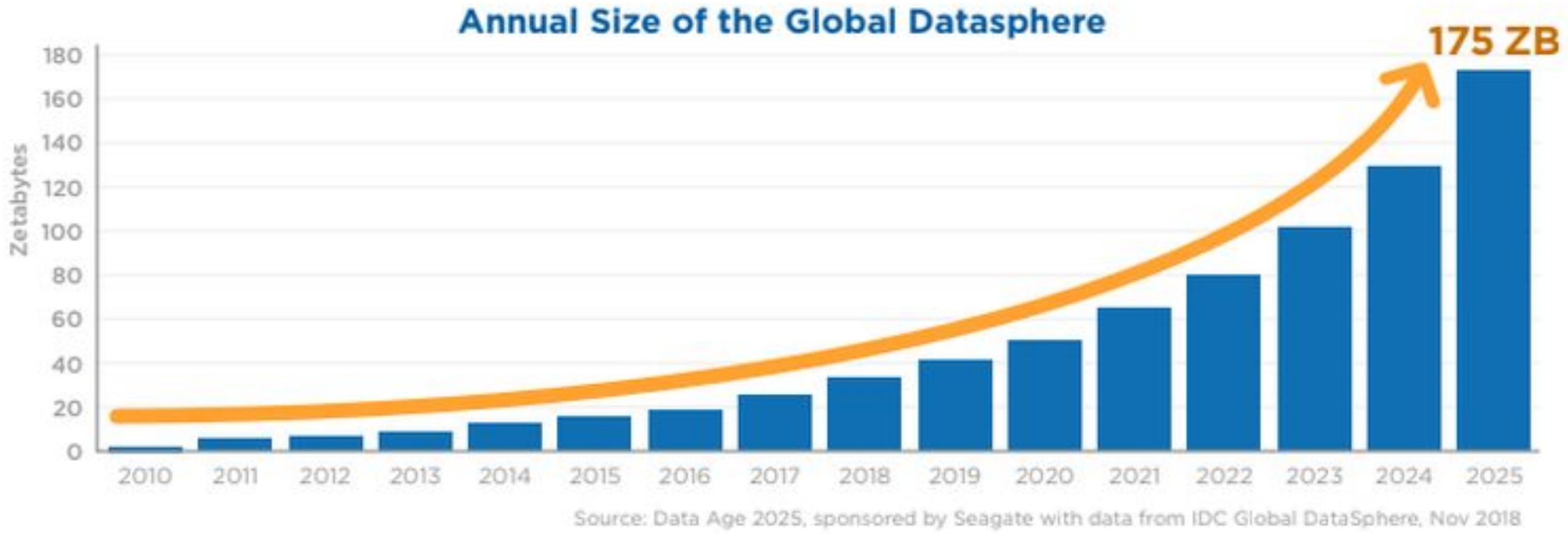
Основы Data science
Кластеризация

- **Data Science** — это работа с большими данными *(англ. Big Data)*.

Figure 1 – Annual Size of the Global Datasphere



1 ZB = 10^21 bytes

1 TB = 10^12 bytes

Evolution of a Terabyte of Data 1956 - 2015

A decade by decade guide to storing 1TB of data from the 1950s to 2015

280MB

1960s

1TB

2013

Эволюция в области хранения и Обработки данных

Кто такой Data Scientist?

proschool
An ims Initiative

DATA SCIENTIST
MUST-HAVE SKILLS

MATH & STATISTICS

- Machine Learning
- Statistical Modeling
- Exploratory Analysis
- Clustering
- Regression Analysis

PROGRAMMING & DATABASE

- Computer Science Fundamentals
- Database Management System
- Data Visualization
- Python
- Big Data

DOMAIN KNOWLEDGE & SOFT SKILLS

- Inclination towards business operations
- Keen on working with data
- Problem solver
- Strategic, proactive, and cooperative
- Interested in hacking

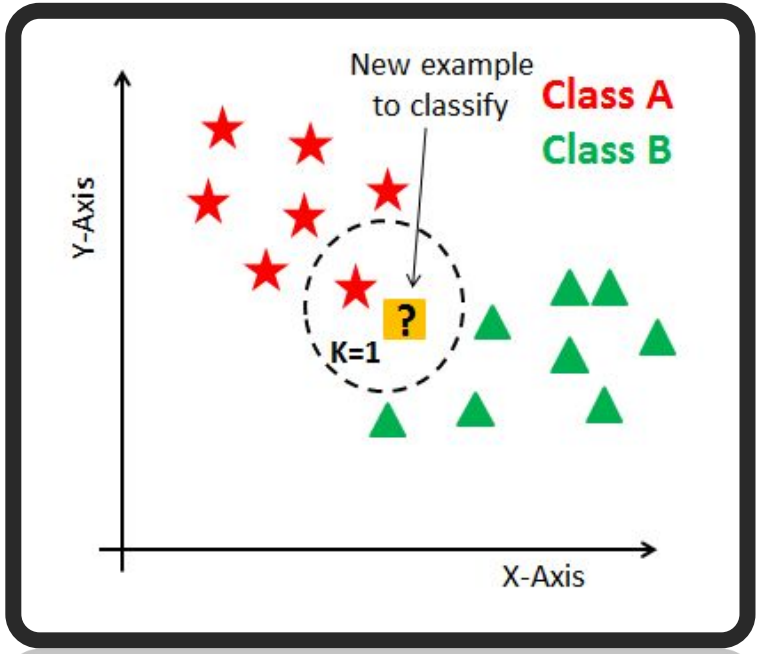
COMMUNICATION & VISUALIZATION

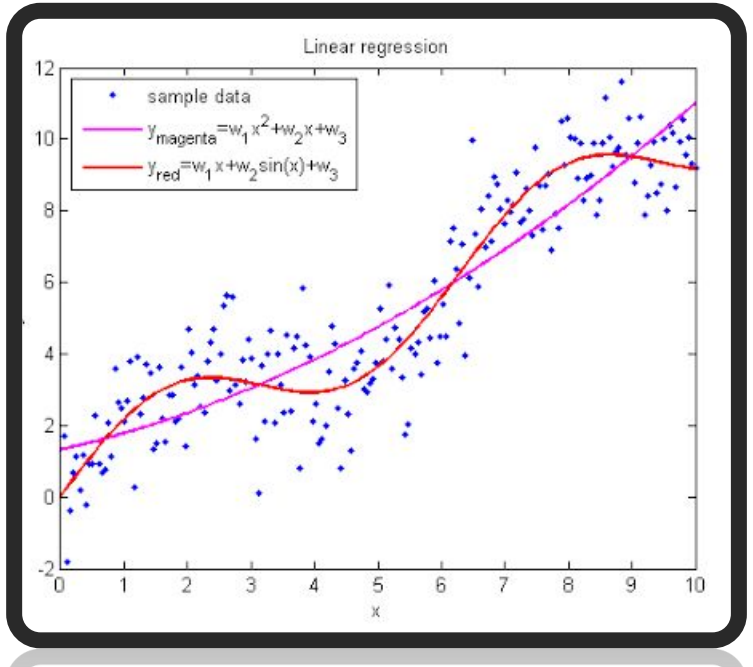
- Storytelling skills
- Convert data-based insights into decisions
- Collaborative with Sr. Management
- Knowledge of tools like Tableau
- Visual art design

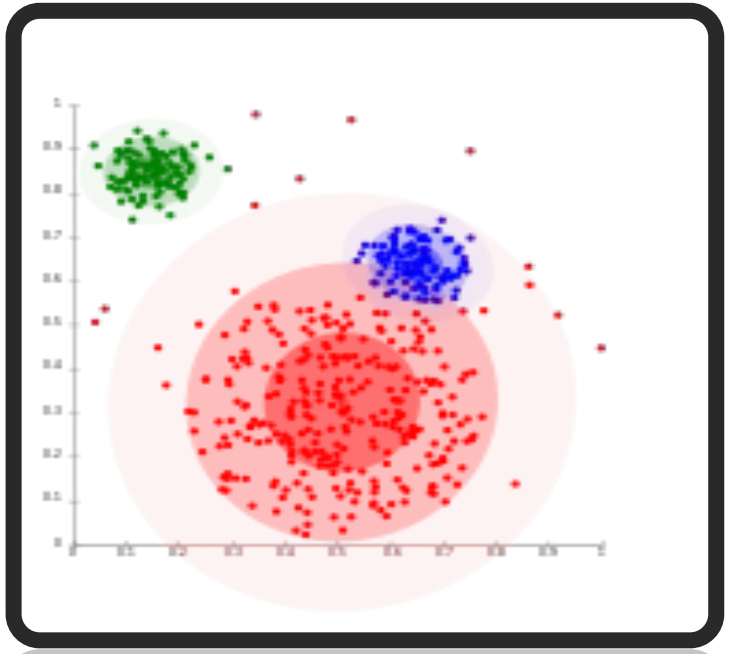
Классификация

Регрессия

Кластеризация



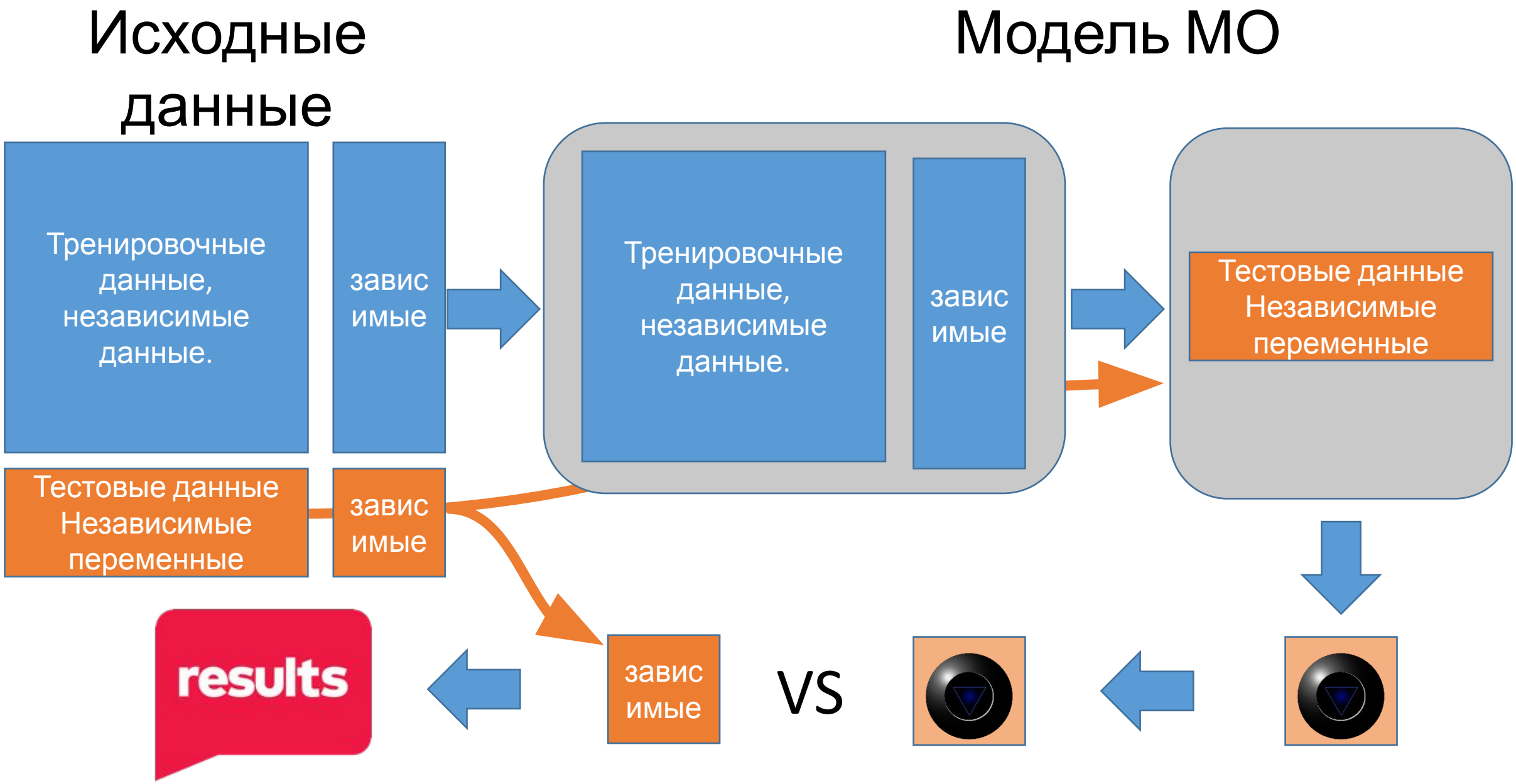


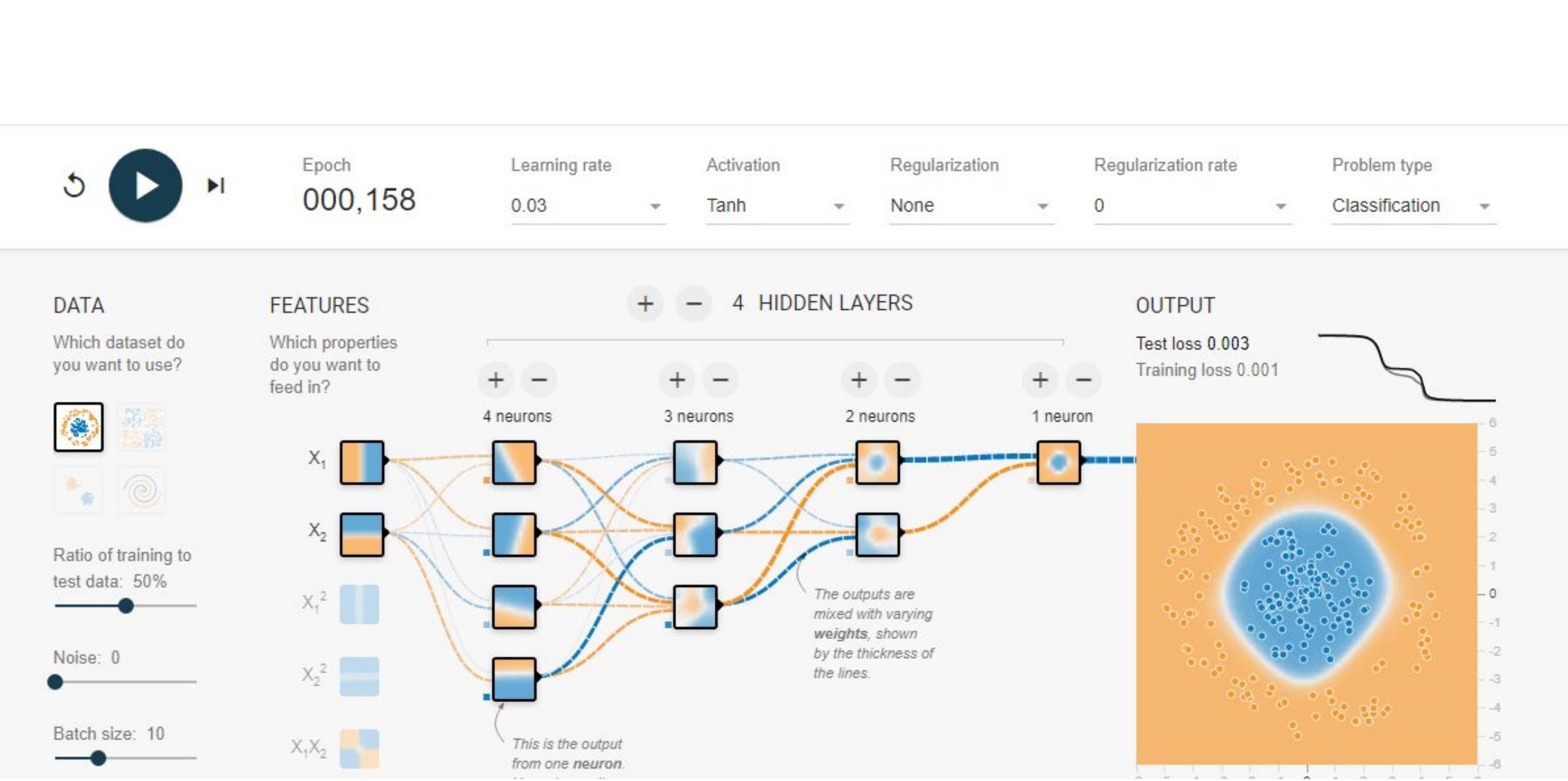


Независимые переменные

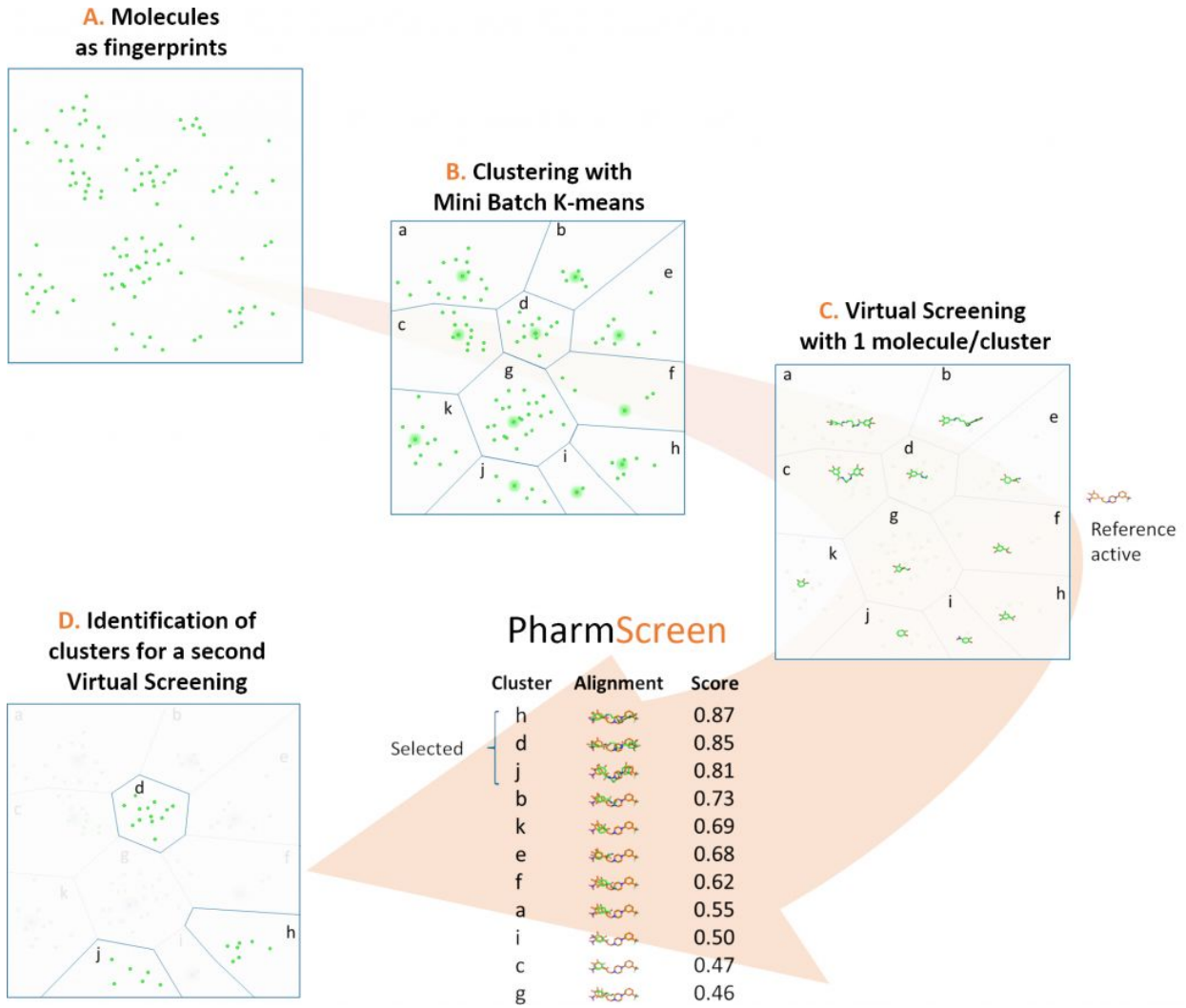
Зависимая

V - 1	V –2	V – 3	V – 4	V – 5	V – 6	V – 7	V - 8	V – 9	V – 10	Num	Class
value	value	value	value	value	value	value	value	value	value	1.003	cat
value	value	value	value	value	value	value	value	value	value	2.008	dog
value	value	value	value	value	value	value	value	value	value	7.256	dog
value	value	value	value	value	value	value	value	value	value	8.240	cat
value	value	value	value	value	value	value	value	value	value	3.001	cat
value	value	value	value	value	value	value	value	value	value	5.443	cat
value	value	value	value	value	value	value	value	value	value	2.754	dog
value	**value**	**value**	**value**	**value**	**value**	**value**	**value**	**value**	**value**	**?**	**?**

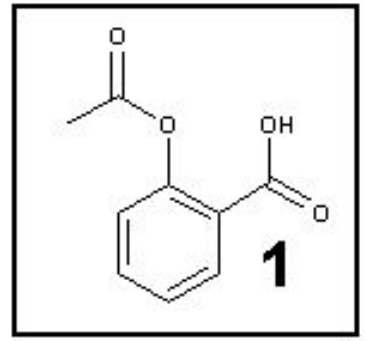

Исходные данные
Модель МО
Тренировочные данные, независимые данные.
зависимые
Тестовые данные Независимые переменные
зависимые
Тренировочные данные, независимые данные.
зависимые
Тестовые данные Независимые переменные
results
зависимые
VS

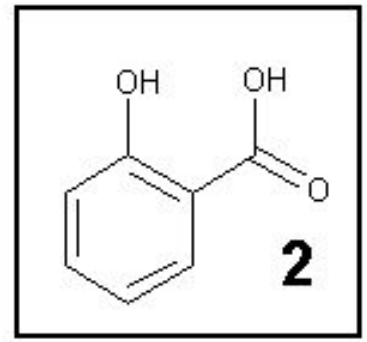

Epoch
000,158
Learning rate
0.03
Activation
Tanh
Regularization
None
Regularization rate
0
Problem type
Classification
DATA
Which dataset do you want to use?
Ratio of training to test data: 50%
Noise: 0
Batch size: 10
FEATURES
Which properties do you want to feed in?
4 HIDDEN LAYERS
4 neurons
3 neurons
2 neurons
1 neuron
The outputs are mixed with varying weights, shown by the thickness of the lines.
This is the output from one neuron.
OUTPUT
Test loss 0.003
Training loss 0.001

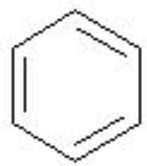
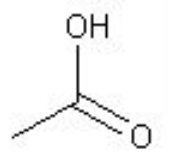
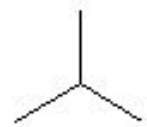
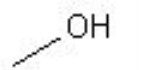
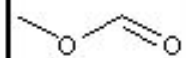
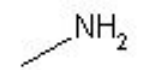
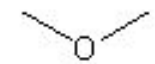
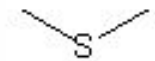
Кластеризация молекул



Similarity Searching



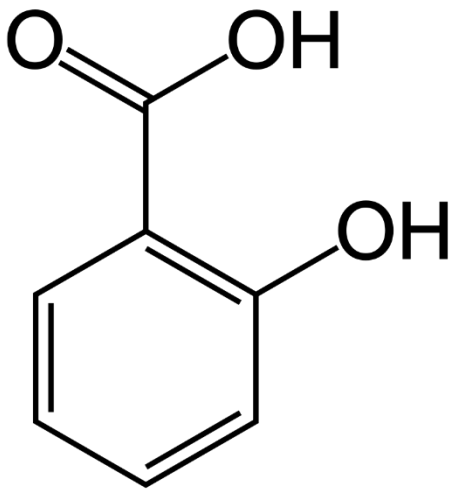


1	1	1	0	1	1	0	1	0
2	1	1	0	1	0	0	0	0
								

A = Number of bits set in both = 3
B = Number of bits set in (1), but not in (2) = 2
C = Number of bits set in (2), but not in (1) = 0

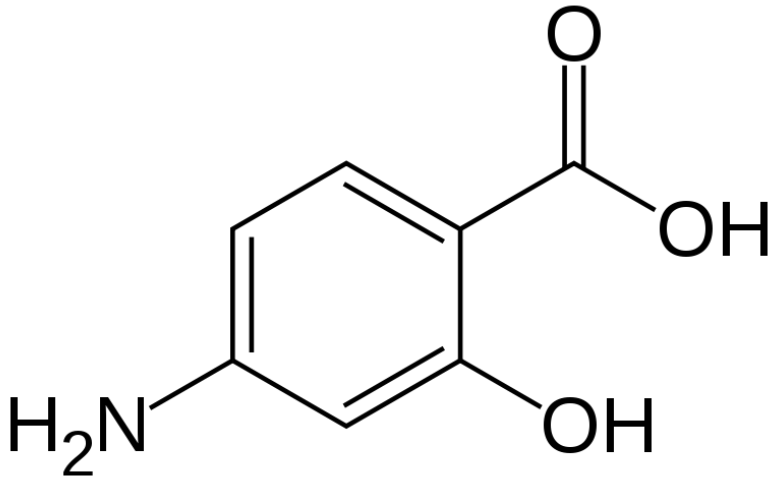
TANIMOTO COEFFICIENT = A / (A + B + C)
= 3 / (3 + 2 + 0) = 0.6 or 60%

Задача на Python



Salicylic acid

c1ccc(c(c1)C(=O)O)O



PASA

C1=CC(=C(C=C1N)O)C(=O)O

Tanimoto coefficient, Tanimoto distance

In [19]:
```
from rdkit import Chem
from rdkit.Chem import Descriptors
from rdkit.Chem import rdFingerprintGenerator
```

In [20]:
```
SA = 'c1ccc(c(c1)C(=O)O)O'
PASA = 'C1=CC(=C(C=C1N)O)C(=O)O'
```

In [21]:
```
SA = Chem.MolFromSmiles(SA)
PASA = Chem.MolFromSmiles(PASA)
```

In [22]:
```
rdkit_gen = rdFingerprintGenerator.GetRDKitFPGenerator(maxPath=5)
```

In [26]:
```
SA_fp = rdkit_gen.GetFingerprint(SA)
PASA_fp = rdkit_gen.GetFingerprint(PASA)
```

In [33]:
```
sim = round(Chem.DataStructs.TanimotoSimilarity(SA_fp, PASA_fp), 3)
sim
```

Out[33]:
```
0.811
```

In [36]:
```
tanimoto_distance = round(1-sim, 3)
tanimoto_distance
```

Out[36]:
```
0.189
```

```
data = pd.read_csv('Data_ML.csv')
```

```
compounds = []
for _, chembl_id, smile in data[['molecule_chembl_id', 'Smiles']].itertuples():
    compounds.append((Chem.MolFromSmiles(smile), chembl_id))
compounds[:5]
```

```
[(<rdkit.Chem.rdchem.Mol at 0x280de08e7b0>, 'CHEMBL3640324'),
 (<rdkit.Chem.rdchem.Mol at 0x280de08e530>, 'CHEMBL3640408'),
 (<rdkit.Chem.rdchem.Mol at 0x280de08ee40>, 'CHEMBL3642557'),
 (<rdkit.Chem.rdchem.Mol at 0x280dec69850>, 'CHEMBL3642442'),
 (<rdkit.Chem.rdchem.Mol at 0x280dec693f0>, 'CHEMBL3955760')]
```

```
rdkit_gen = rdFingerprintGenerator.GetRDKitFPGenerator(maxPath=5)
fingerprints = [rdkit_gen.GetFingerprint(mol) for mol, indx in compounds]
```

```
fingerprints[0:5]
```

Сложности..

У нас есть список из 5 молекул (1 – 5). Нужно рассчитать коэфф. Танимото для каждой пары из молекул без повторений.

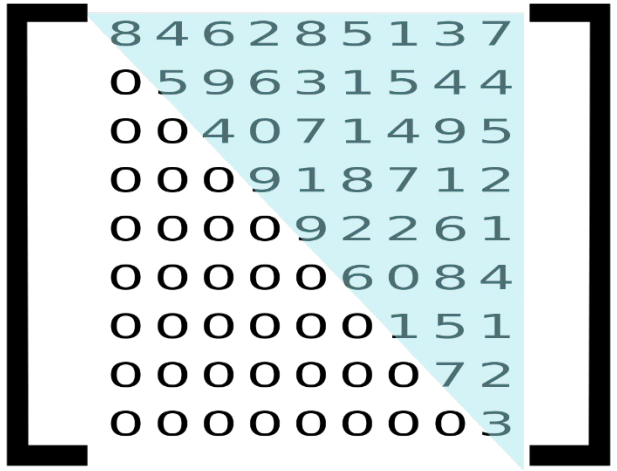
[1 2 3 4 5]

1 – 2, 1 – 3, 1 – 4, 1 – 5

2 – 3, 2 – 4, 2 – 5

3 – 4, 3 – 5,

4 – 5.

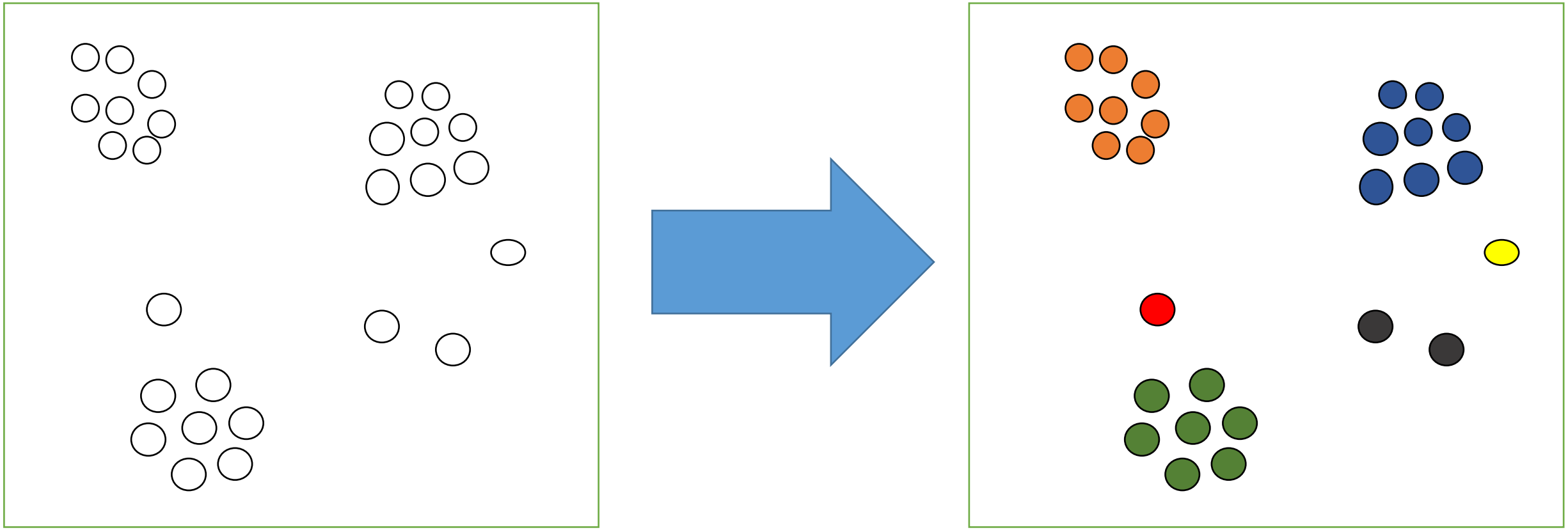


Трудности…

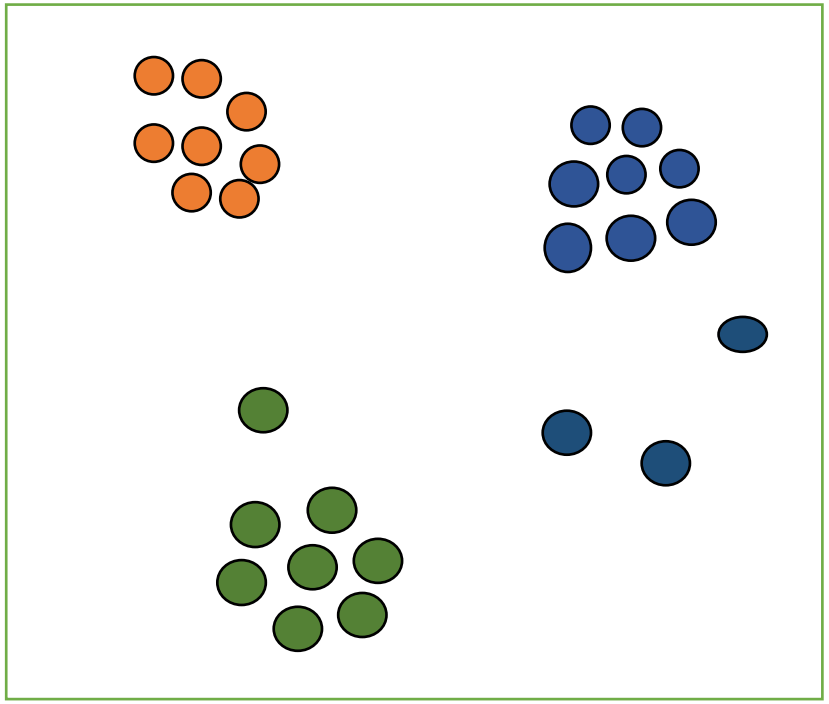
```
def tanimoto_distance_matrix(fp_list):
    dissimilarity_matrix = []
    for i in range(1, len(fp_list)):
        similarities = DataStructs.BulkTanimotoSimilarity(fp_list[i], fp_list[:i])
        dissimilarity_matrix.extend([1 - x for x in similarities])
    return dissimilarity_matrix
```

```
tdm = tanimoto_distance_matrix(fingerprints)
```

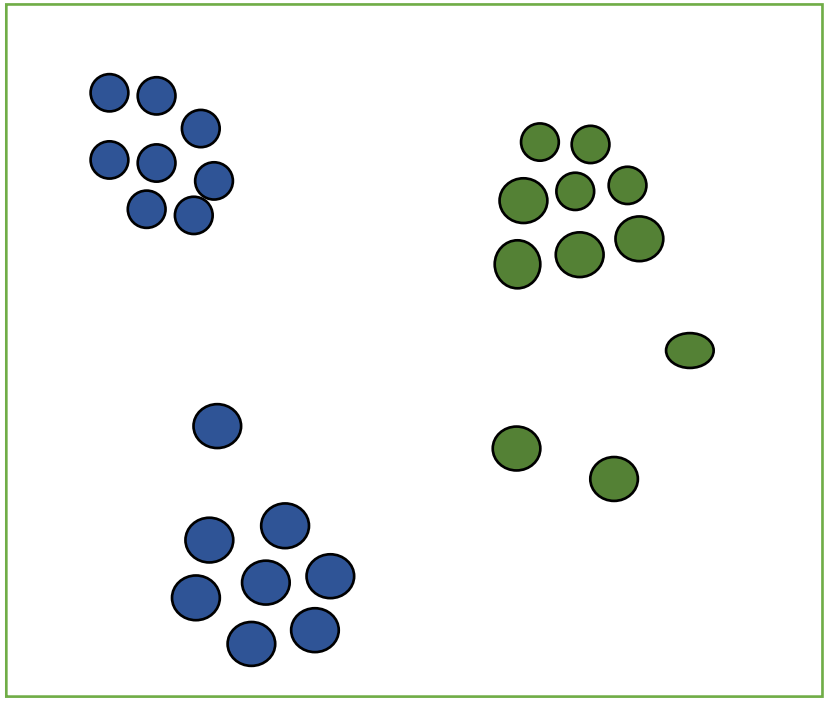
Принцип кластеризации



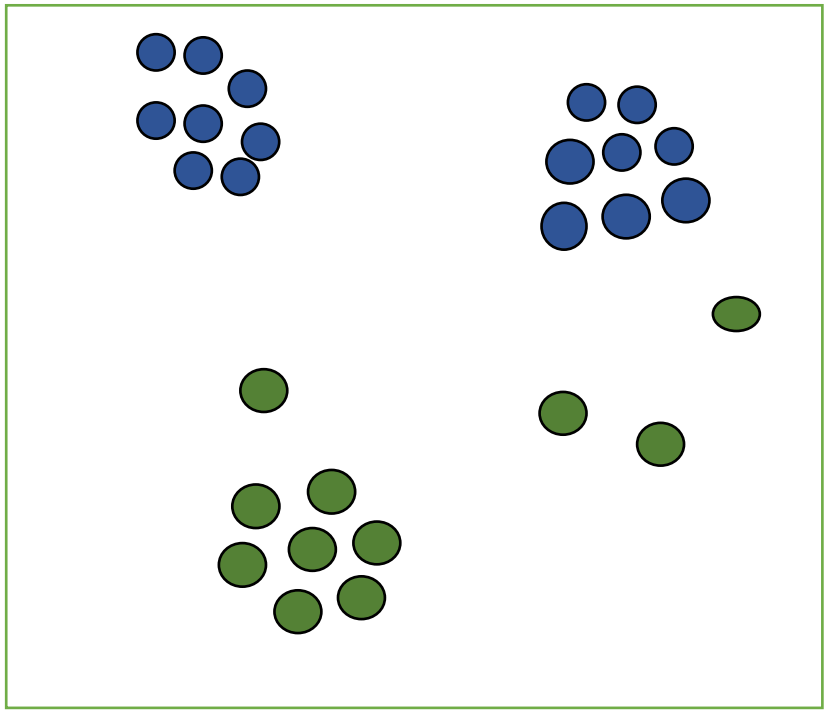
A



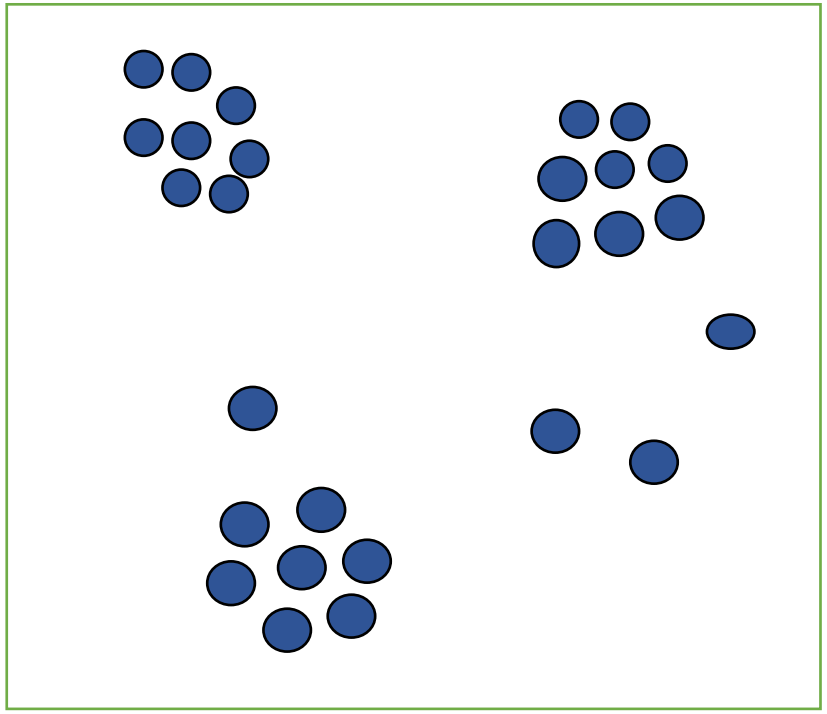
B



C



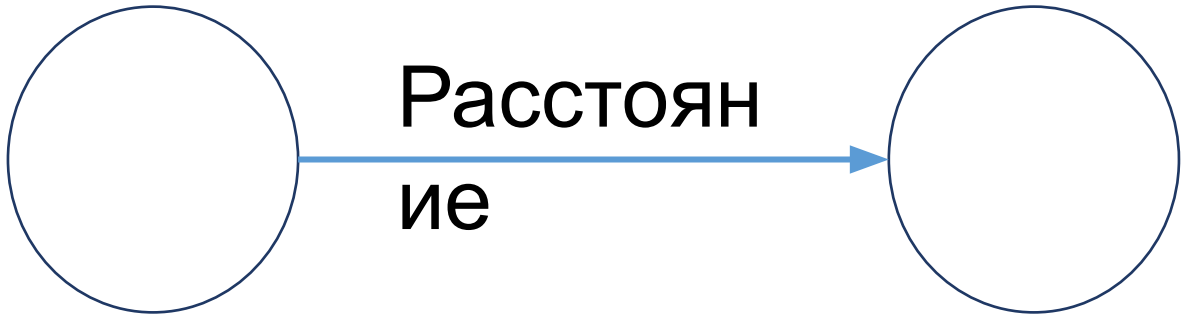
D

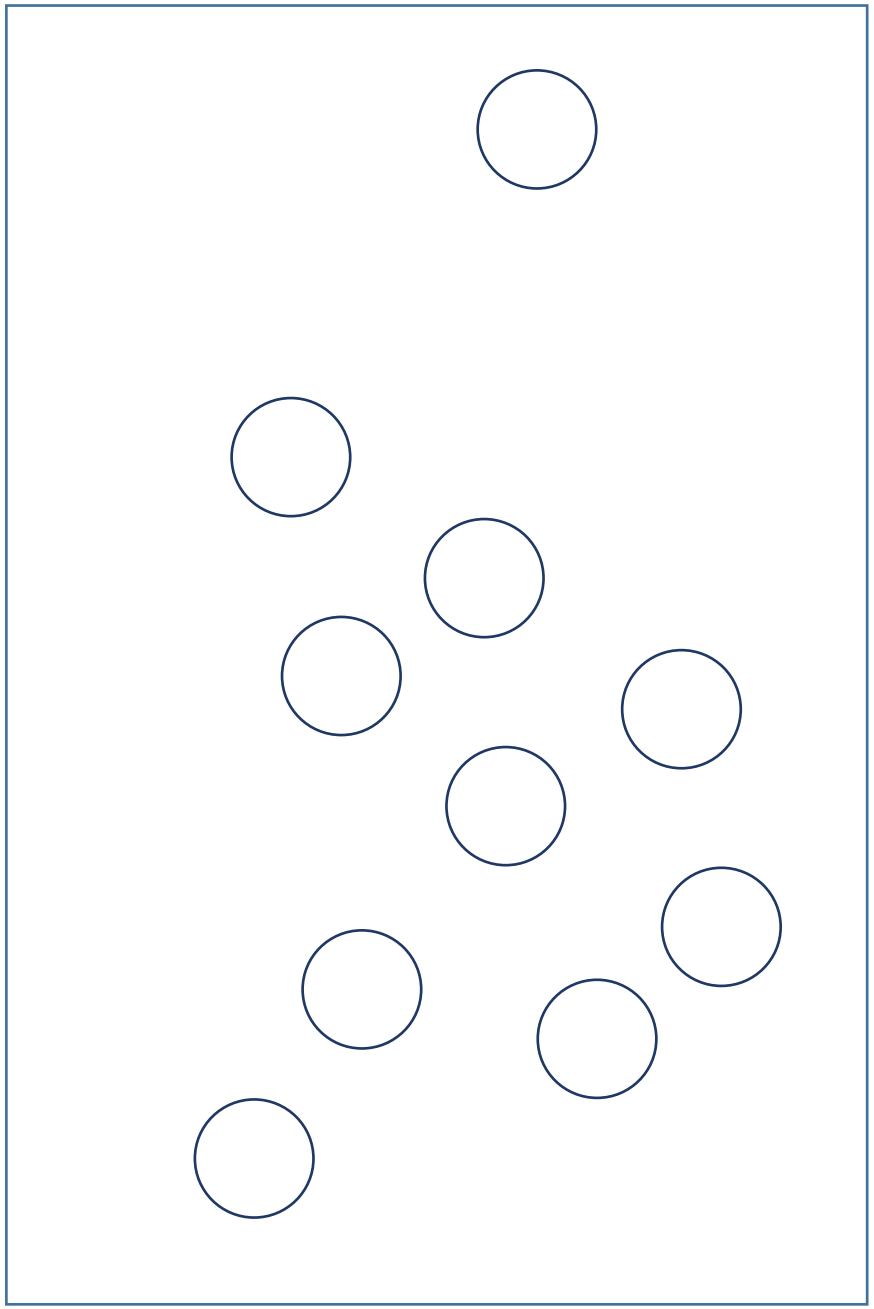


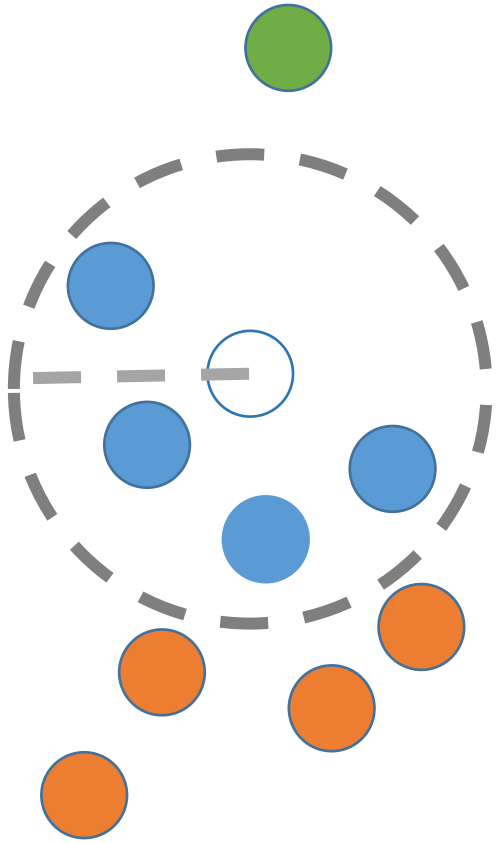
Для кластеризации необходимы:

1. Расстояние
2. Центроиды

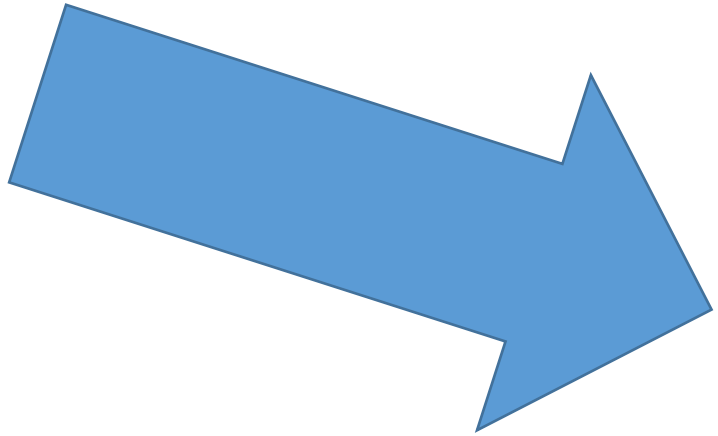
Цель – найти оптимальные центройды при данном расстоянии



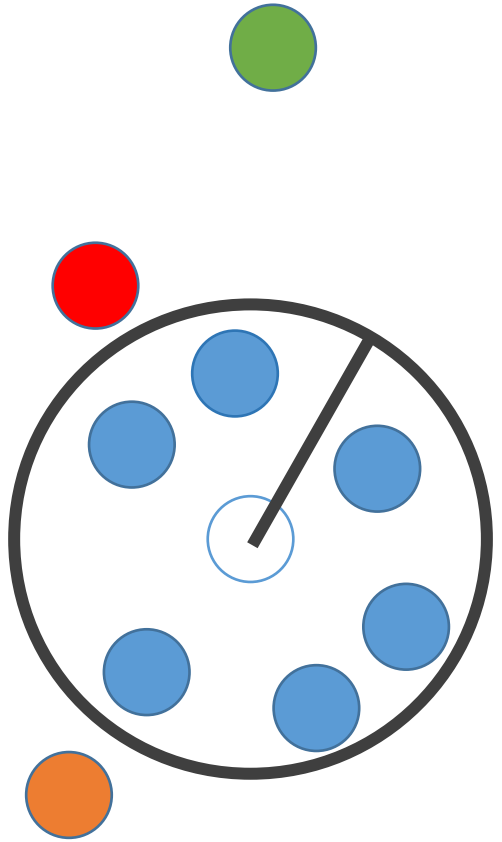




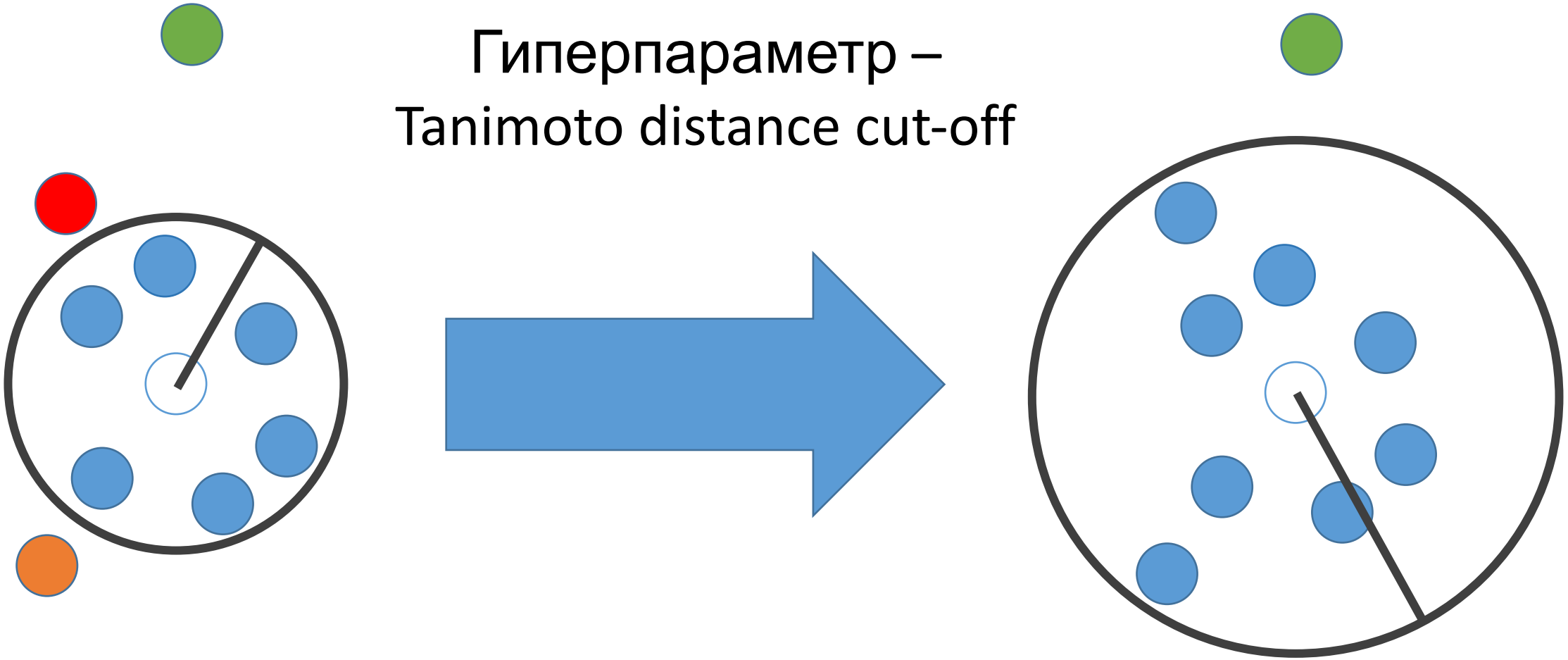
Не оптимальный центроид



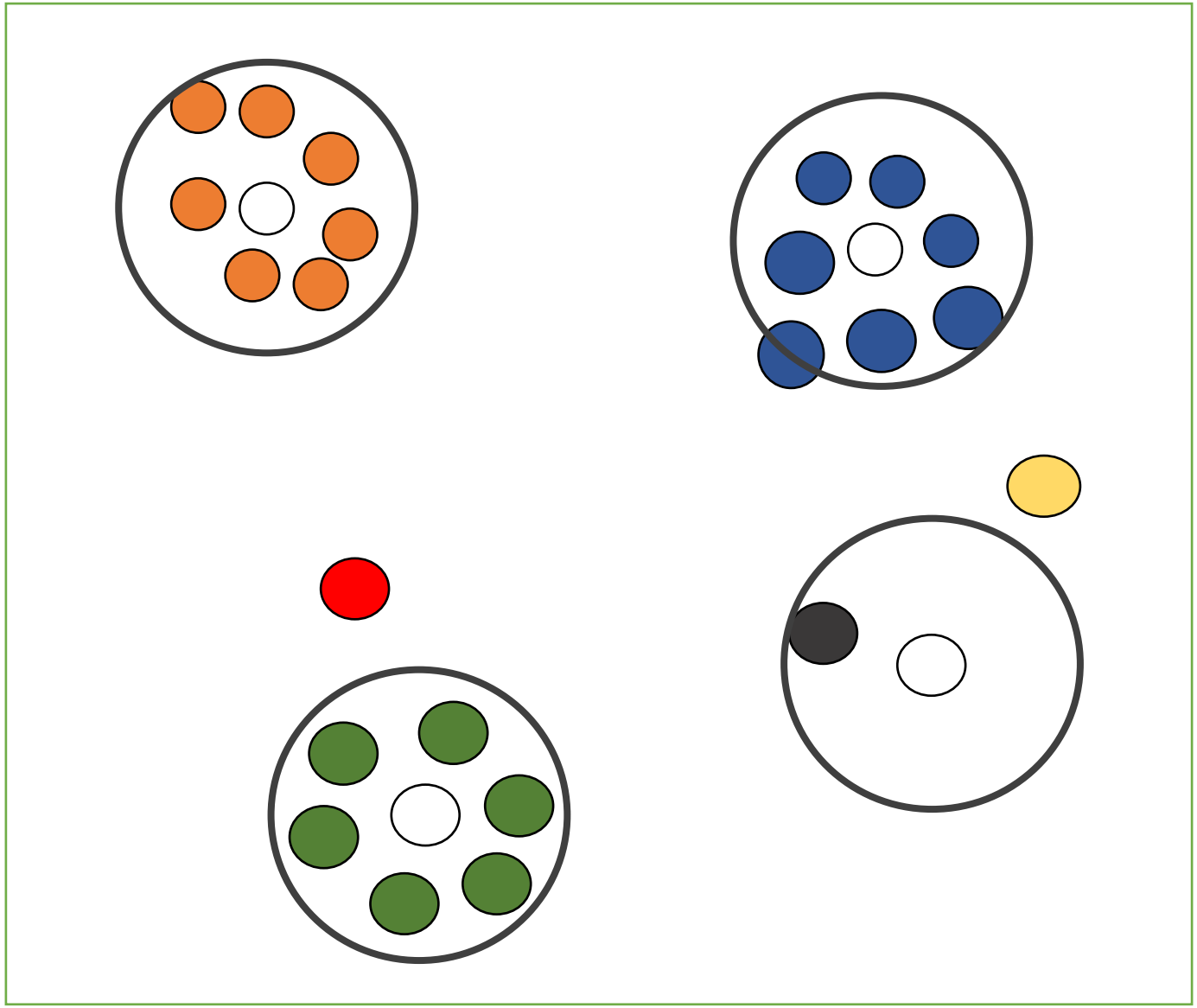
Оптимальный центроид



Гиперпараметр –
Tanimoto distance cut-off



Чем больше значение расстояния –
тем больше кластеры содержат элементов.
Тем меньше кластеров



```python
def cluster_fingerprints(fingerprints, cutoff=0.2):
    tdm = tanimoto_distance_matrix(fingerprints)
    clusters = Butina.ClusterData(tdm, len(fingerprints), cutoff, isDistData=True)
    clusters = sorted(clusters, key=len, reverse=True)
    return clusters
```

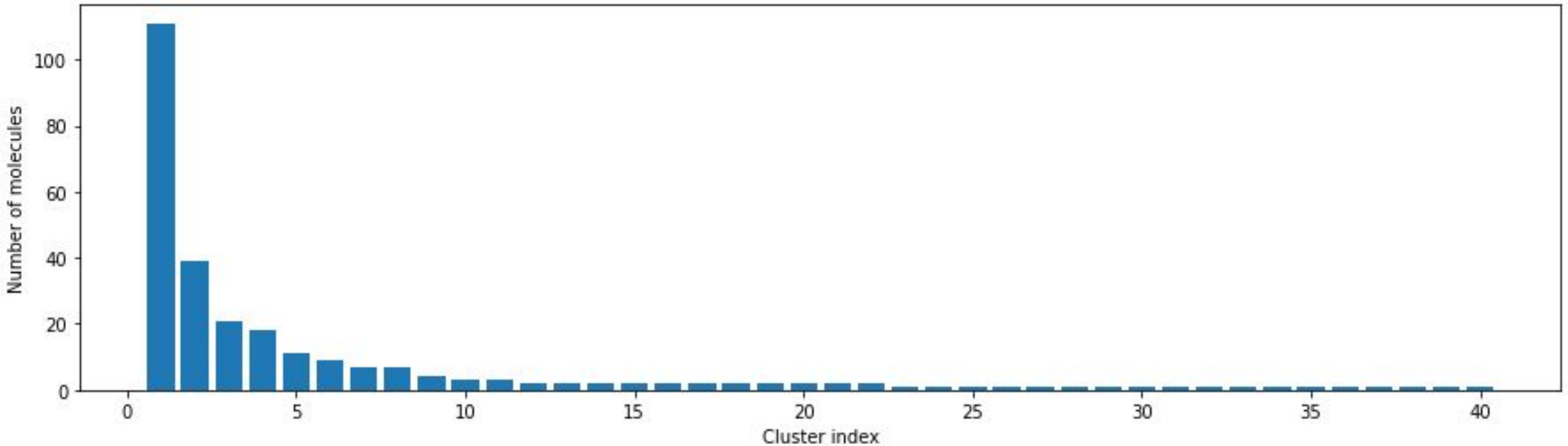
```python
clusters = cluster_fingerprints(fingerprints, cutoff=0.35)

num_clust_g1 = sum(1 for c in clusters if len(c) == 1)
num_clust_g5 = sum(1 for c in clusters if len(c) > 5)
num_clust_g25 = sum(1 for c in clusters if len(c) > 25)
num_clust_g100 = sum(1 for c in clusters if len(c) > 100)

print("total # clusters: ", len(clusters))
print("# clusters with only 1 compound: ", num_clust_g1)
print("# clusters with >5 compounds: ", num_clust_g5)
print("# clusters with >25 compounds: ", num_clust_g25)
print("# clusters with >100 compounds: ", num_clust_g100)
```

```
total # clusters:  18
# clusters with only 1 compound:  6
# clusters with >5 compounds:  3
# clusters with >25 compounds:  2
# clusters with >100 compounds:  1
```

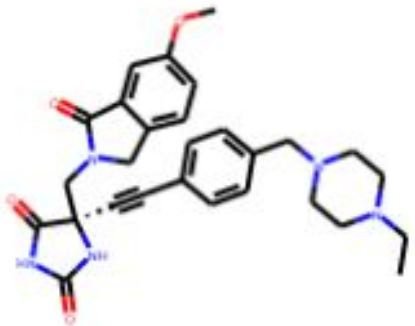
```
fig, ax = plt.subplots(figsize=(15, 4))
ax.set_xlabel("Cluster index")
ax.set_ylabel("Number of molecules")
ax.bar(range(1, len(clusters) + 1), [len(c) for c in clusters], lw=5);
```



Play with cut-off

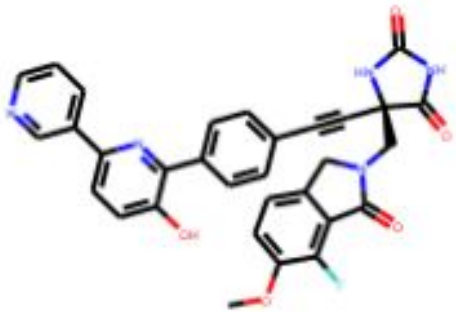
```
print("Centroid molecules from first 7clusters:")
# Draw molecules
Draw.MolsToGridImage(
    [compounds[clusters[i][0]][0] for i in range(7)],
    legends=[compounds[clusters[i][0]][1] for i in range(7)],
    molsPerRow=5,
)
```

Centroid molecules from first 7clusters:

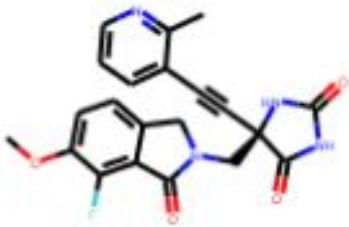


CHEMBL1287881

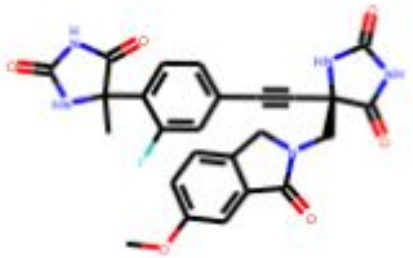
CHEMBL3947142



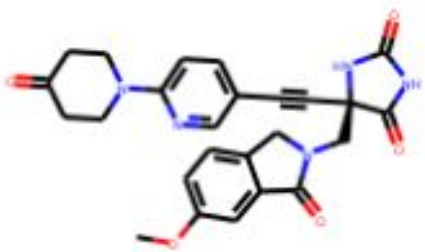
CHEMBL3640366



CHEMBL3642535



CHEMBL3642544



Спасибо за внимание