РОССИЙСКИЙ УНИВЕРСИТЕТ ДРУЖБЫ НАРОДОВ

Факультет физико-математических и естественных наук

Кафедра математического моделирования и искусственного интеллекта

ОТЧЕТ ПО ЛАБОРАТОРНОЙ РАБОТЕ № 3

Дисциплина: Интеллектуальный анализ данных

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Группа: НПИбд-01-21

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Вариант № 1

Annealing Data Set

Название файла: anneal.data

Ссылка: https://archive.ics.uci.edu/ml/machine-learning-databases/annealing/

Первый признак: thick (столбец No 33)

Второй признак: width (столбец No 34)

Класс: classes (столбец No 39)

Алгоритмы: K-means, Agglomerative Clustering, DBSCAN, Gaussian Mixture Model

Меры качества: чистота (purity), парные меры TP, FN, FP, TN, индекс Фоулкса – Мэллоуса

Найти лучший алгоритм кластеризации относительно меры качества: чистота (purity)

1. открыть базу данных и прочитать значения

In [2]:
```
from ucimlrepo import fetch_ucirepo

# fetch dataset
annealing = fetch_ucirepo(id=3)
```

In [3]:
```
annealing['data'].keys()
```

Out[3]:
```
dict_keys(['ids', 'features', 'targets', 'original', 'headers'])
```

In [4]:
```
import pandas as pd
df = pd.DataFrame(annealing['data']['targets'])
df['thick'] = annealing['data']['features']['thick']
df['width'] = annealing['data']['features']['width']
df
```

Out[4]:

	class	thick	width
0	3	0.700	610.0
1	3	3.200	610.0
2	3	0.700	1300.0
3	3	2.801	385.1
4	3	0.801	255.0
...	...	...	...
893	2	1.599	610.0
894	2	1.601	830.0
895	2	1.599	150.0
896	U	0.400	20.0
897	U	4.000	610.0

898 rows × 3 columns

2. починка пропусков

In [5]:
```
df['class'].notna().all()
```

Out[5]:
```
np.True_
```

In [6]:
```
df['thick'].notna().all()
```

Out[6]:
```
np.True_
```

In [7]:
```
df['width'].notna().all()
```

Out[7]:
```
np.True_
```

Починка не требуется.

3. объединение классов

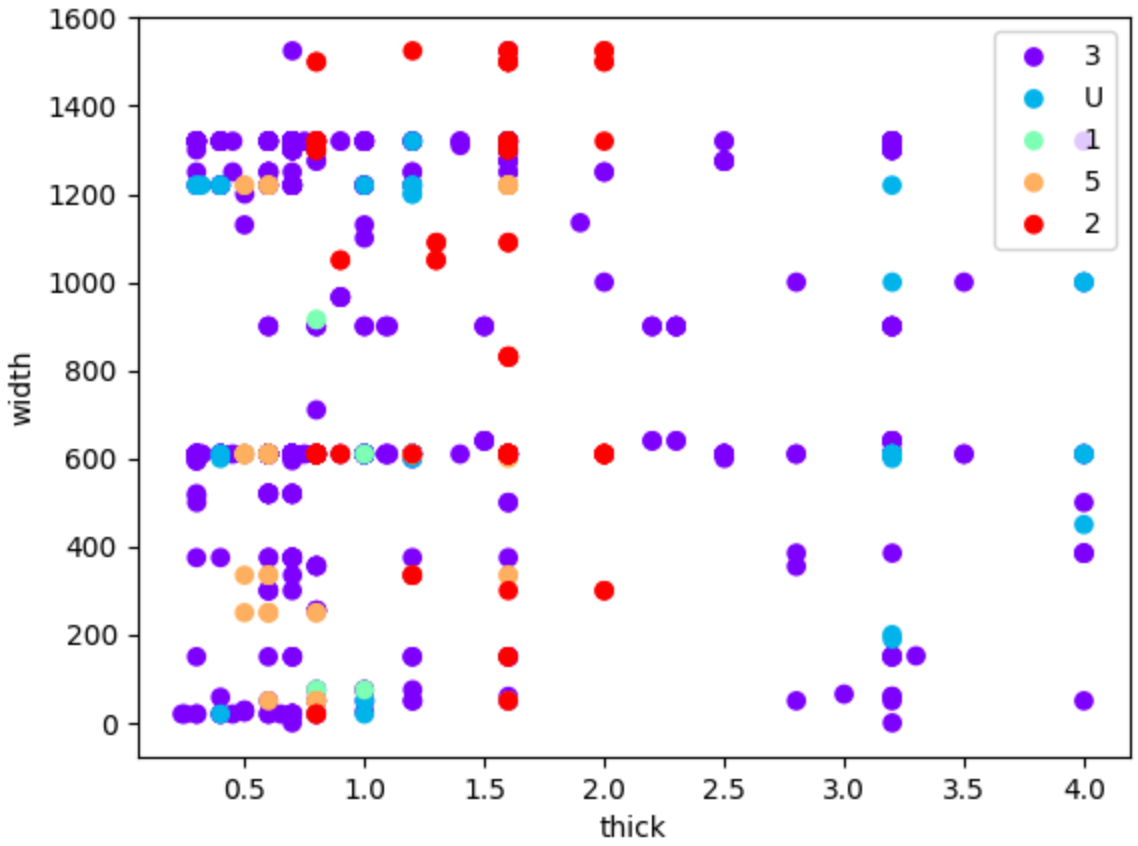
In [8]:
```
df['class'].unique()
```

Out[8]:
```
array(['3', 'U', '1', '5', '2'], dtype=object)
```

Классов не больше 5, поэтому объединение не требуется.

4. визуализация

In [9]:
```
import matplotlib.pyplot as plt

klass = ['3', 'U', '1', '5', '2']

for k in klass:
    df_k = df[df['class'] == k]
    plt.scatter(df_k['thick'], df_k['width'], label=k, c=[klass.index(k) for

plt.xlabel('thick')
plt.ylabel('width')

plt.legend()
plt.show()
```



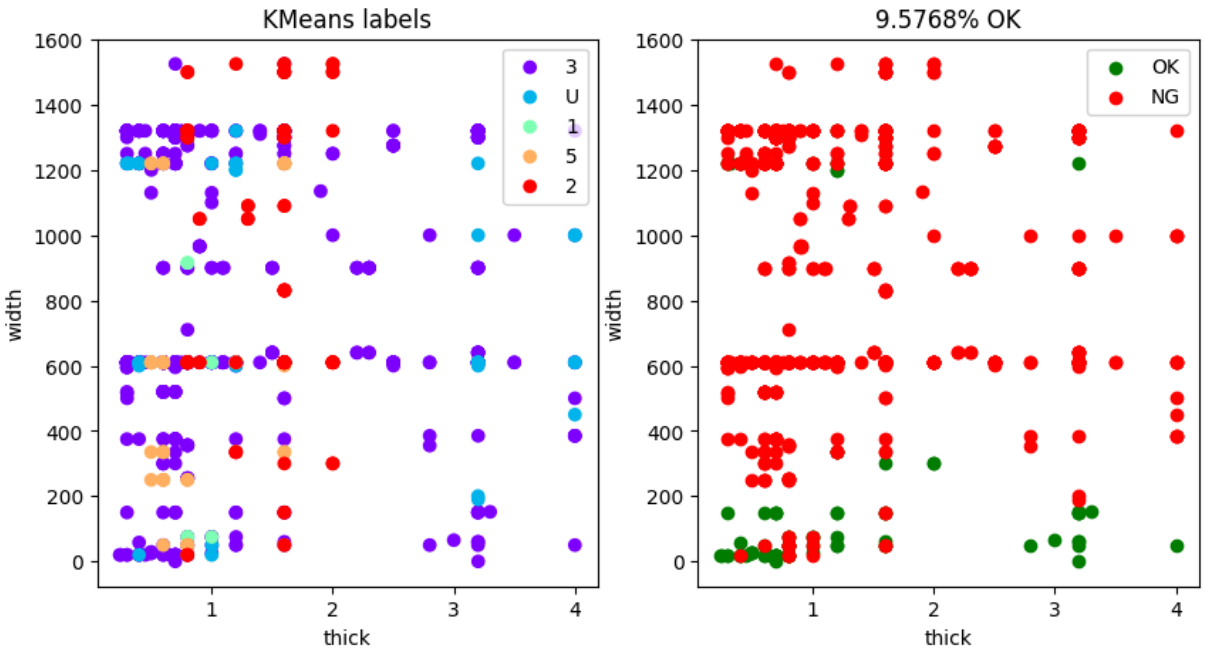
5. кластеризация

In [10]:
```
def draw_clusters(df, predicted_labels, title):
    # two panels, left with predicted data, right with correct and incorrect
    fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(10, 5))

    all_thick = list(df['thick'])
    all_width = list(df['width'])
    all_class = list(df['class'])


    for k in range(5):
        thick = []
        width = []
        for i in range(len(df)):
            if all_class[i] == klass[k]:
                thick.append(all_thick[i])
                width.append(all_width[i])
        ax1.scatter(thick, width, label=klass[k], c=[k for i in range(len(th

    ax1.set_xlabel('thick')
    ax1.set_ylabel('width')

    ax1.legend()

    ax1.set_title(title)
```

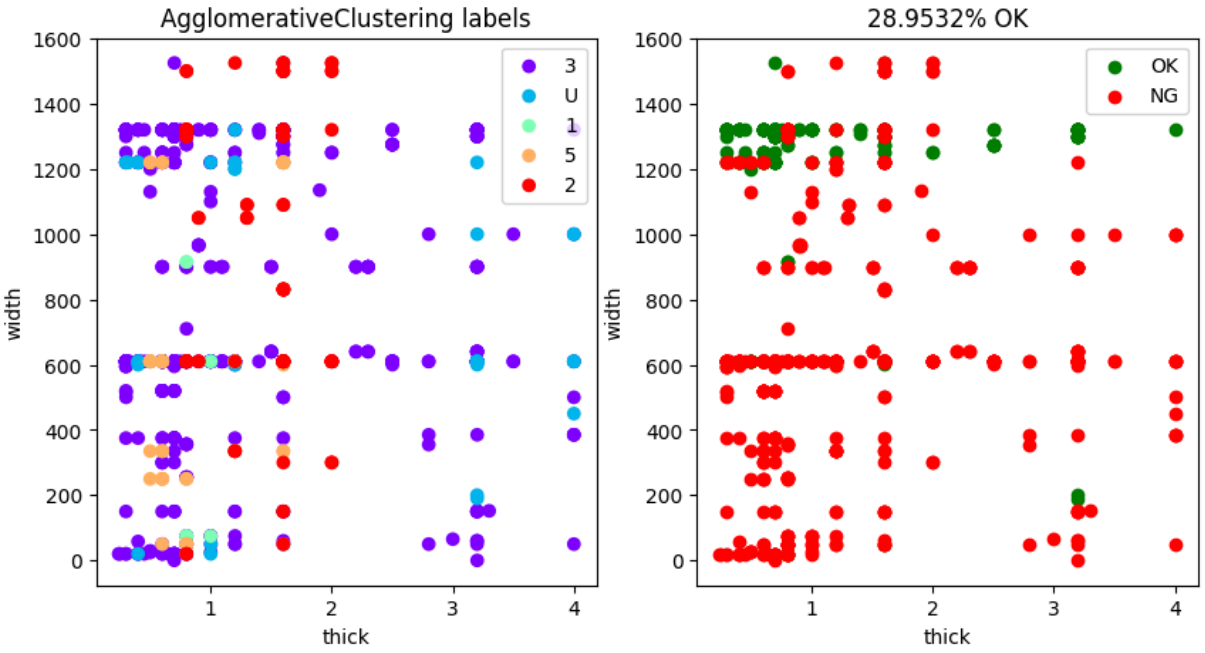
```
    prediction_correct_thick = []
    prediction_correct_width = []
    prediction_incorrect_thick = []
    prediction_incorrect_width = []

    for i in range(len(df)):
        if all_class[i] == predicted_labels[i]:
            prediction_correct_thick.append(all_thick[i])
            prediction_correct_width.append(all_width[i])
        else:
            prediction_incorrect_thick.append(all_thick[i])
            prediction_incorrect_width.append(all_width[i])

    ax2.scatter(prediction_correct_thick, prediction_correct_width, label='C
    ax2.scatter(prediction_incorrect_thick, prediction_incorrect_width, labe

    ax2.set_xlabel('thick')
    ax2.set_ylabel('width')

    ax2.legend()
    ax2.set_title(str(round((len(prediction_correct_thick) / len(all_thick))

    plt.show()
```

In [11]:

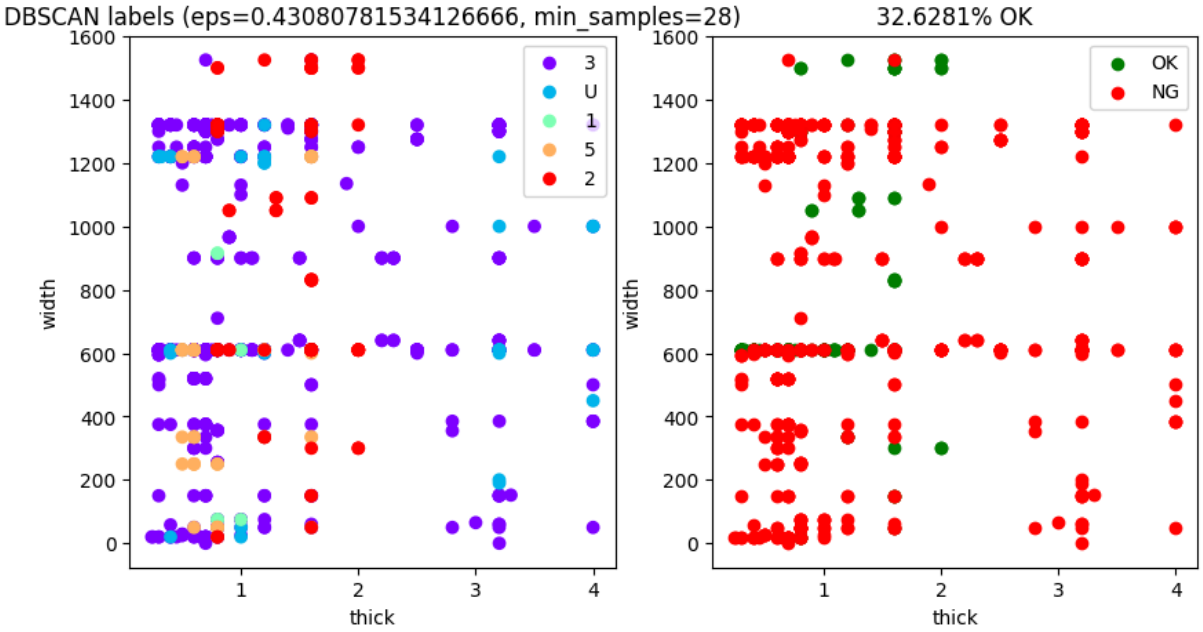
```
# K-means, Agglomerative Clustering, DBSCAN, Gaussian Mixture Model

from sklearn.cluster import KMeans
from sklearn.cluster import AgglomerativeClustering
from sklearn.cluster import DBSCAN
from sklearn.mixture import GaussianMixture

kmeans = KMeans(n_clusters=5)
kmeans_labels = kmeans.fit_predict(df[['thick', 'width']])
kmeans_labels = [klass[i] for i in kmeans_labels]
draw_clusters(df, kmeans_labels, "KMeans labels")
```

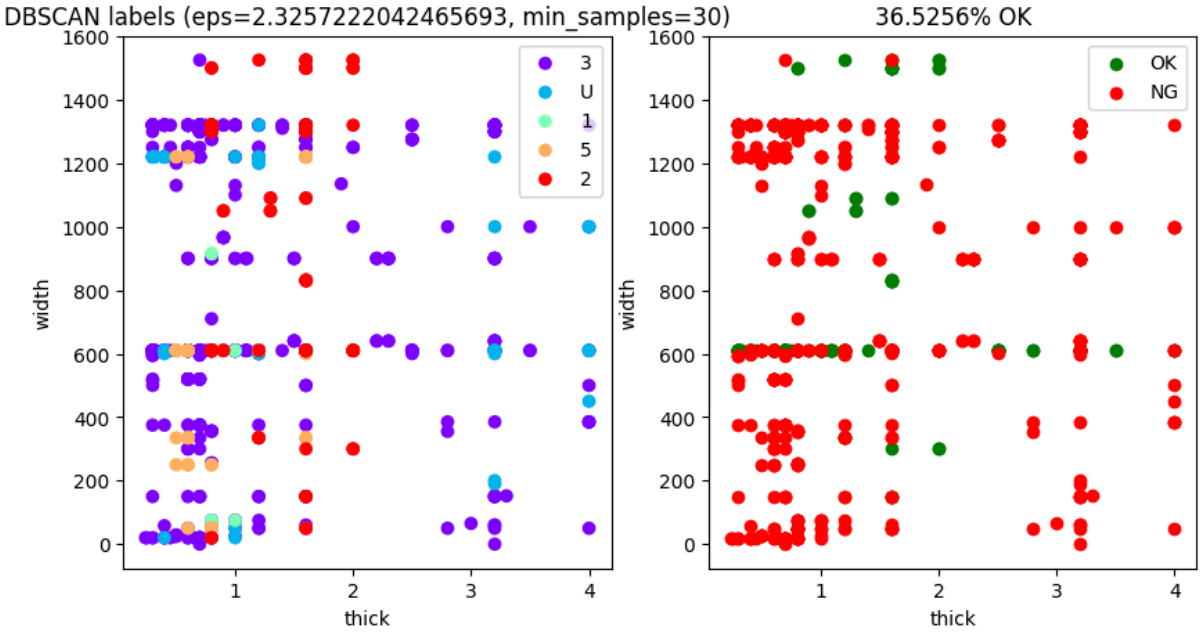


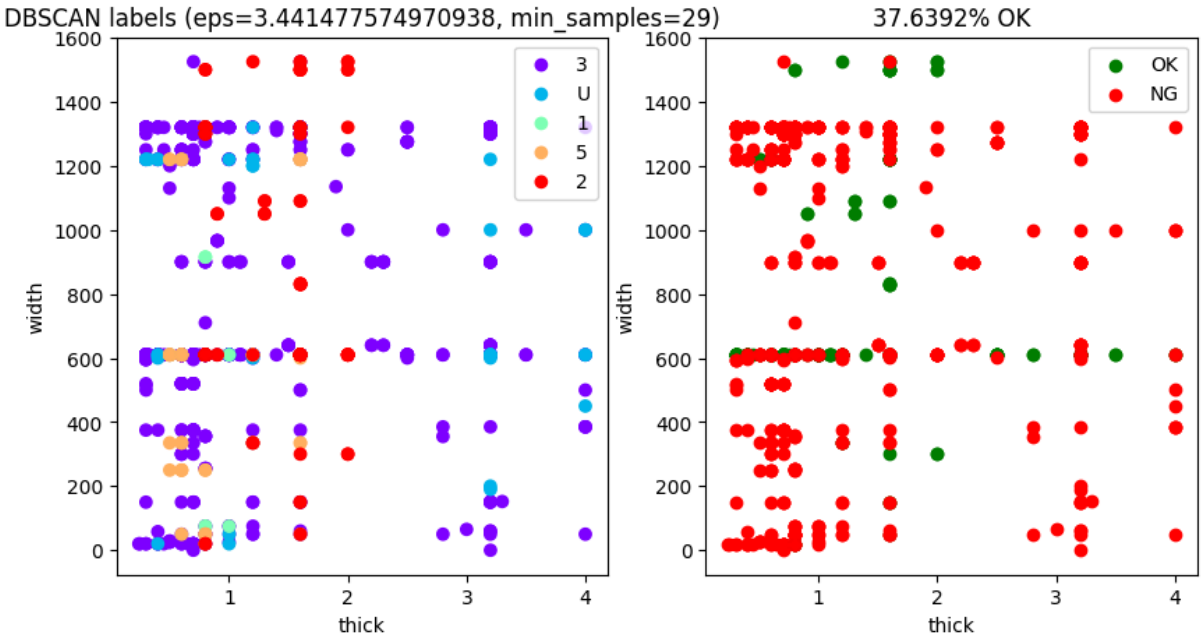
In [12]:
```
aggloclusterer = AgglomerativeClustering(n_clusters=5)
aggloclusterer_labels = aggloclusterer.fit_predict(df[['thick', 'width']])
aggloclusterer_labels = [klass[i] for i in aggloclusterer_labels]
draw_clusters(df, aggloclusterer_labels, "AgglomerativeClustering labels")
```



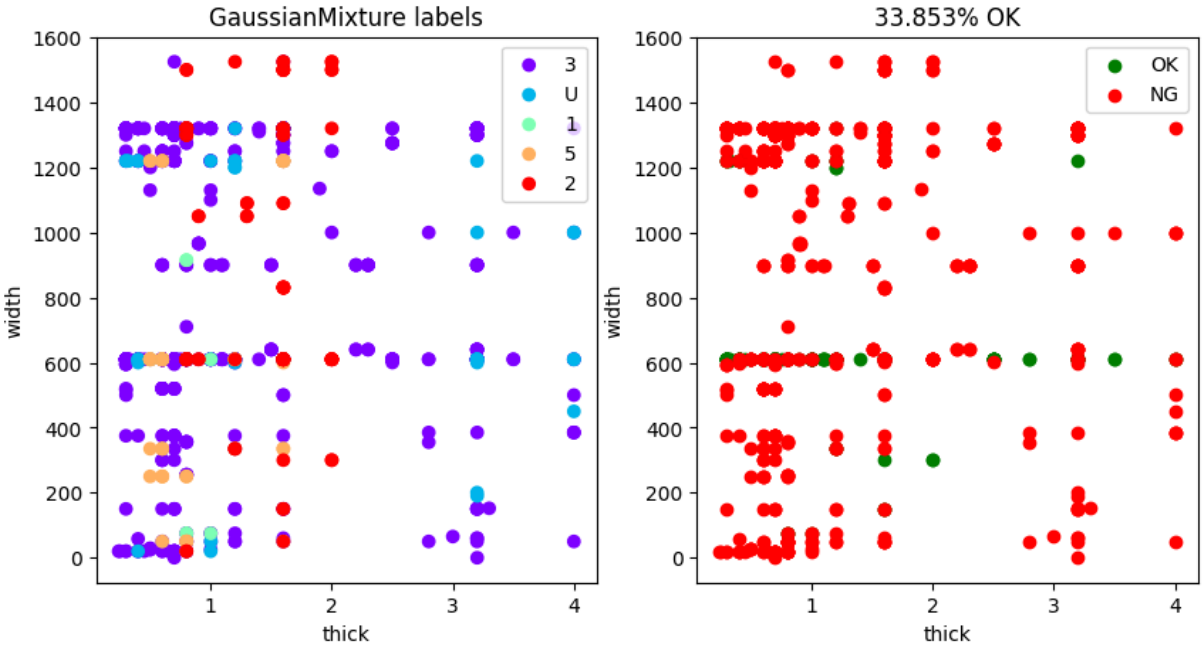
In [13]:
```
import random
for i in range(3):
    eps = 0.5
    min_samples = 5
    set_ok = False
    while not set_ok:
        eps = random.uniform(0.1, 5)
        min_samples = random.randint(2, 50)
        dbscan = DBSCAN(eps=eps, min_samples=min_samples)
        dbscan_labels = dbscan.fit_predict(df[['thick', 'width']])
        if len(set(dbscan_labels)) == 5:
            set_ok = True

    dbscan_labels = [klass[i] for i in dbscan_labels]
    draw_clusters(df, dbscan_labels, f"DBSCAN labels ({eps=}, {min_samples=}
```


DBSCAN labels (eps=0.43080781534126666, min_samples=28)
32.6281% OK
width
thick
3
U
1
5
2
OK
NG


DBSCAN labels (eps=2.3257222042465693, min_samples=30)
36.5256% OK
width
thick
3
U
1
5
2
OK
NG



In [14]:
```
gaussmix = GaussianMixture(n_components=5)
gaussmix_labels = gaussmix.fit_predict(df[['thick', 'width']])
gaussmix_labels = [klass[i] for i in gaussmix_labels]
draw_clusters(df, gaussmix_labels, "GaussianMixture labels")
```



6. матрица сопряженности

Во всех таблицах, строчки -- это настоящие классы, а столбцы -- предсказания.

In [15]:
```
from sklearn.metrics.cluster import contingency_matrix
```

```
true_labels = [i for i in list(df['class'])]
kmeans_contingency = contingency_matrix(true_labels, kmeans_labels)
pd.DataFrame(kmeans_contingency).style.background_gradient(cmap='Blues')
```

Out[15]:

	0	1	2	3	4
0	3	0	3	2	0
1	42	5	5	13	34
2	328	32	64	37	223
3	33	14	7	0	13
4	17	2	4	3	14

In [16]:
```
agglocluster_contingency = contingency_matrix(true_labels, agglocluster_labe
pd.DataFrame(agglocluster_contingency).style.background_gradient(cmap='Blues
```

Out[16]:

	0	1	2	3	4
0	2	3	0	3	0
1	13	3	34	42	7
2	40	50	220	328	46
3	0	7	13	33	14
4	3	3	14	18	2

In [17]:
```
dbscan_contingency = contingency_matrix(true_labels, dbscan_labels)
pd.DataFrame(dbscan_contingency).style.background_gradient(cmap='Blues')
```

Out[17]:

	0	1	2	3	4
0	0	5	3	0	0
1	15	37	42	0	5
2	140	204	288	27	25
3	0	22	32	13	0
4	3	14	14	9	0

In [18]:
```
gaussmix_contingency = contingency_matrix(true_labels, gaussmix_labels)
pd.DataFrame(gaussmix_contingency).style.background_gradient(cmap='Blues')
```

Out[18]:

	0	1	2	3	4
0	3	0	3	2	0
1	3	7	42	11	36
2	43	101	280	36	224
3	7	15	32	0	13
4	3	6	14	3	14

In [19]:
```
import numpy as np
# https://stackoverflow.com/a/51672699
def purity_score(contingency_matrix):
    return np.sum(np.amax(contingency_matrix, axis=0)) / np.sum(contingency_
```

In [20]:
```
print("KMeans purity: ", purity_score(kmeans_contingency))
print("AgglomerativeClustering purity: ", purity_score(aggloclusterr_continge
print("DBSCAN purity: ", purity_score(dbscan_contingency))
print("GaussianMixture purity: ", purity_score(gaussmix_contingency))
```

```
KMeans purity:  0.7616926503340757
AgglomerativeClustering purity:  0.7616926503340757
DBSCAN purity:  0.7616926503340757
GaussianMixture purity:  0.7616926503340757
```

In [21]:
```
# pairwise TN, FN, FP, TP
def pairwise_tf_fn(true_labels, test_labels):
    out = []
    for k in klass:
        tp = 0
        fp = 0
        fn = 0
        tn = 0
        for i in range(len(true_labels)):
            if true_labels[i] == k and test_labels[i] == k:
                tp += 1
            elif true_labels[i] != k and test_labels[i] == k:
                fp += 1
            elif true_labels[i] == k and test_labels[i] != k:
                fn += 1
            else:
                tn += 1
        out.append([tp, fp, fn, tn])
    return np.array(out).sum(axis=0)
```

In [22]:
```
import math
def fowkes_mallows(tp, fp, fn):
    return math.sqrt( (tp / (tp+fp)) * (tp / (tp + fn)) )
```

In [23]:
```
tp,fp,fn,tn = pairwise_tf_fn(true_labels, kmeans_labels)
print("Fowkes-Mallows KMeans:", fowkes_mallows(tp,fp,fn))
tp,fp,fn,tn = pairwise_tf_fn(true_labels, aggloclusterr_labels)
print("Fowkes-Mallows AgglomerativeClustering:", fowkes_mallows(tp,fp,fn))
tp,fp,fn,tn = pairwise_tf_fn(true_labels, dbscan_labels)
print("Fowkes-Mallows DBSCAN:", fowkes_mallows(tp,fp,fn))
tp,fp,fn,tn = pairwise_tf_fn(true_labels, gaussmix_labels)
print("Fowkes-Mallows GaussianMixture:", fowkes_mallows(tp,fp,fn))
```

```
Fowkes-Mallows KMeans: 0.0957683741648107
Fowkes-Mallows AgglomerativeClustering: 0.289532293986637
Fowkes-Mallows DBSCAN: 0.37639198218262804
Fowkes-Mallows GaussianMixture: 0.33853006681514475
```

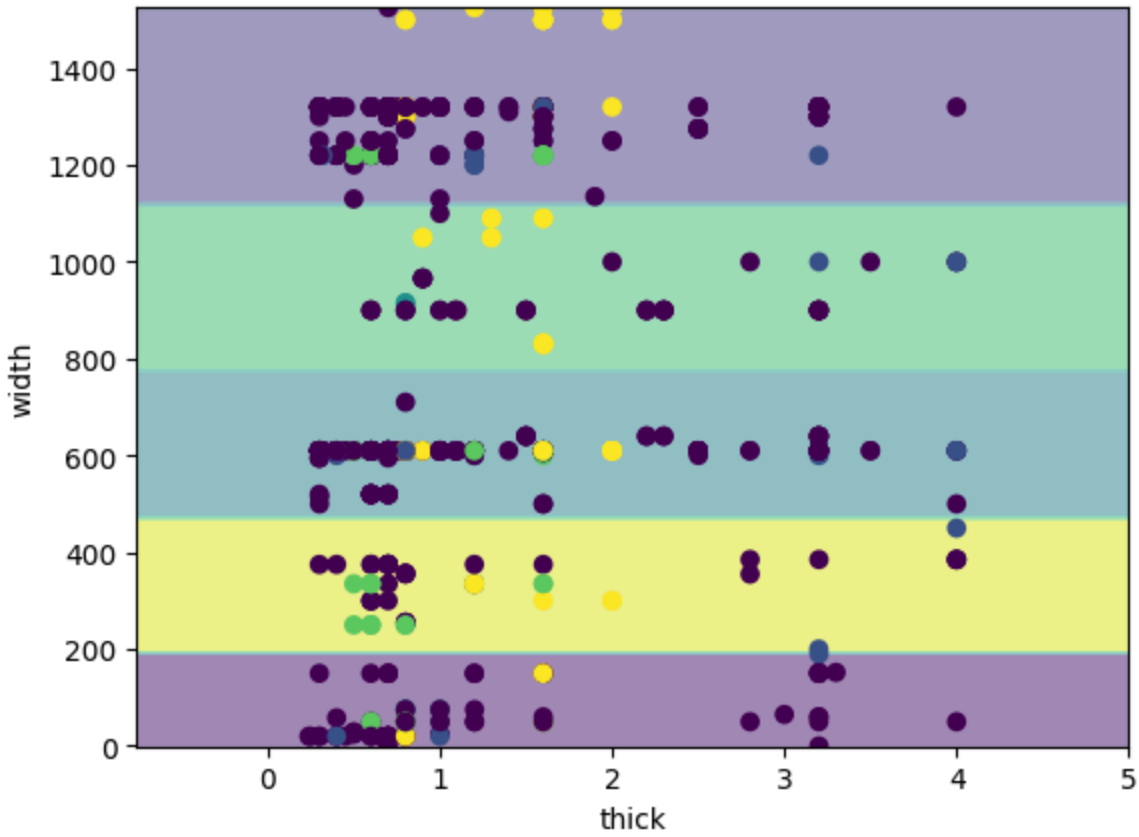
7. лучший алгоритм

In [24]:
```
purity_scores = [
    ("KMeans", purity_score(kmeans_contingency)),
    ("AgglomerativeClustering", purity_score(agglocluster_contingency)),
    ("DBSCAN", purity_score(dbscan_contingency)),
    ("GaussianMixture", purity_score(gaussmix_contingency)),
]

purity_scores.sort(key=lambda x: x[1], reverse=True)
print("Best:")
for i, score in enumerate(purity_scores):
    print(f"{i+1}. {score[0]}:\t\t{score[1]}")
```

```
Best:
1. KMeans:              0.7616926503340757
2. AgglomerativeClustering:             0.7616926503340757
3. DBSCAN:              0.7616926503340757
4. GaussianMixture:             0.7616926503340757
```

8. области принятия решений

In [29]:
```
# decision boundary plot for KMeans

from sklearn.inspection import DecisionBoundaryDisplay

disp = DecisionBoundaryDisplay.from_estimator(kmeans, df[['thick', 'width']]
disp.ax_.scatter(df['thick'], df['width'], c=[klass.index(k) for k in df['cl
plt.show()
```



In [ ]: