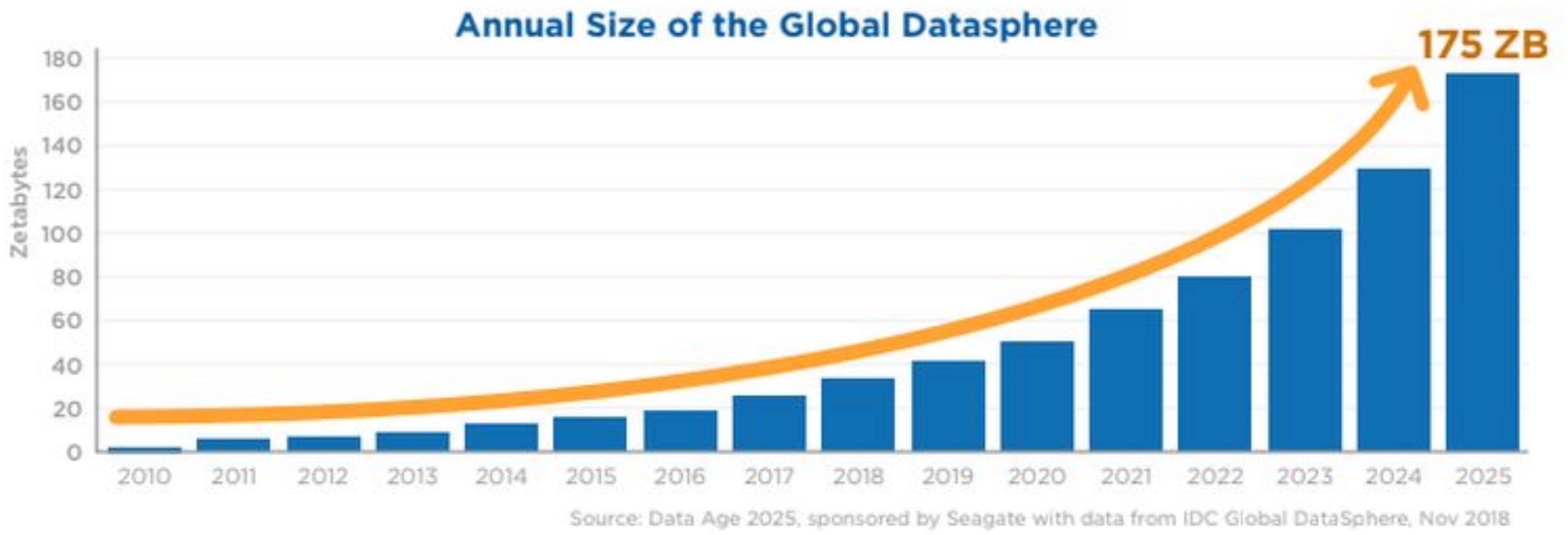
Основы Data science
Кластеризация

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

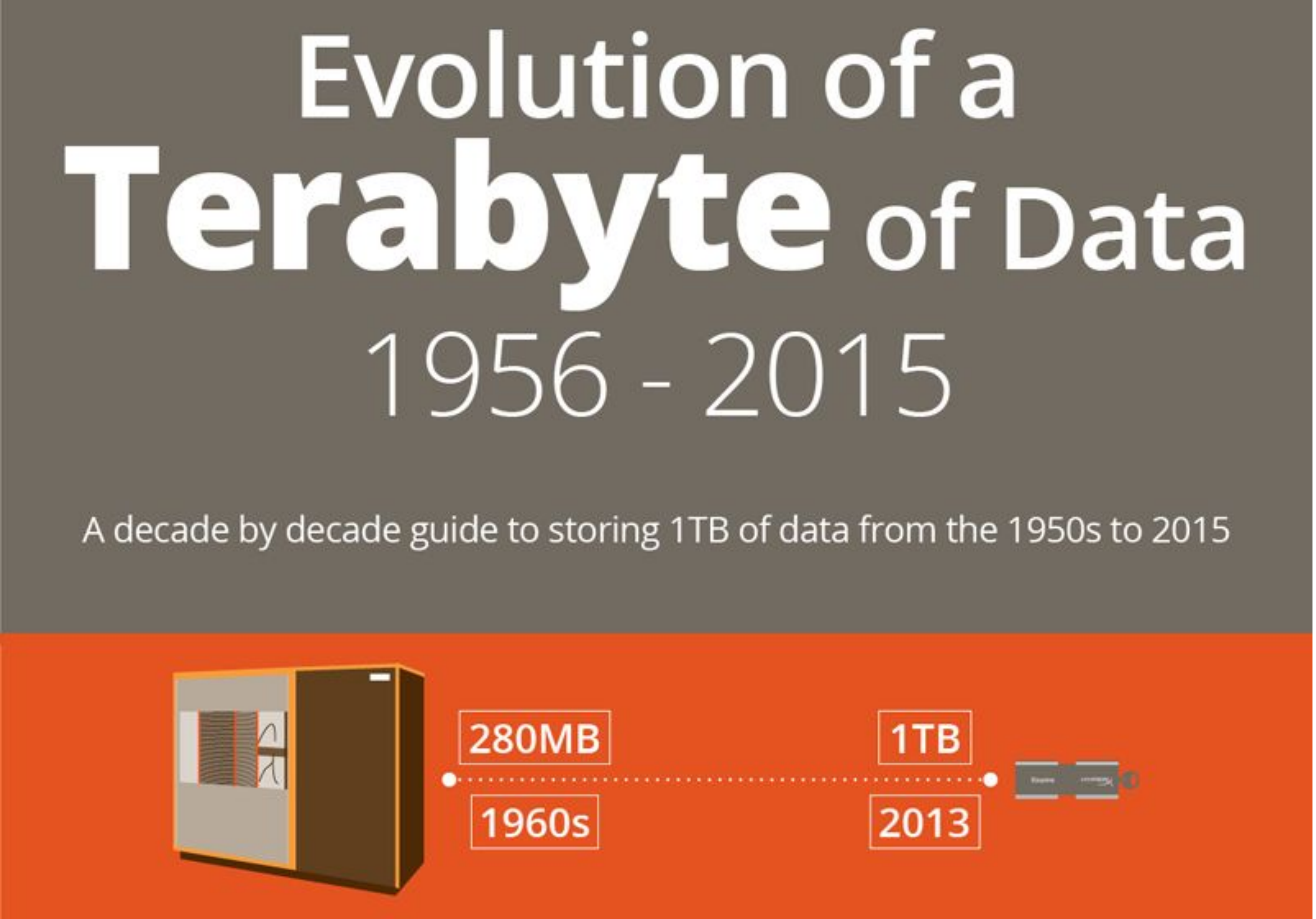
Figure 1 - Annual Size of the Global Datasphere



1 ZB = 10^21 bytes

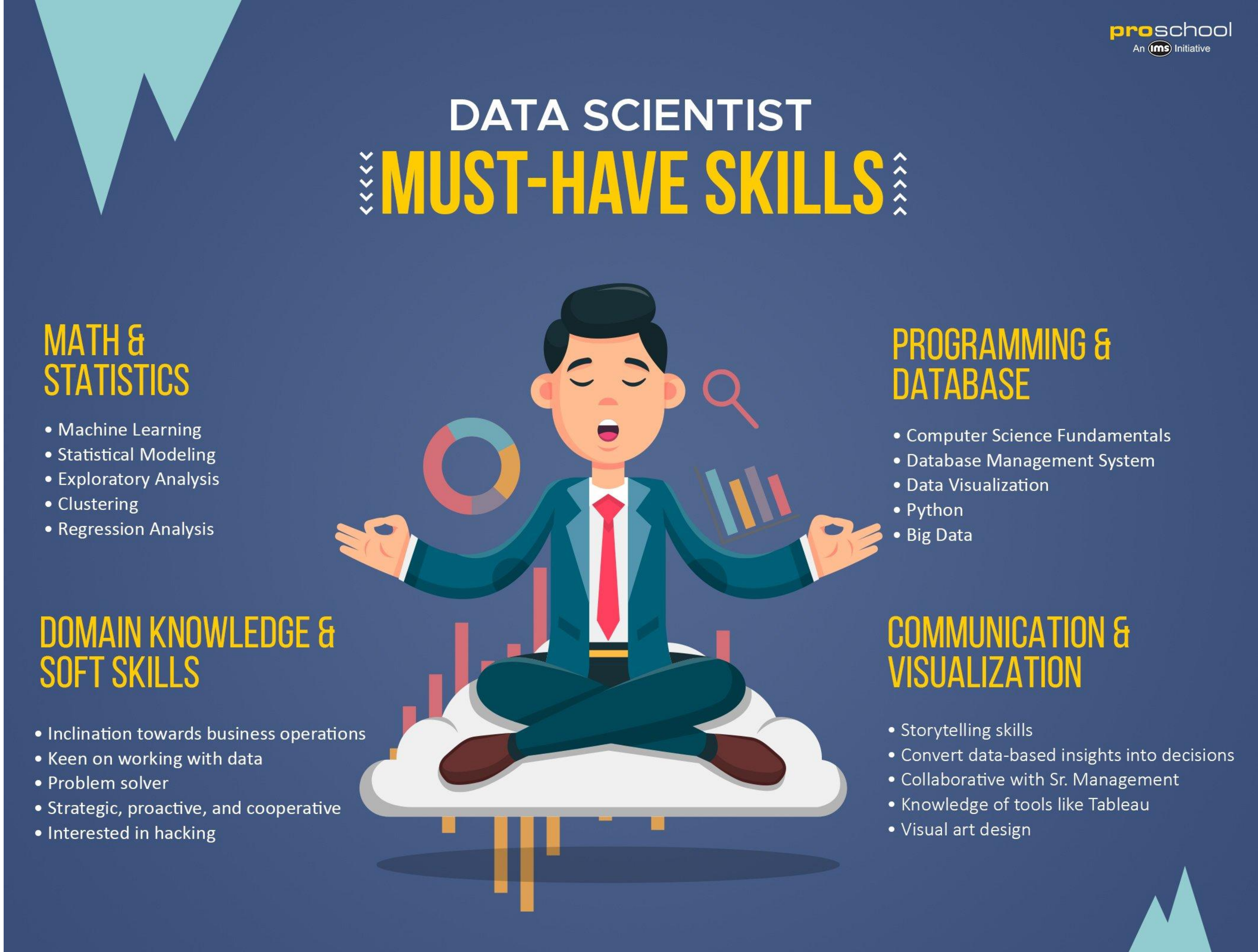
1 TB = 10^12 bytes

Эволюция в области хранения и Обработки данных


Evolution of a Terabyte of Data 1956 - 2015

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

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

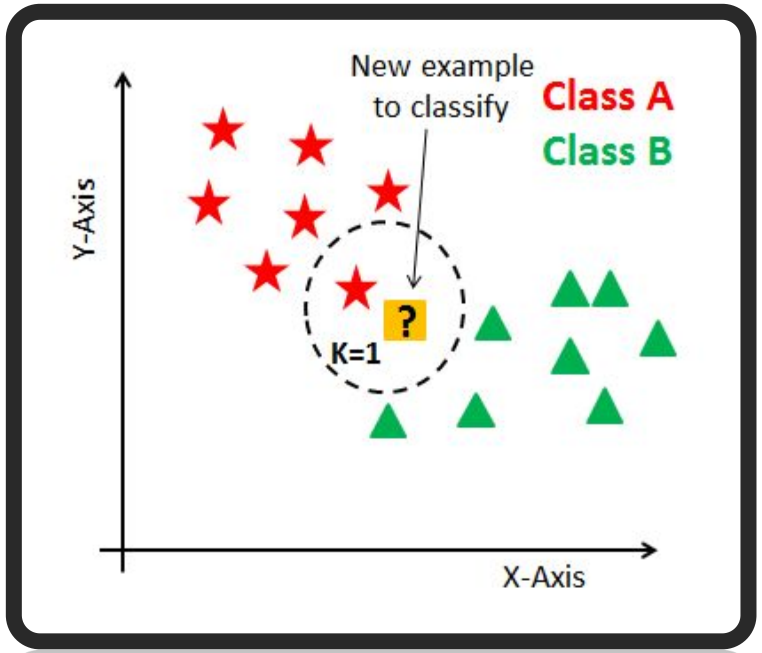
COMMUNICATION & VISUALIZATION

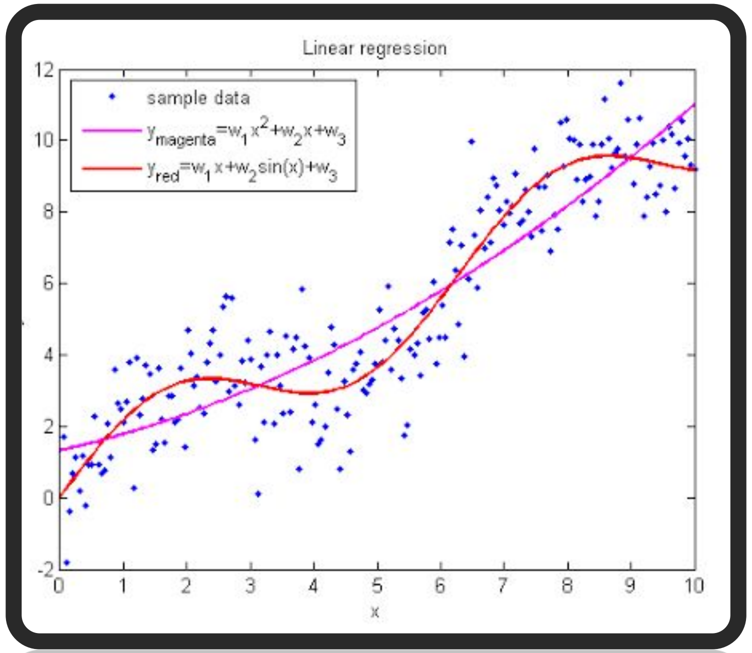
- Storytelling skills
- Convert data-based insights into decisions
- Collaborative with Sr. Management
- Knowledge of tools like Tableau
- Visual art design

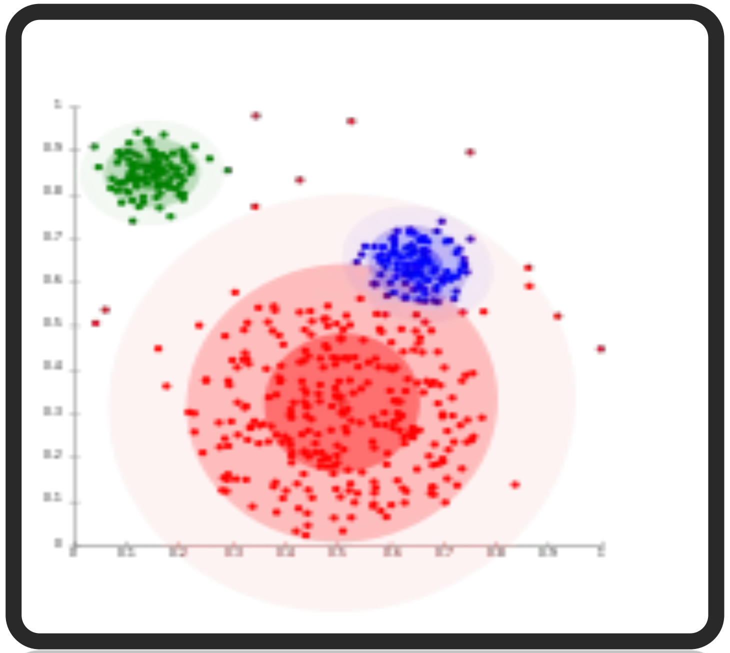
Классификац
ия

Регрессия

Кластеризац
ия





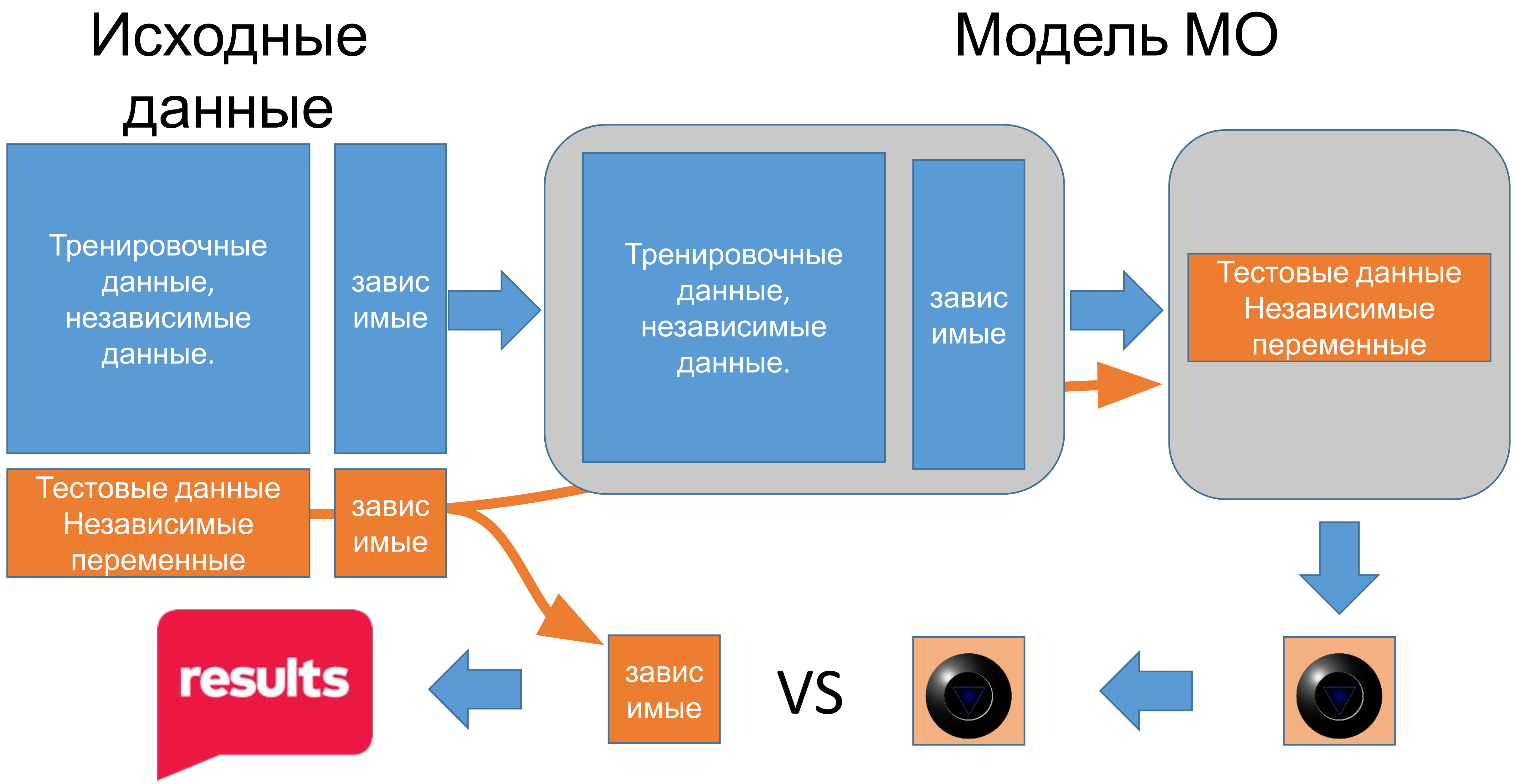


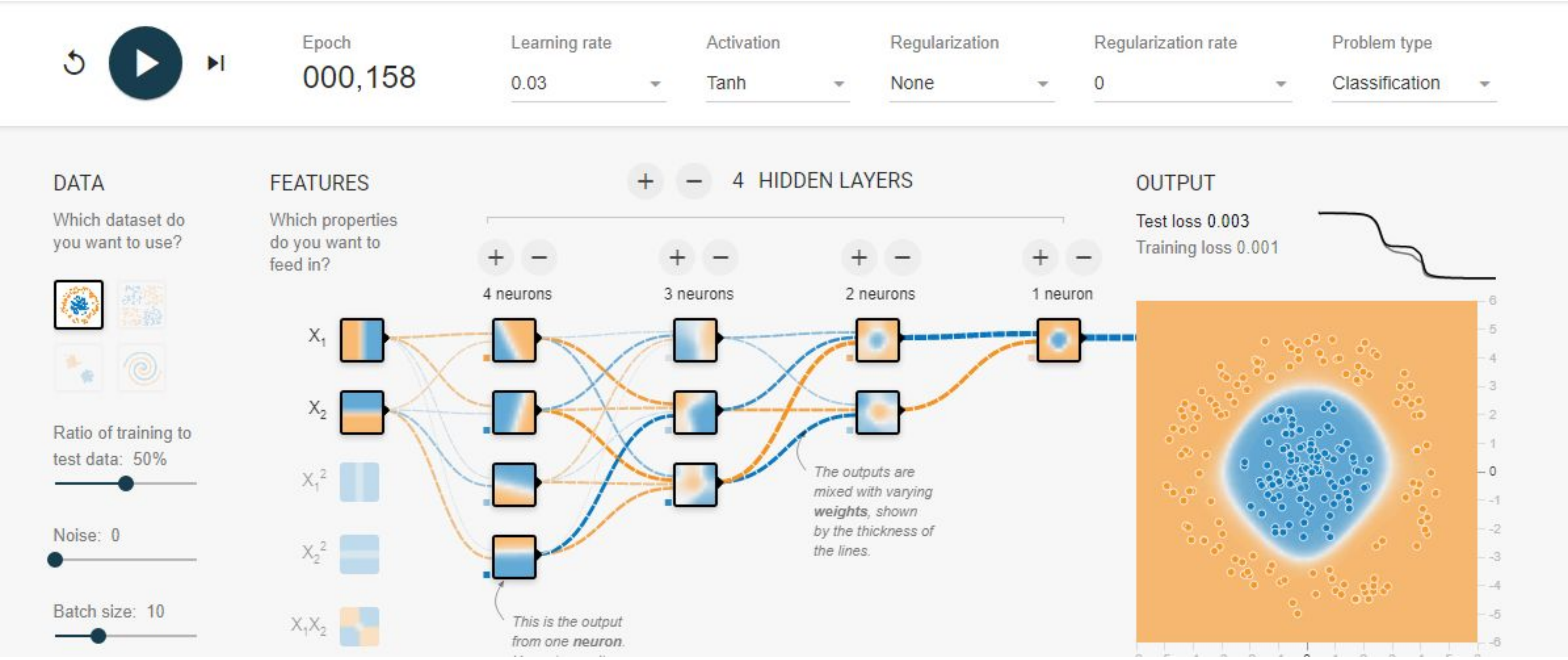
Независимые переменные

V - 1	V –2	V – 3	V – 4	V – 5	V – 6	V – 7	V - 8	V – 9	V – 10
value	value	value	value	value	value	value	value	value	value
value	value	value	value	value	value	value	value	value	value
value	value	value	value	value	value	value	value	value	value
value	value	value	value	value	value	value	value	value	value
value	value	value	value	value	value	value	value	value	value
value	value	value	value	value	value	value	value	value	value
value	value	value	value	value	value	value	value	value	value
value	**value**	**value**	**value**	**value**	**value**	**value**	**value**	**value**	**value**

Зависимая

Num	Class
1.003	cat
2.008	dog
7.256	dog
8.240	cat
3.001	cat
5.443	cat
2.754	dog
?	**?**


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

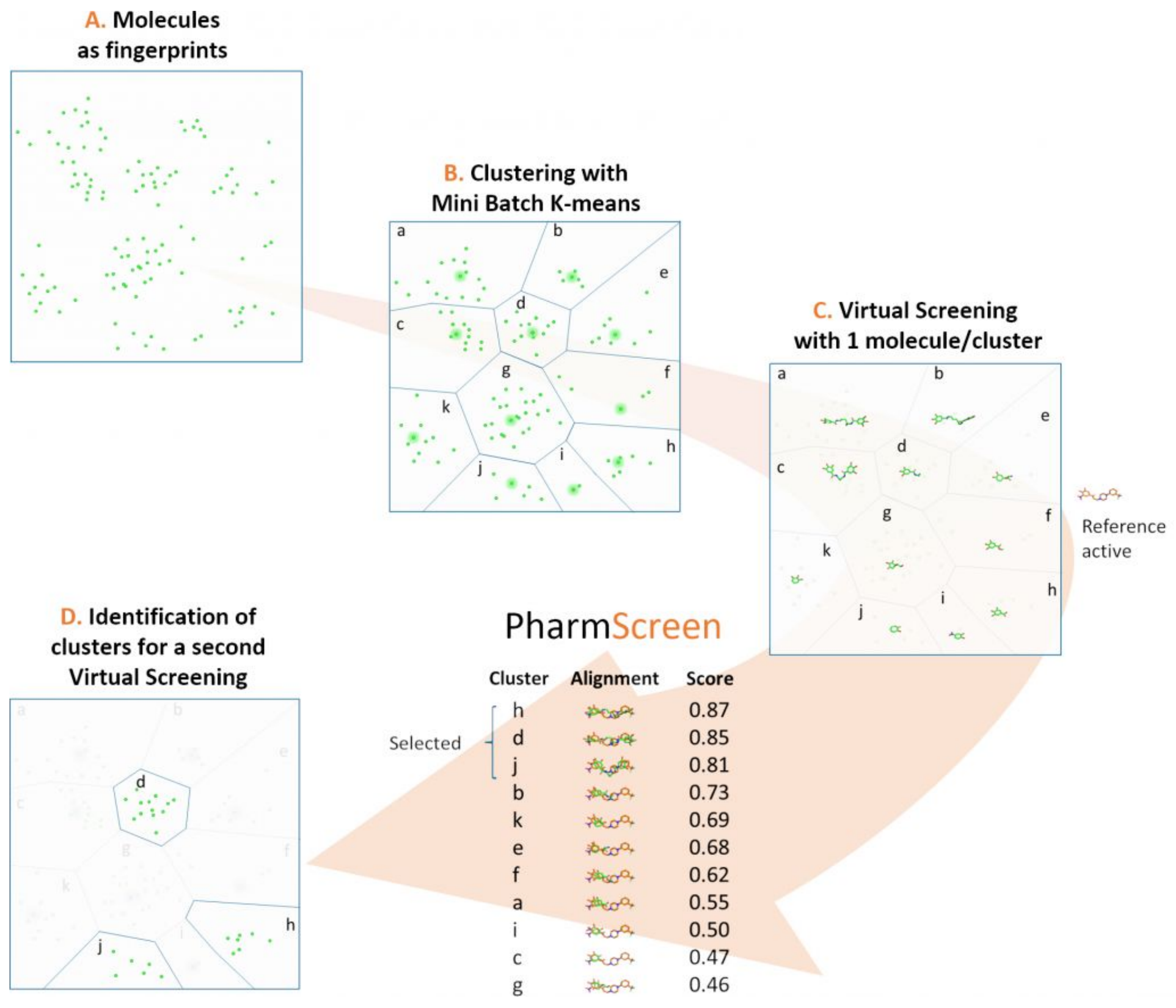
*This is the output from one **neuron**.*

OUTPUT

Test loss 0.003

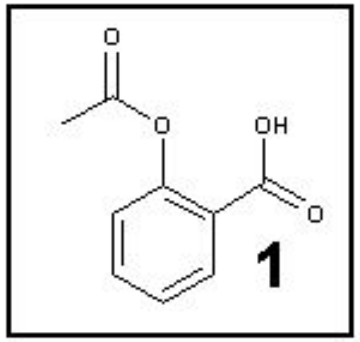
Training loss 0.001

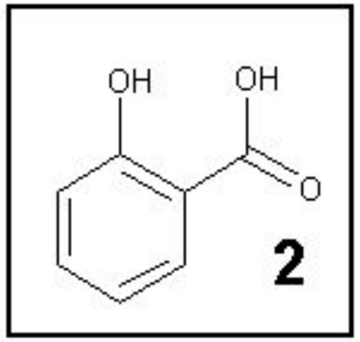
Кластеризация молекул

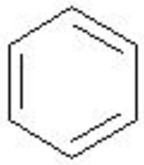
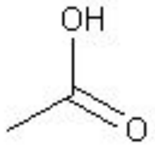
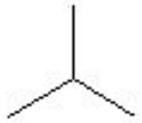
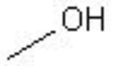
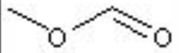
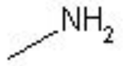
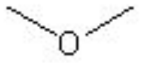
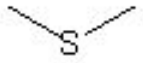

A. Molecules as fingerprints
B. Clustering with Mini Batch K-means
a
b
c
d
e
f
g
h
i
j
k
C. Virtual Screening with 1 molecule/cluster
Reference active
D. Identification of clusters for a second Virtual Screening
PharmScreen
Selected

Cluster	Alignment	Score
h		0.87
d		0.85
j		0.81
b		0.73
k		0.69
e		0.68
f		0.62
a		0.55
i		0.50
c		0.47
g		0.46

Similarity Searching


1

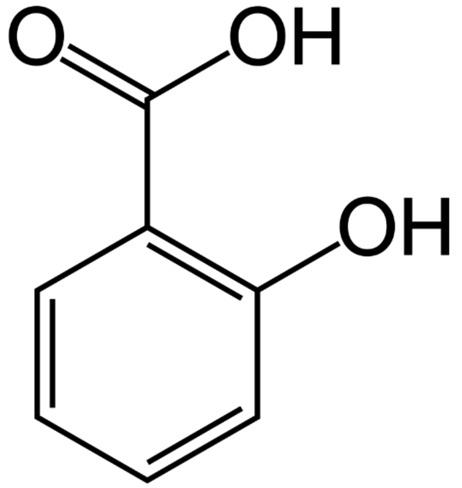

2

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

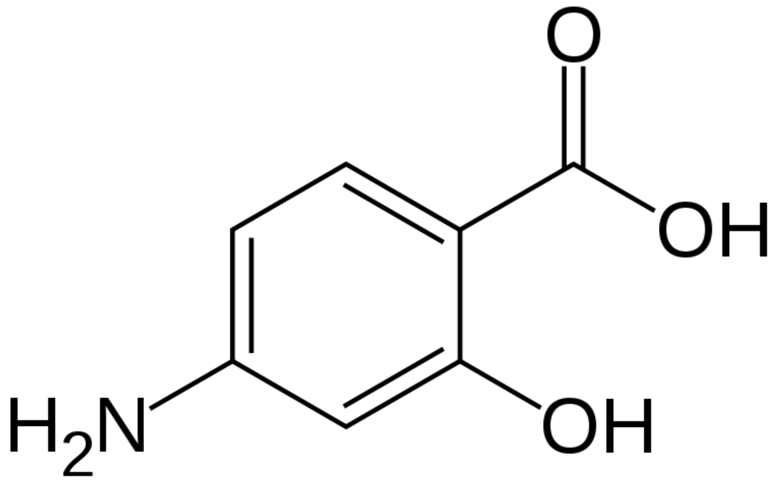
TANIMOTO COEFFICIENT = A / (A + B + C)
= 3 / (3 + 2 + 0) = 0.6 or 60%

Задача на Python



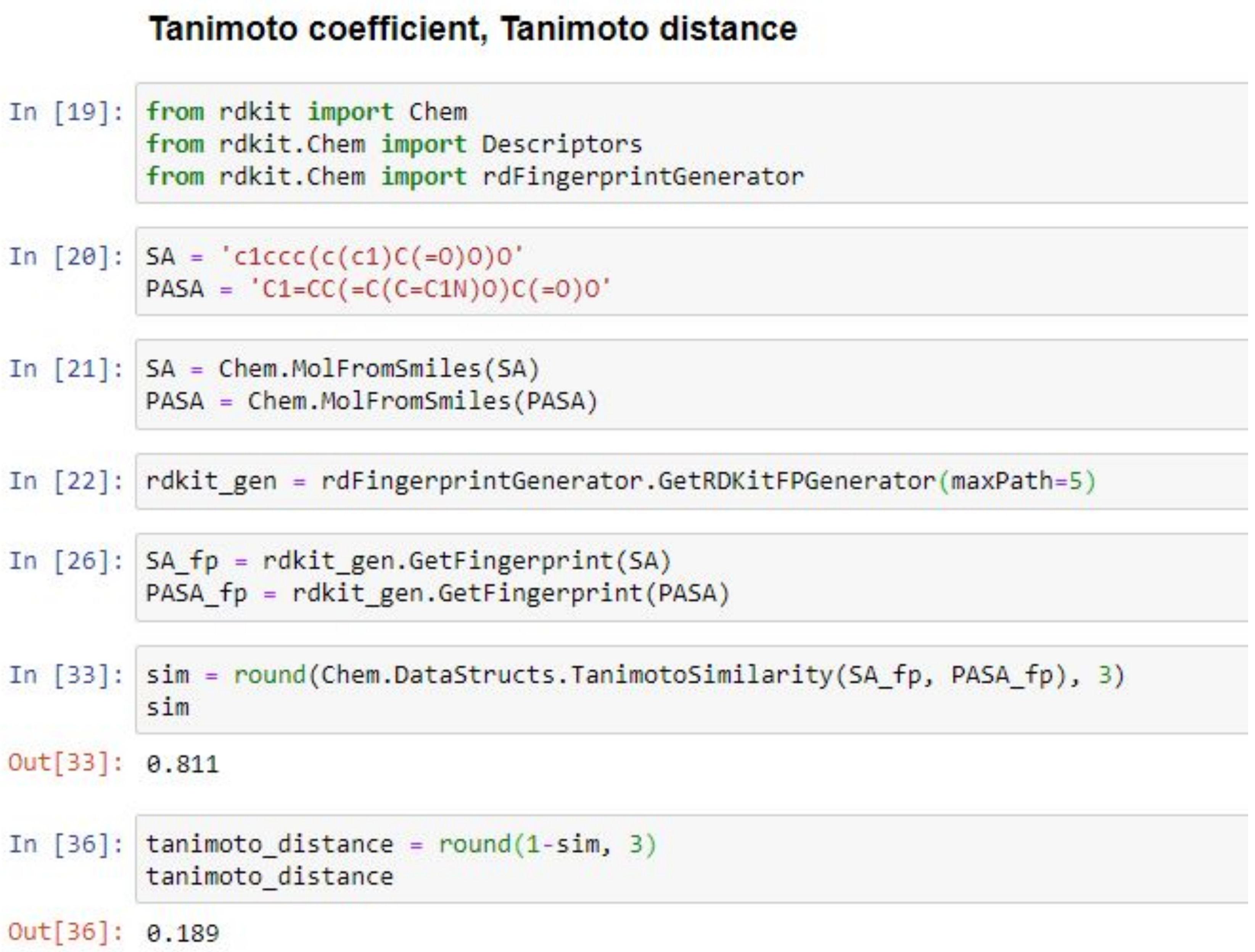
Salicylic acid

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



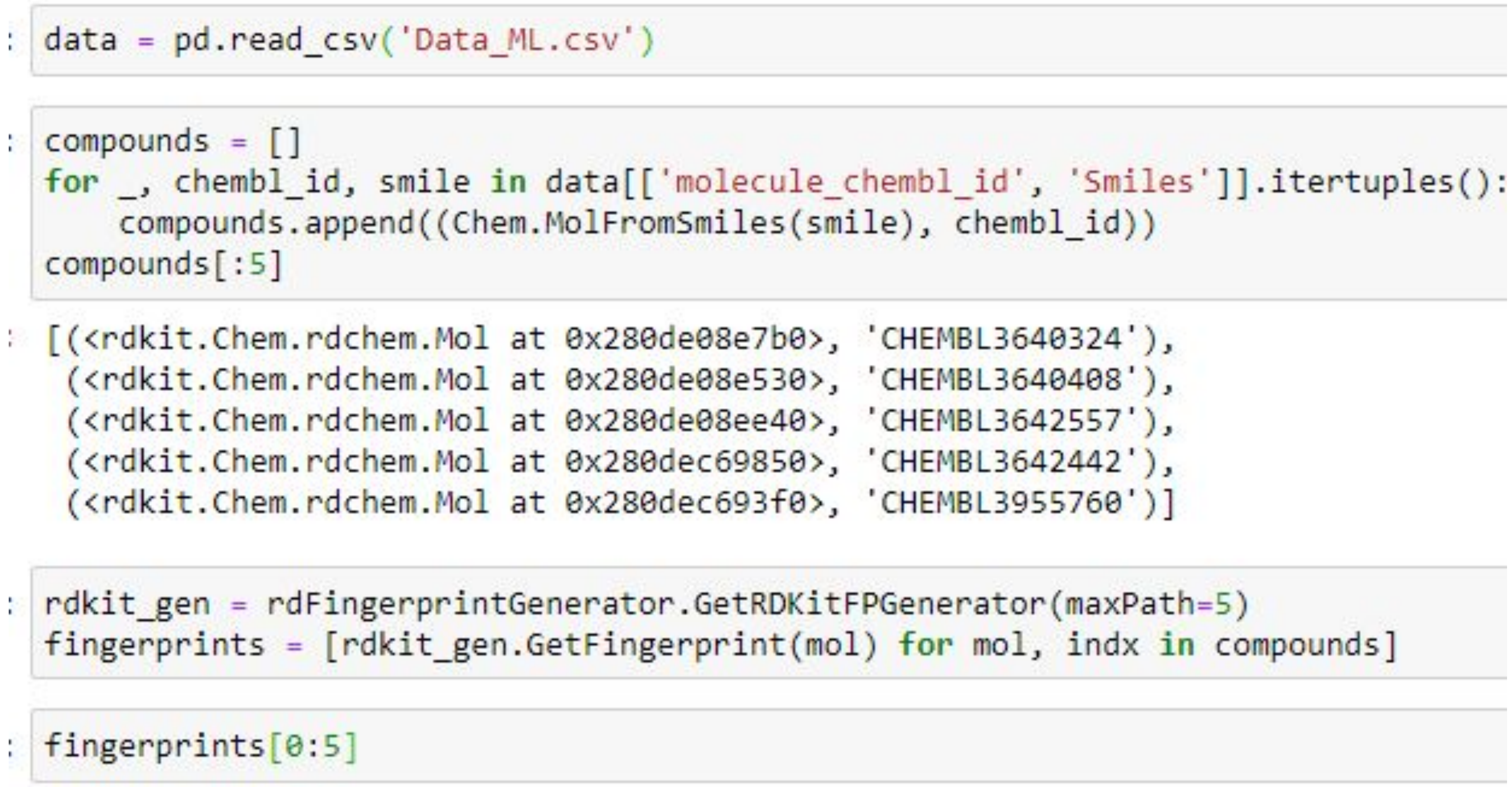
PASA

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
```



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

```python
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')]
```

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

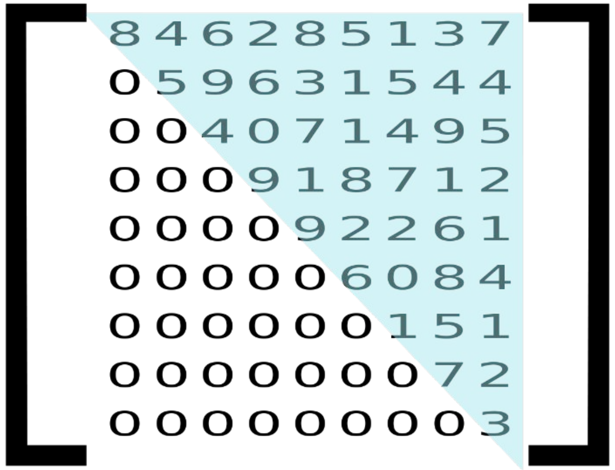
```python
fingerprints[0:5]
```

Сложности..

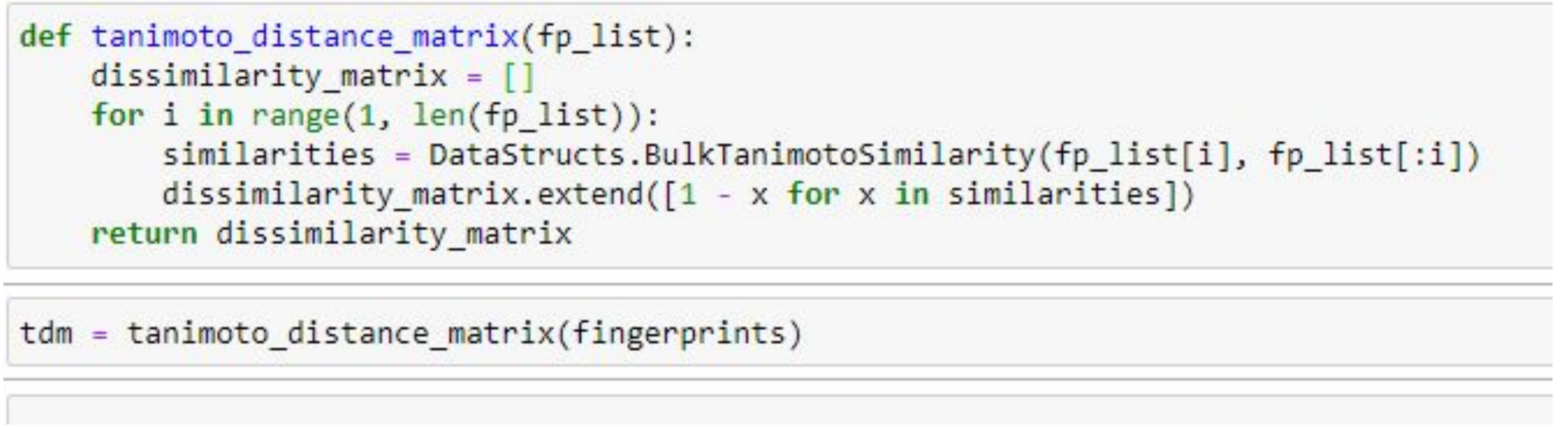
У нас есть список из 5 молекул (1 – 5). Нужно рассчитать коэфф. Танимото для каждой пары из молекул без повторений.

[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.



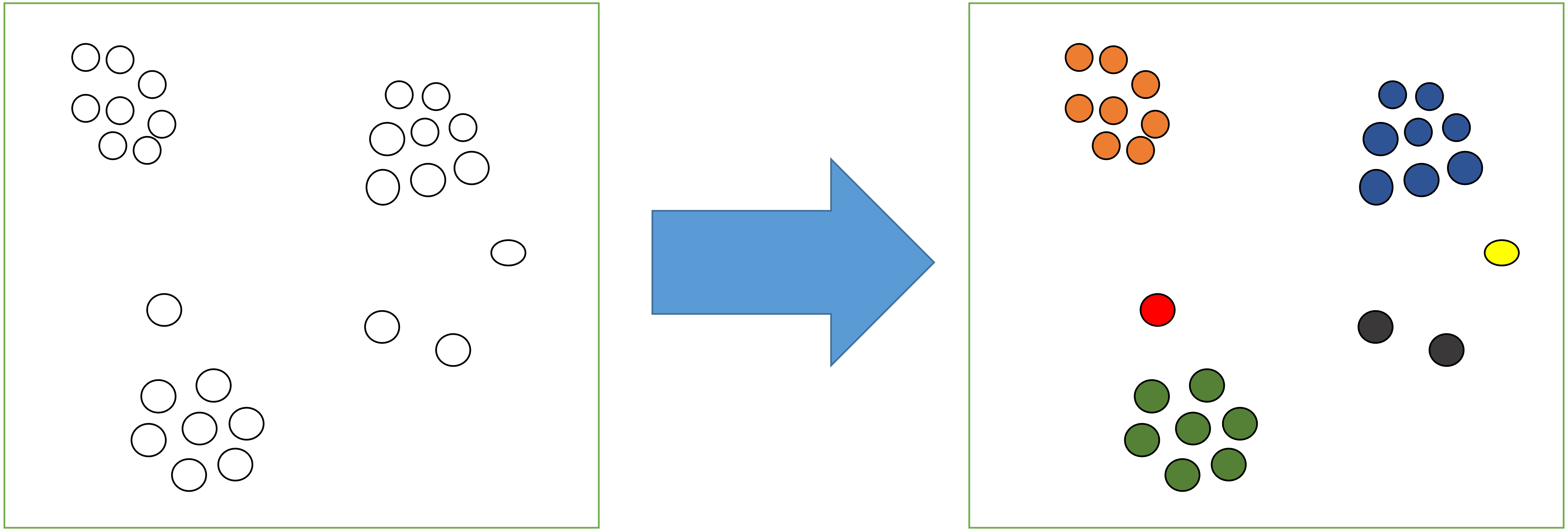
Трудности…



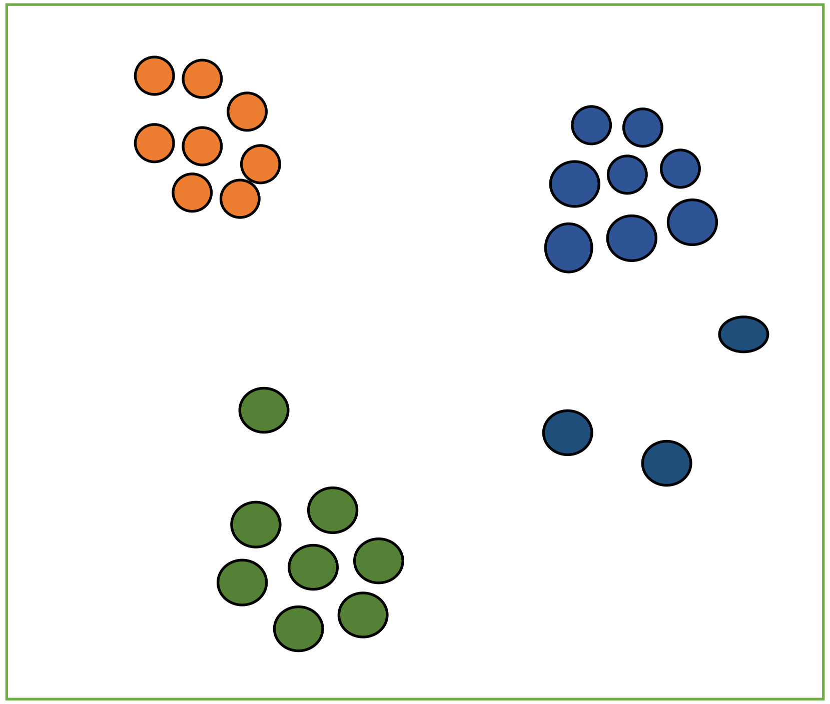
```
def tanimoto_distance_matrix(fp_list):
    dissimilarity_matrix = []
    for i in range(1, len(fp_list)):
        similarities = DataStructs.BulkTanimotoSimilarity(fp_list[i], fp_list[:i])
        dissimilarity_matrix.extend([1 - x for x in similarities])
    return dissimilarity_matrix
```

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

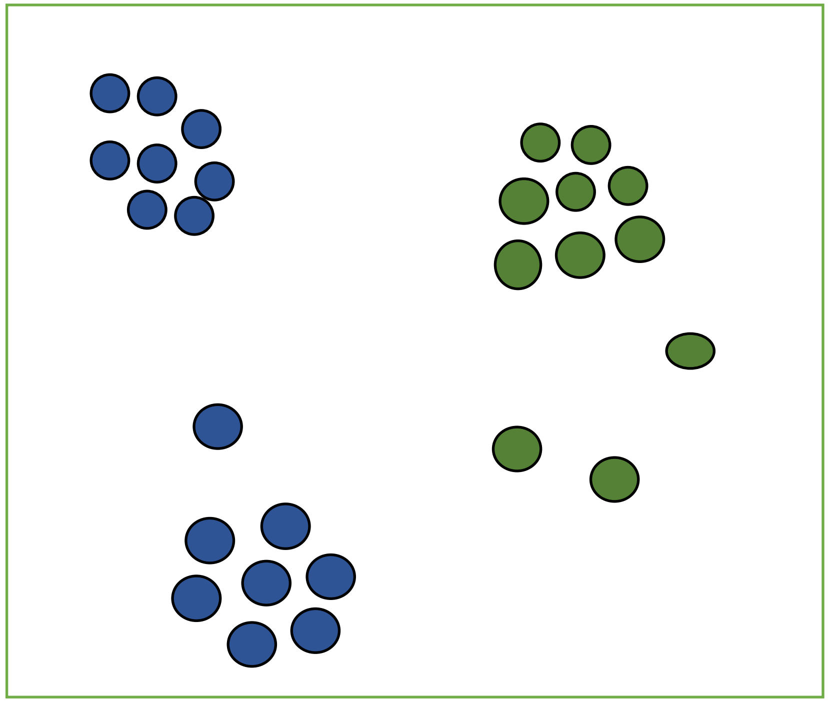
Принцип кластеризации



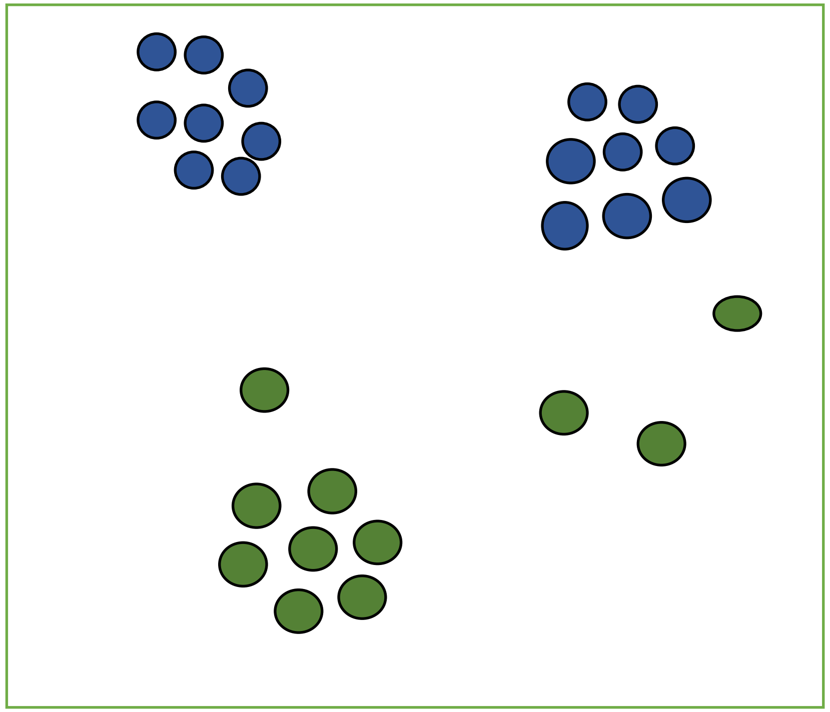
A



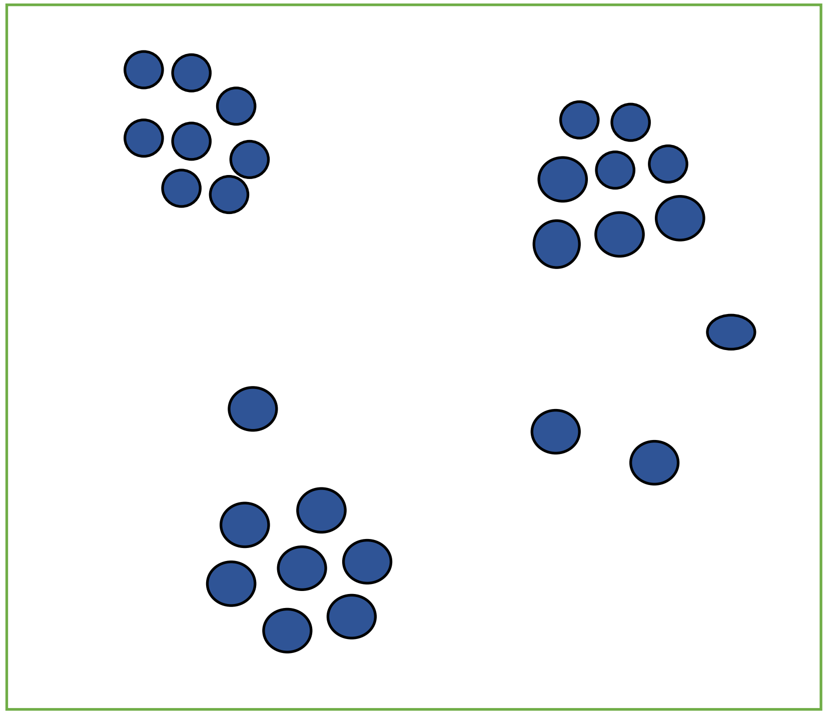
B



C



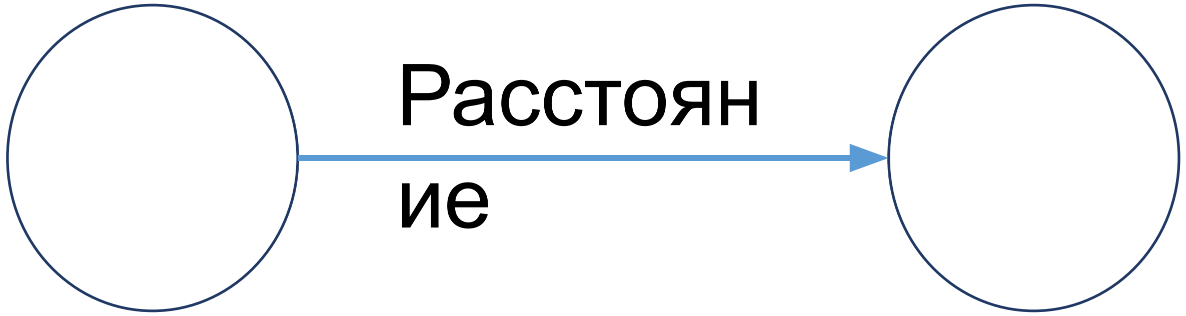
D

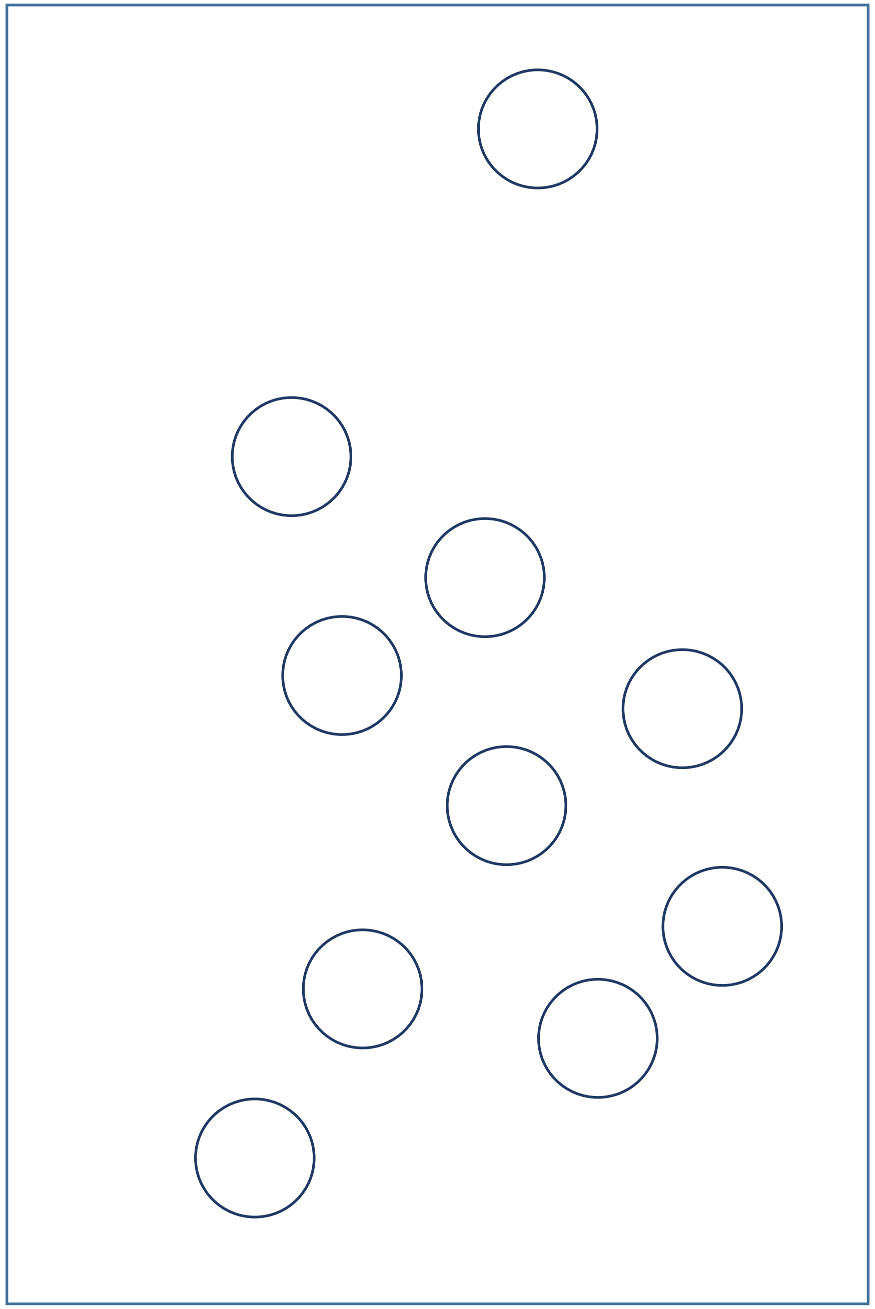


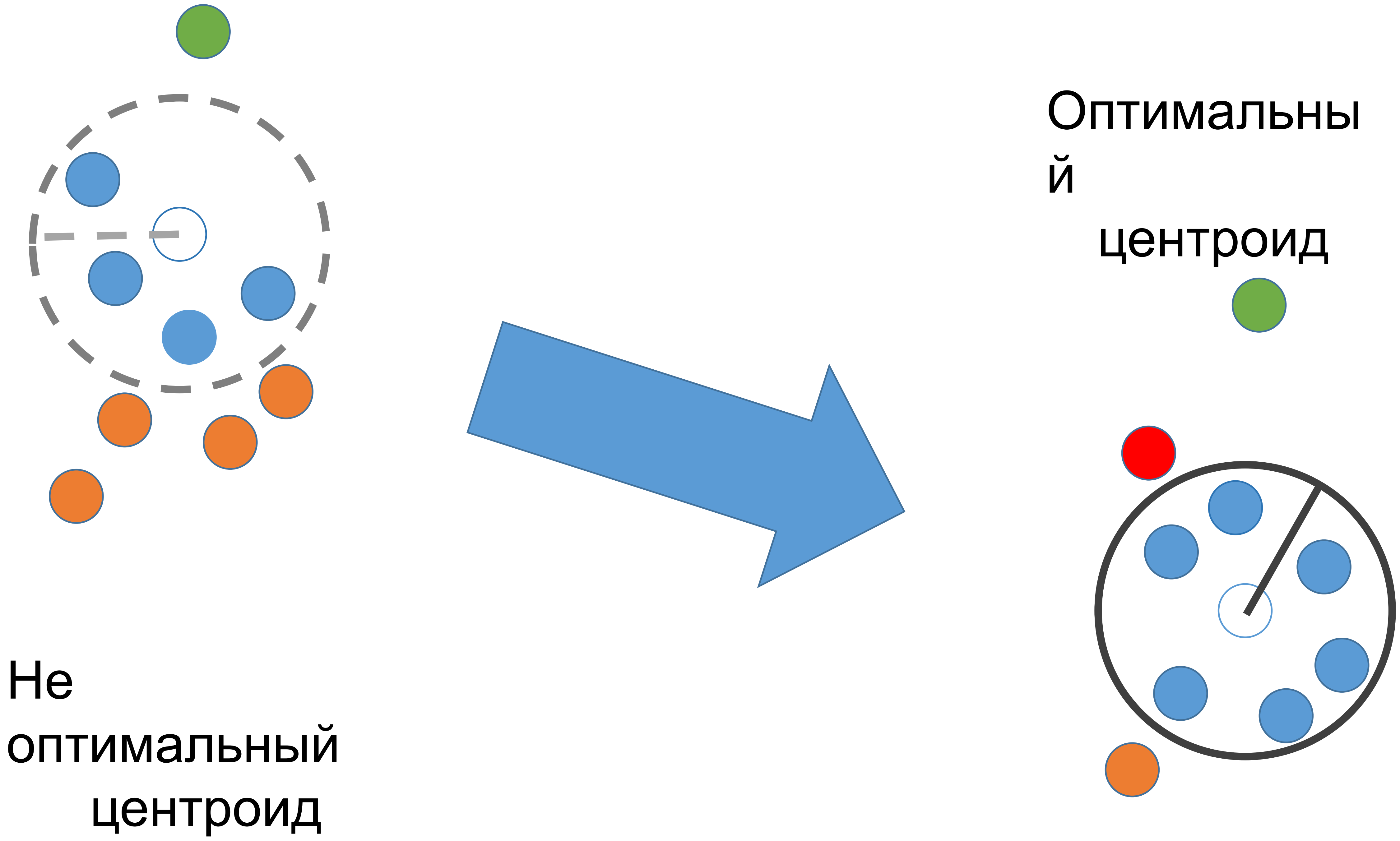
Для кластеризации необходимы:

1. Расстояние
2. Центроиды

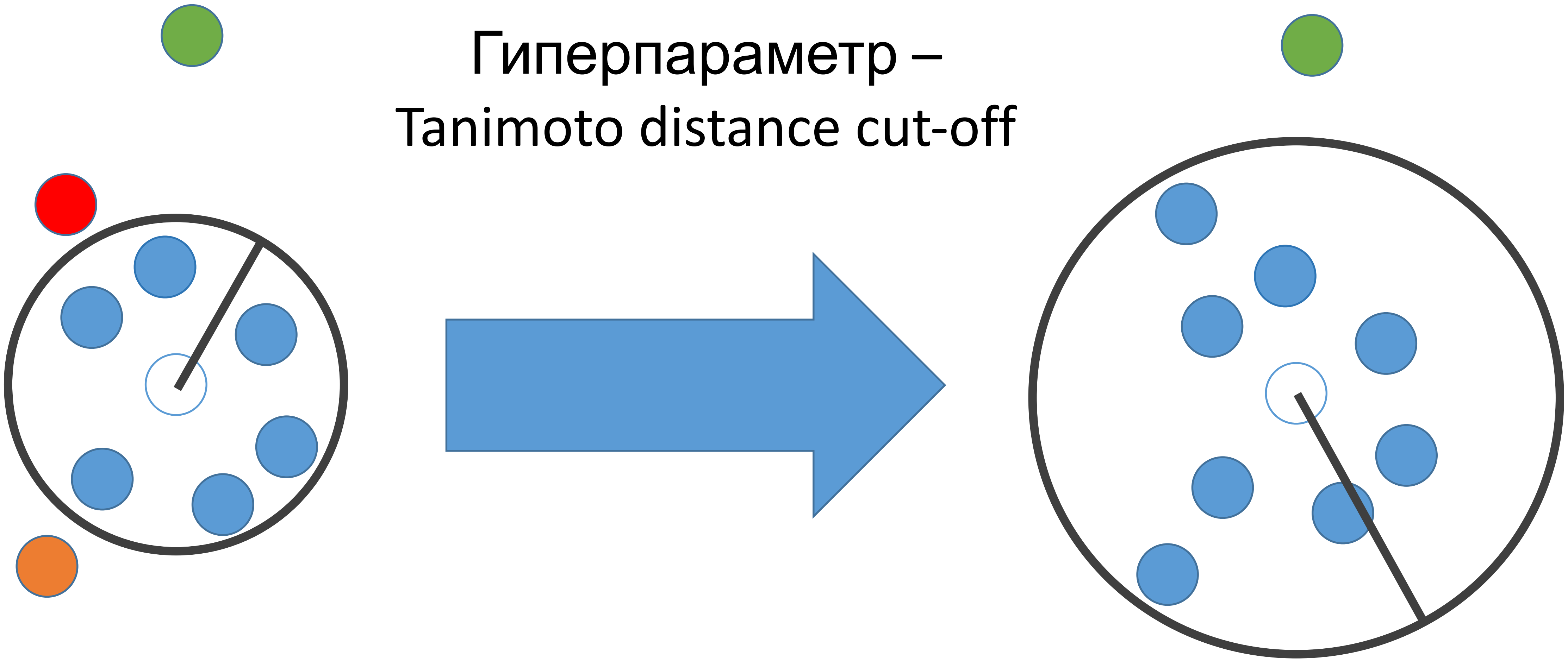
Цель – найти оптимальные центройды при данном расстоянии



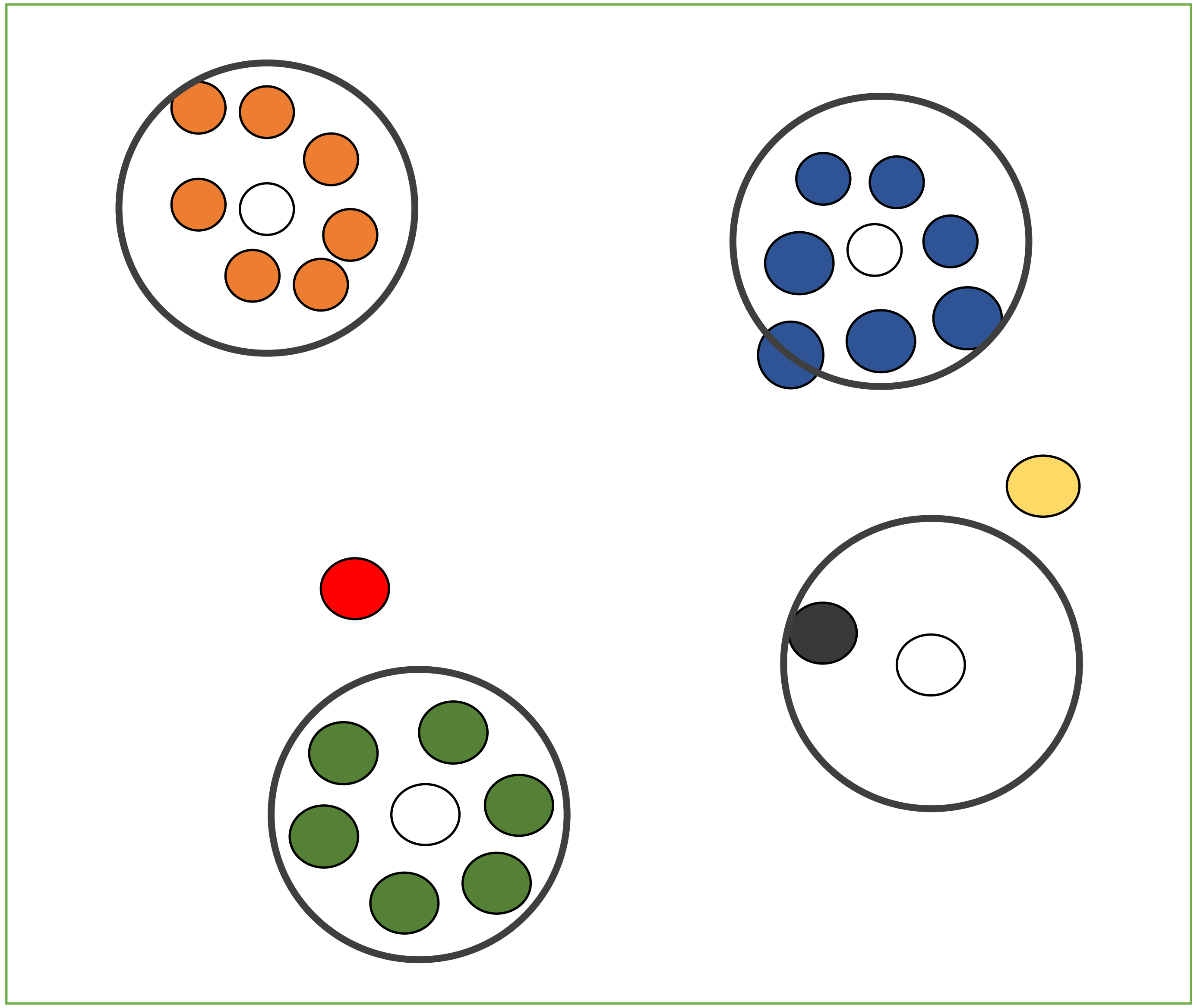


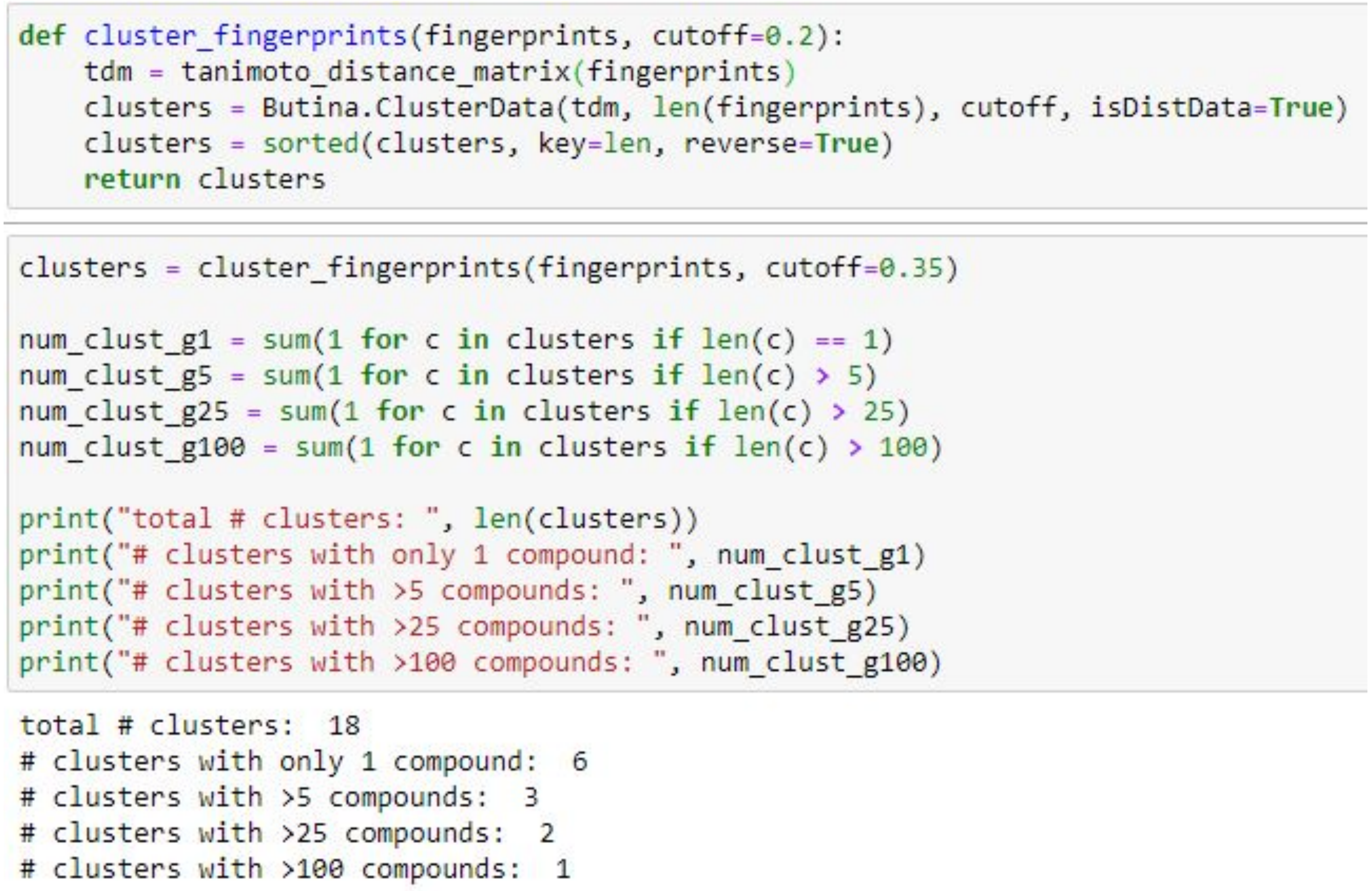

Не оптимальный центроид
Оптимальный центроид

Гиперпараметр – Tanimoto distance cut-off



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

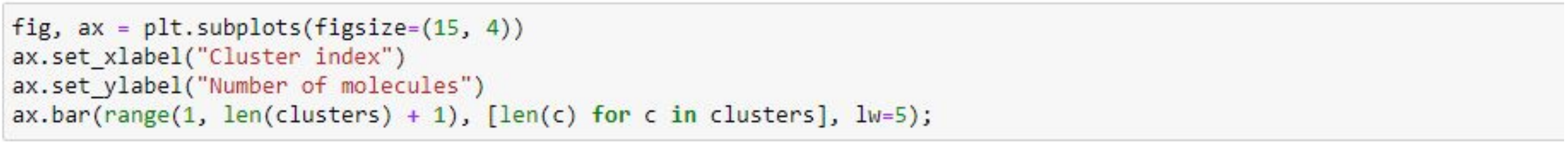




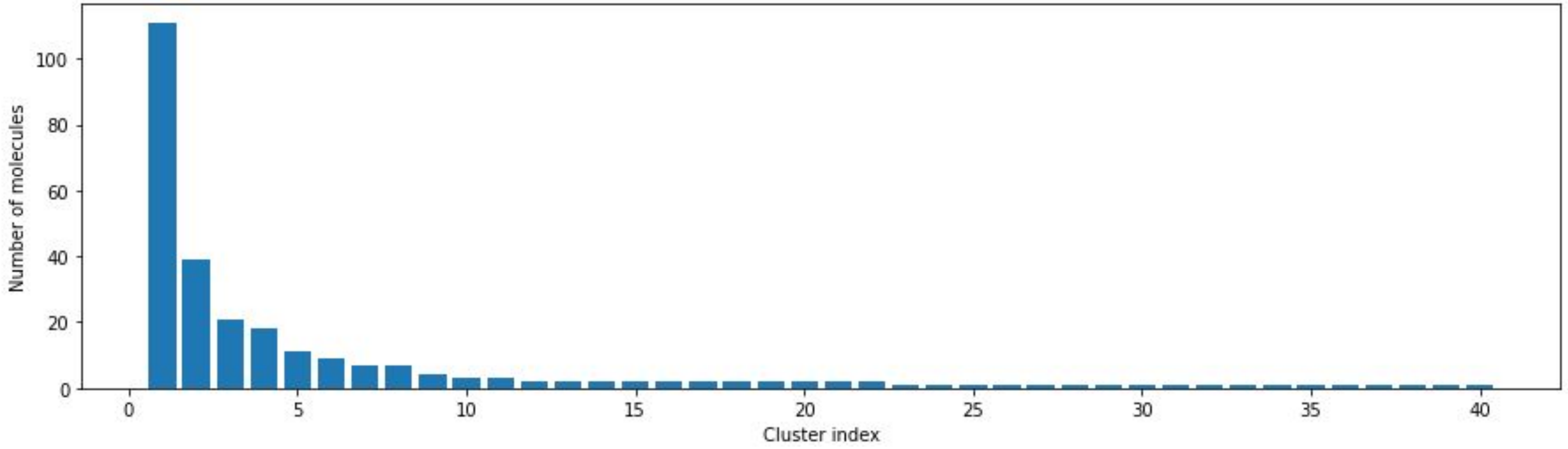
```python
def cluster_fingerprints(fingerprints, cutoff=0.2):
    tdm = tanimoto_distance_matrix(fingerprints)
    clusters = Butina.ClusterData(tdm, len(fingerprints), cutoff, isDistData=True)
    clusters = sorted(clusters, key=len, reverse=True)
    return clusters
```

```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
```



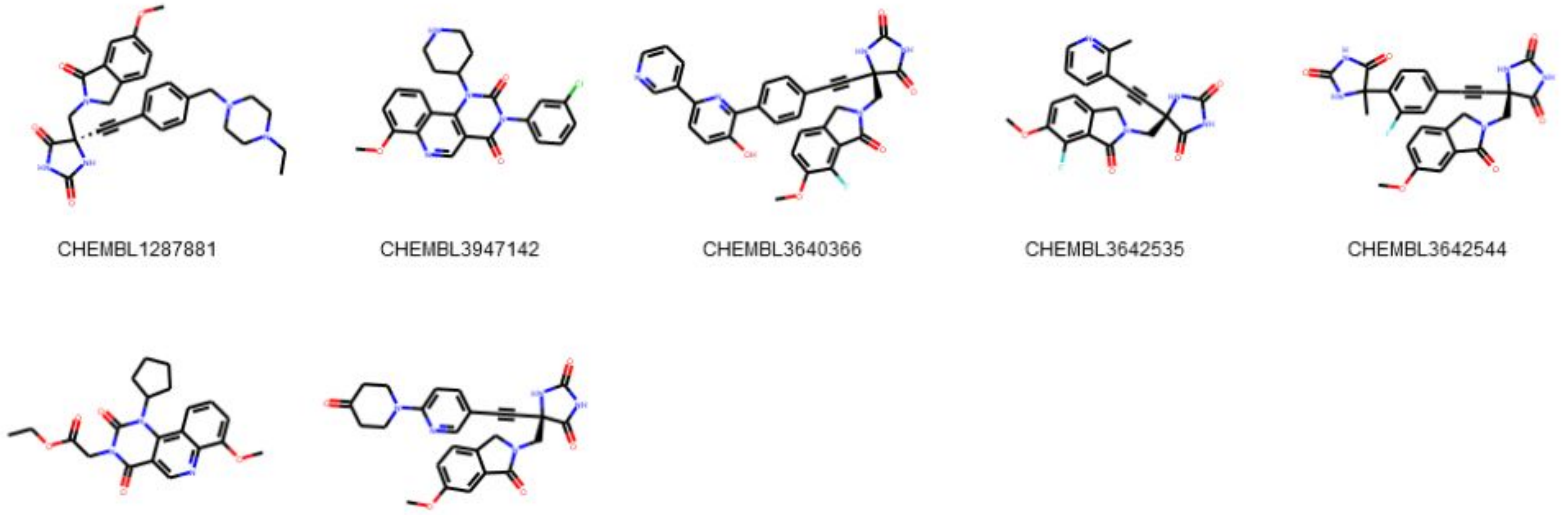
```
fig, ax = plt.subplots(figsize=(15, 4))
ax.set_xlabel("Cluster index")
ax.set_ylabel("Number of molecules")
ax.bar(range(1, len(clusters) + 1), [len(c) for c in clusters], lw=5);
```



Play with cut-off

```python
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:
```



Спасибо за внимание