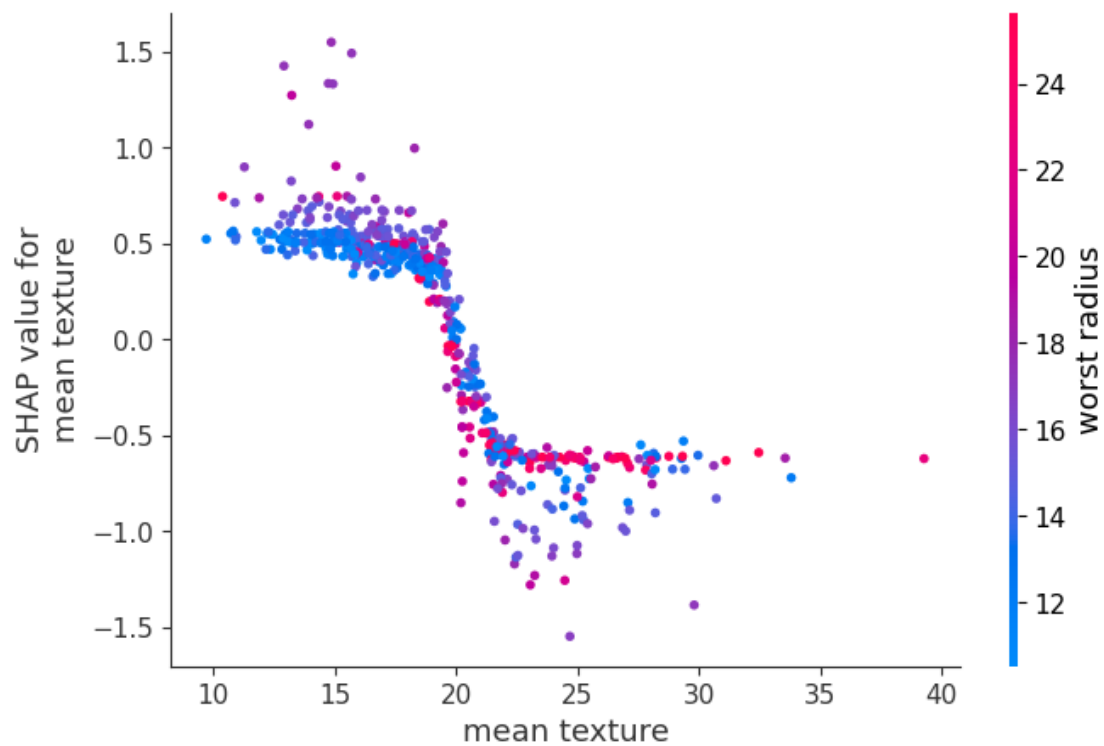


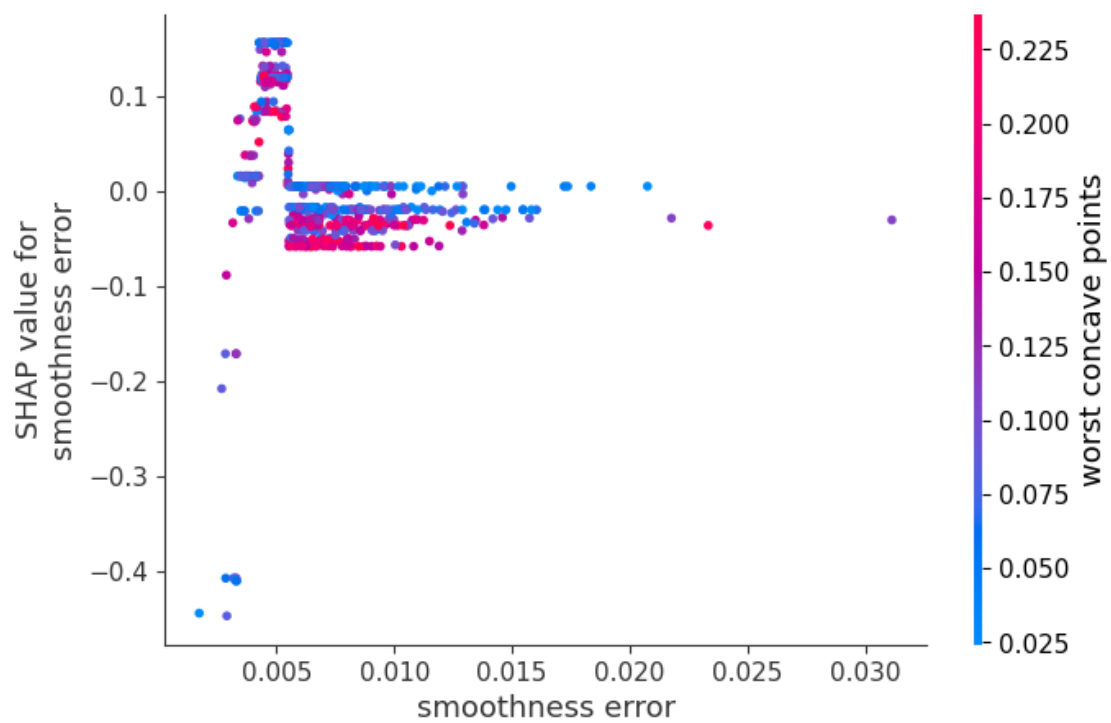
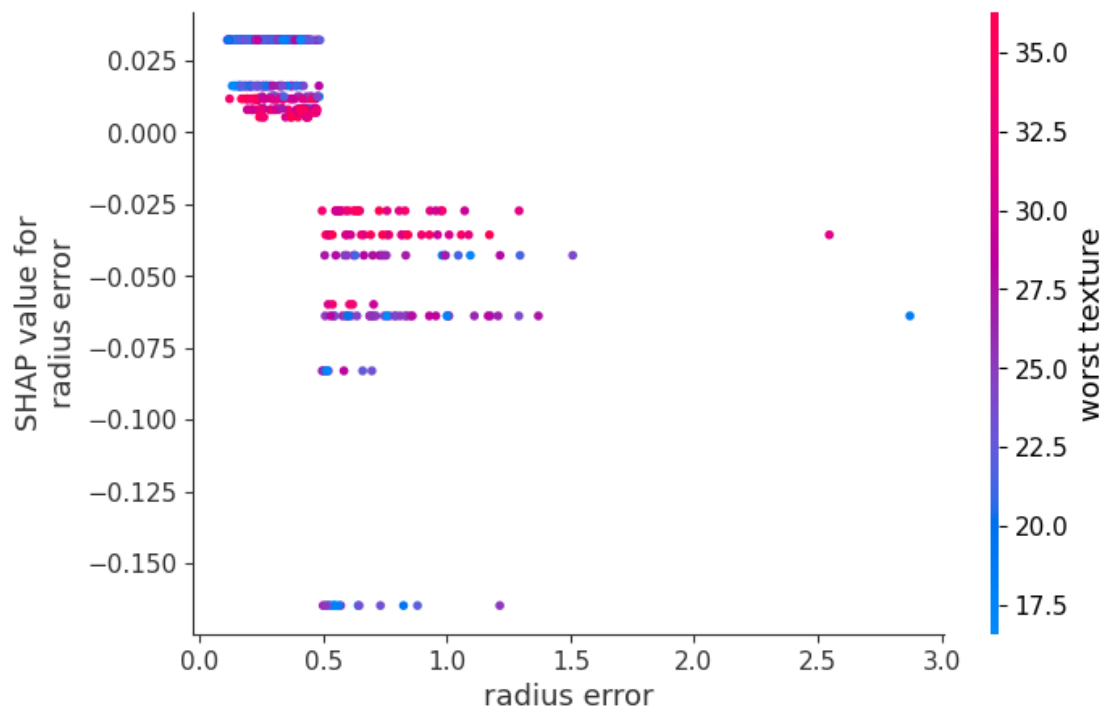


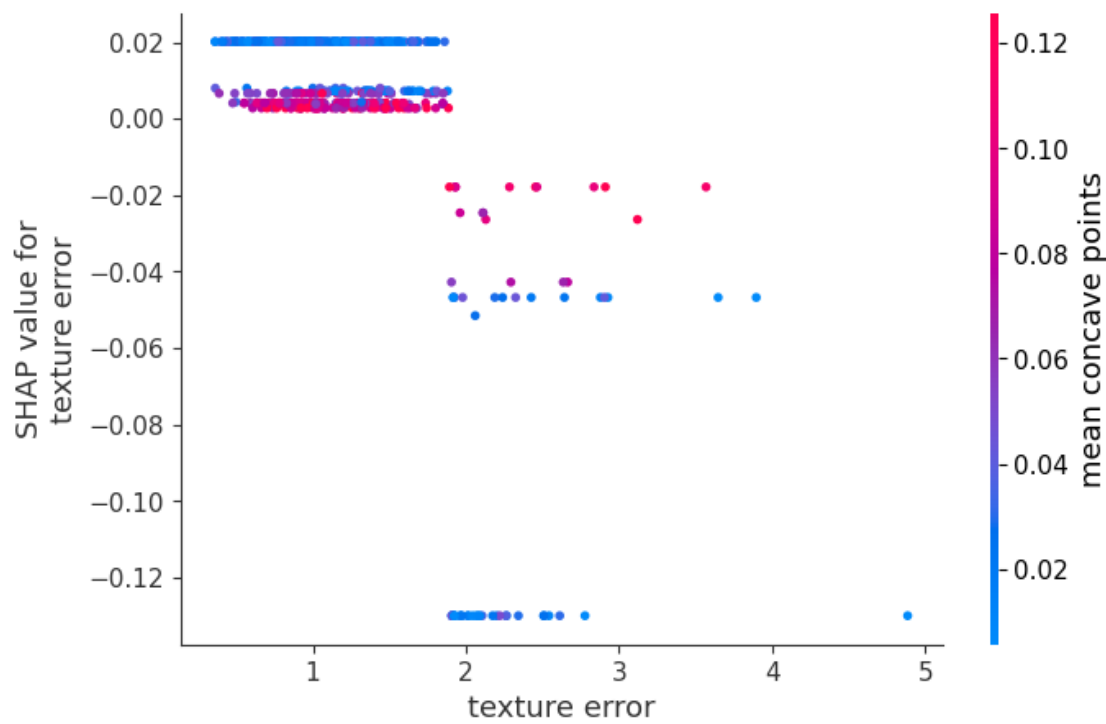
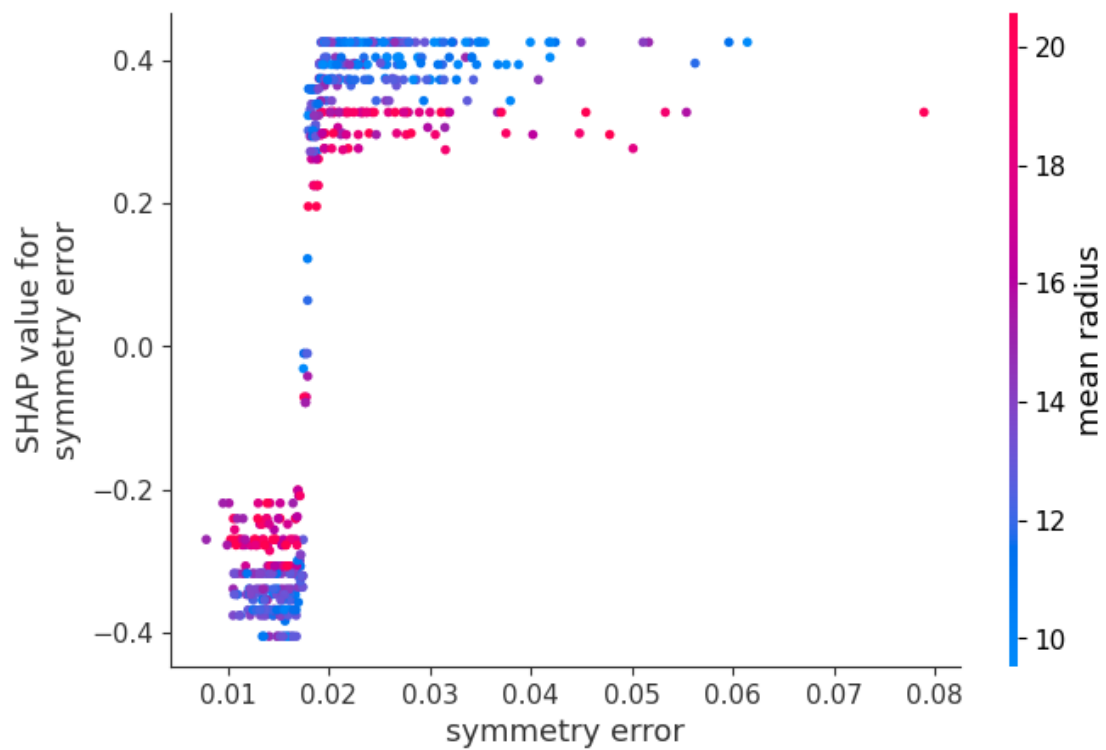


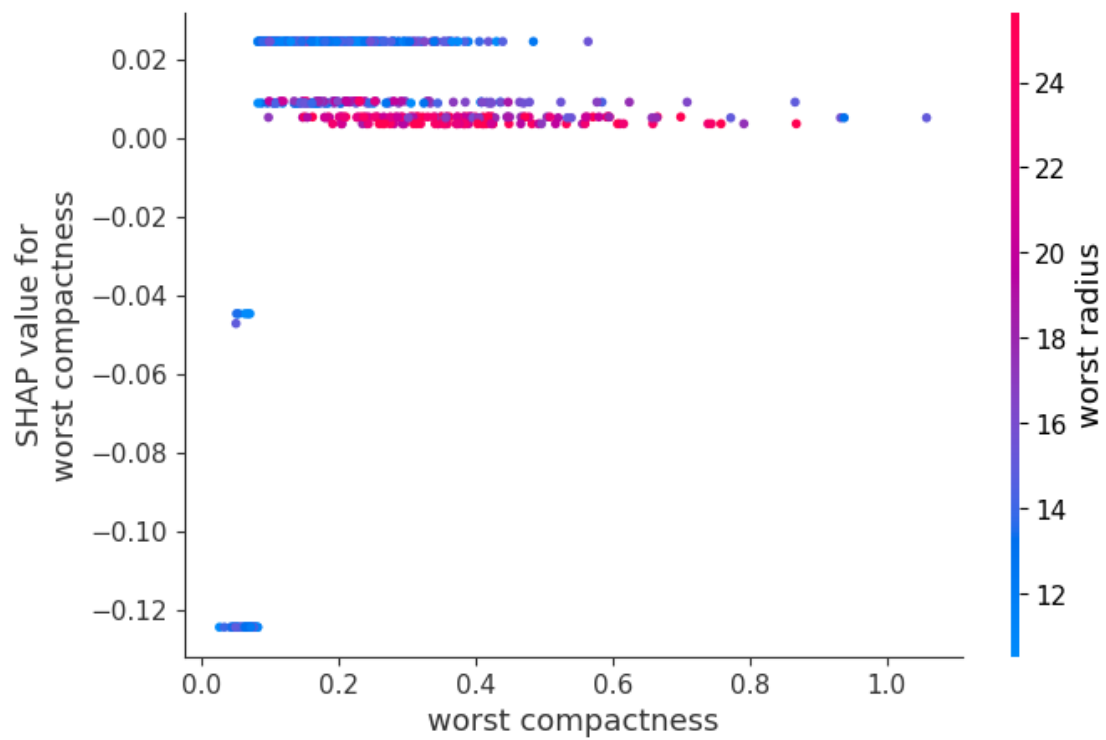
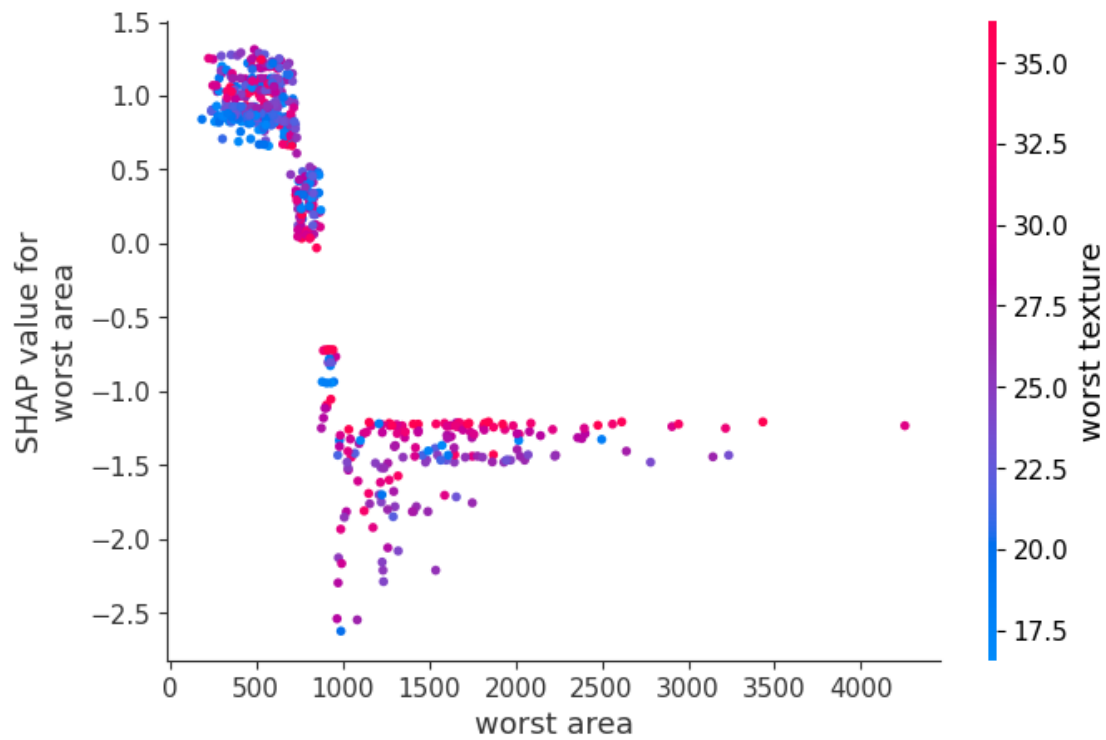




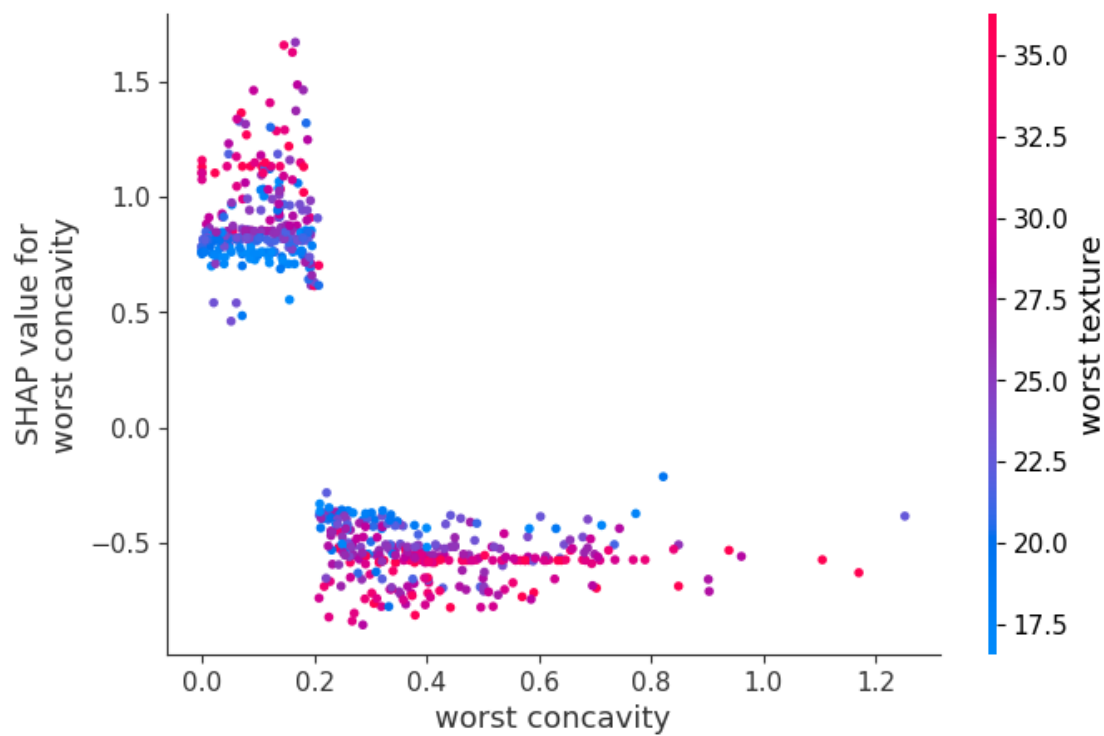
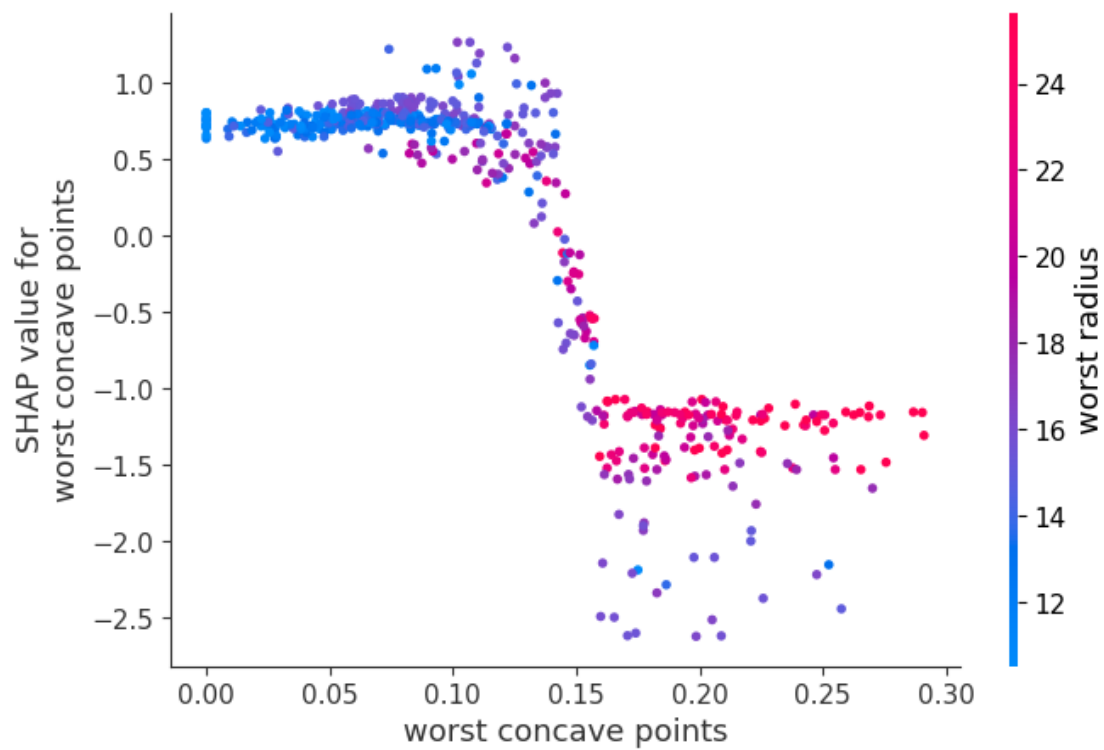


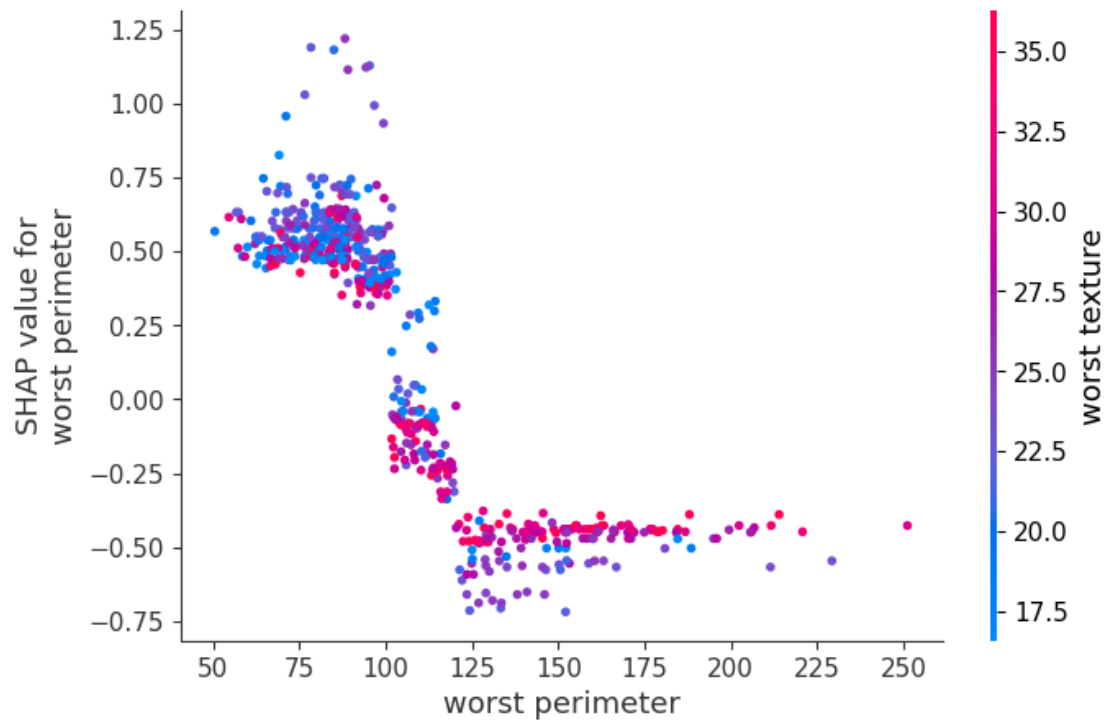
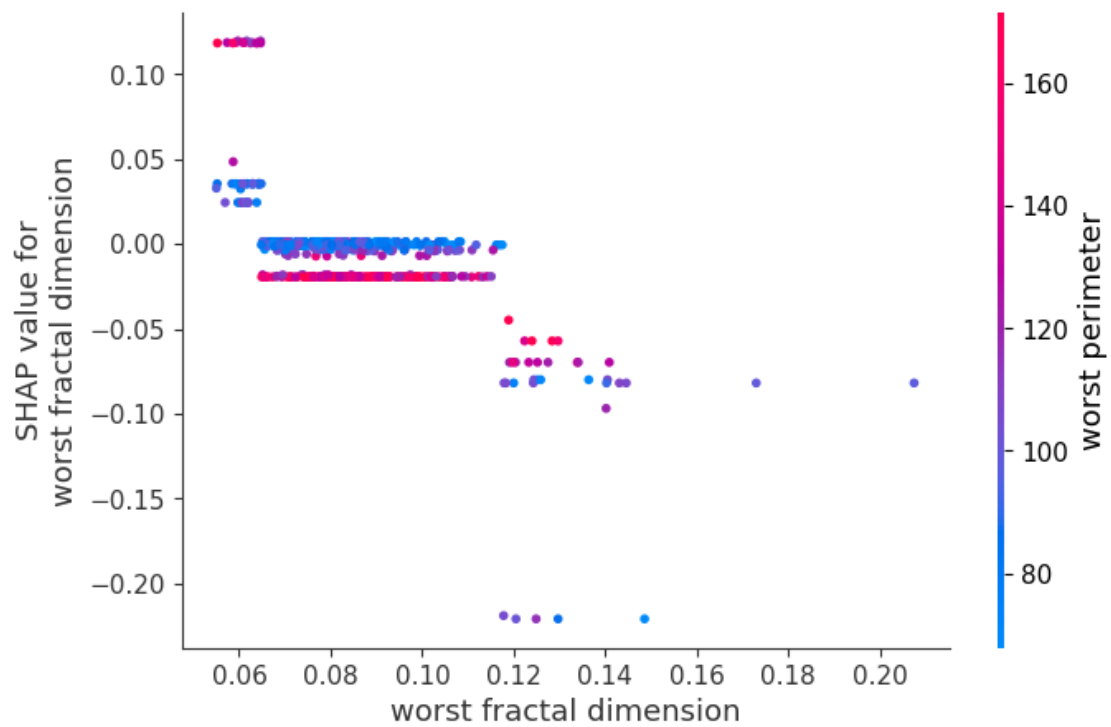


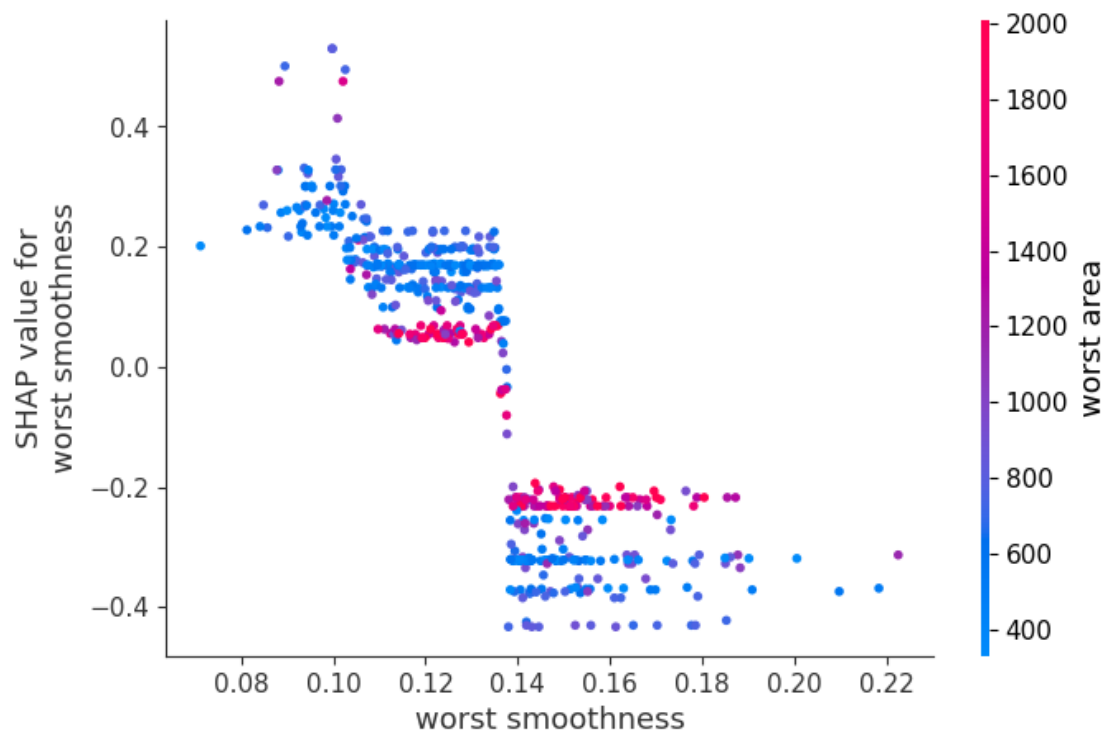
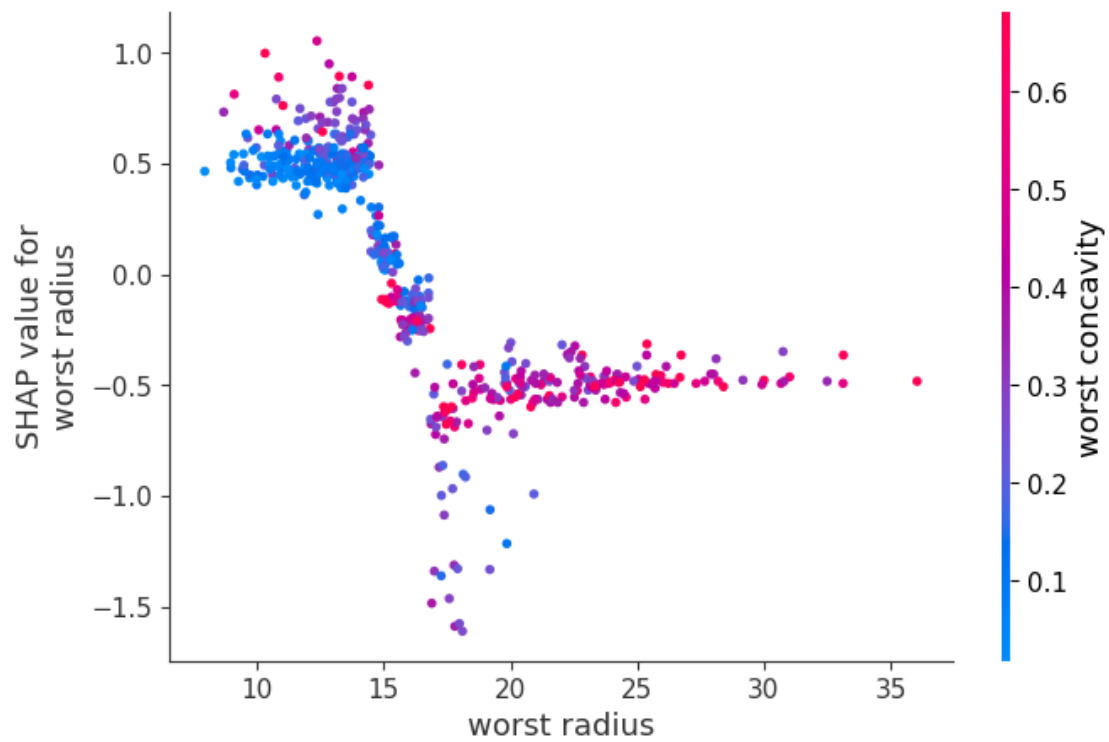


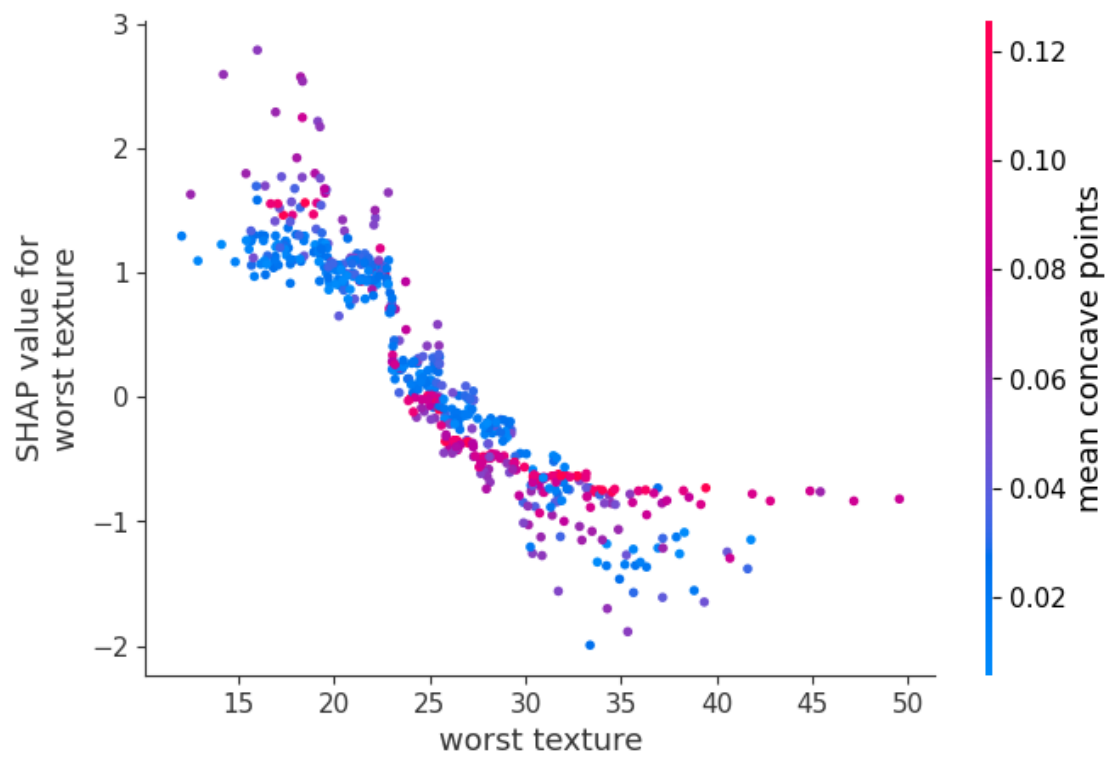
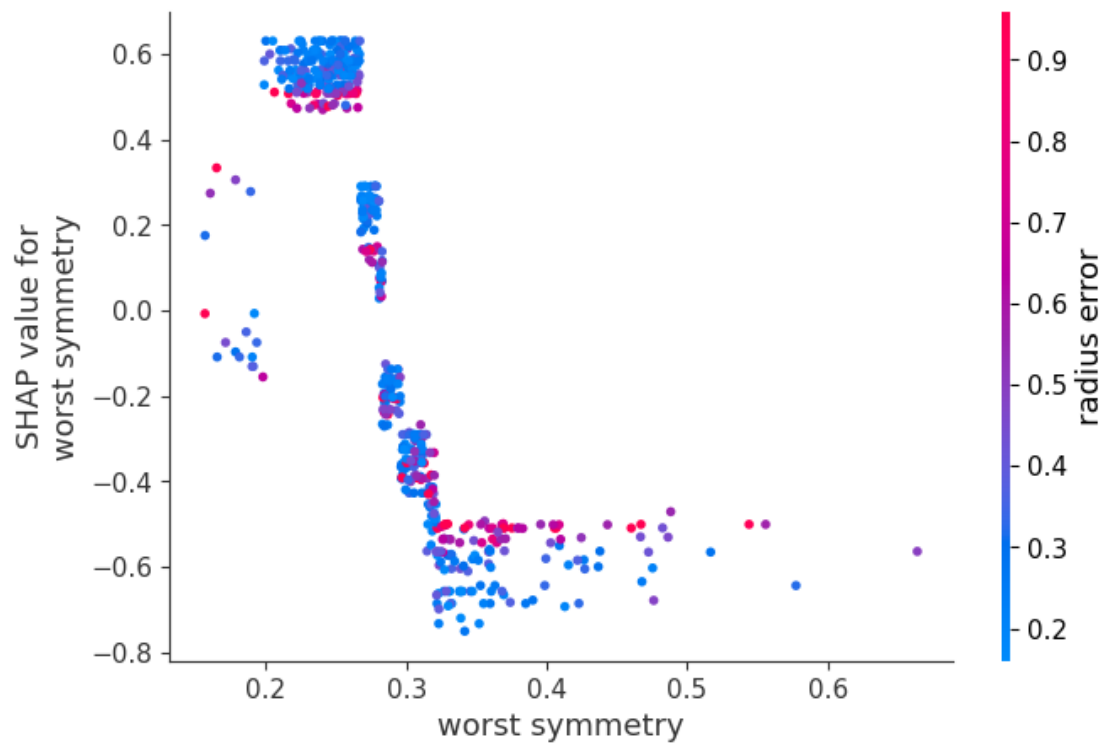


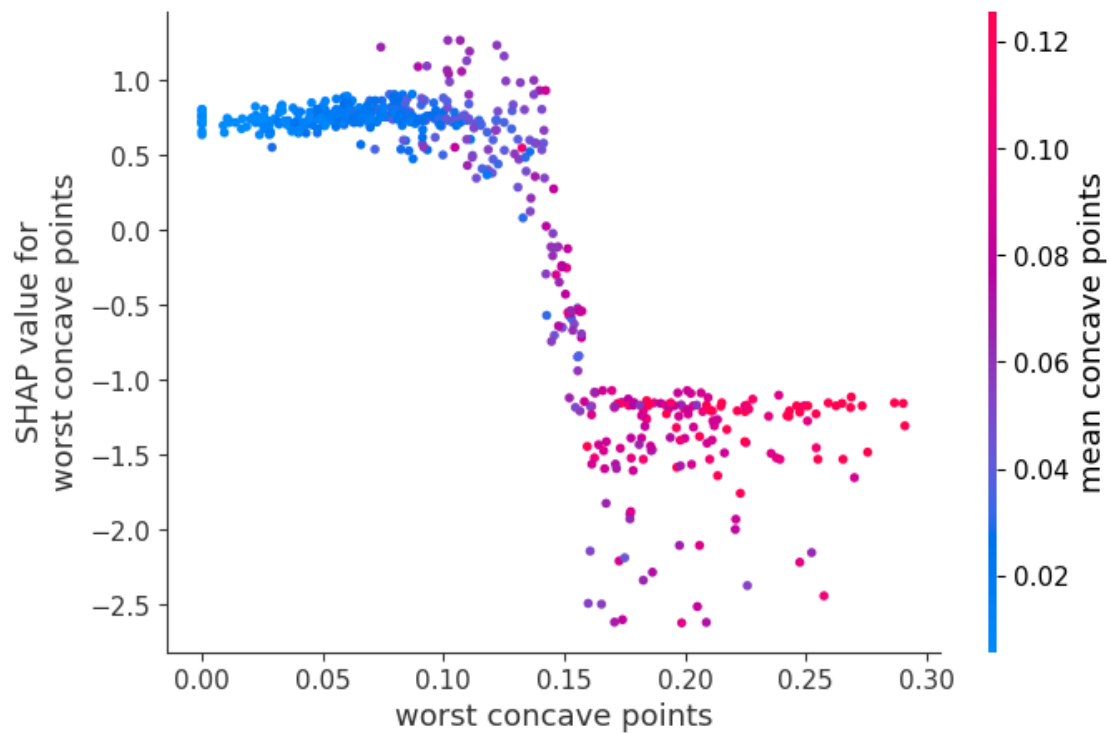












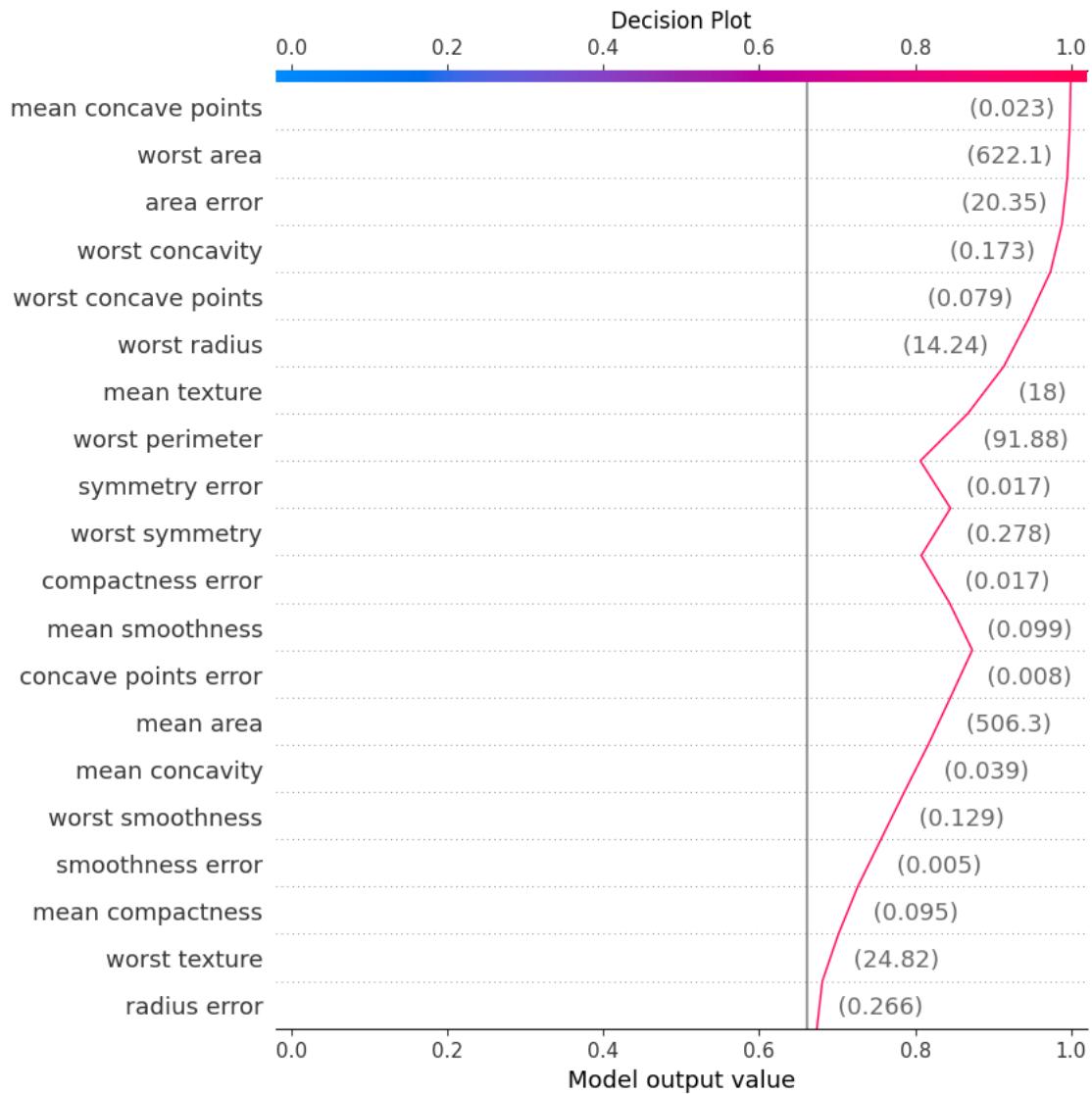
### 3.7 SHAP - Force plots (não é necessário fazer esses)

Adicionar aspas

```
[ ]: # Generate force plot - Multiple rows
shap.force_plot(explainer.expected_value, shap_values[:100,:], X.iloc[:100,:])
```

```
[ ]: # Generate force plot - Single
shap.force_plot(explainer.expected_value, shap_values[0,:], X.iloc[0,:])
```

```
[ ]: # Generate Decision plot
shap.decision_plot(expected_value, shap_values[79],
                    link='logit', features=X.loc[79,:],
                    feature_names=(X.columns.tolist()),
                    show=True, title="Decision Plot")
```



#Push the limits of explainability — an ultimate guide to SHAP library

<https://medium.com/swlh/push-the-limits-of-explainability-an-ultimate-guide-to-shap-library-a110af566a02>

[ ]: