Dimensionality reduction

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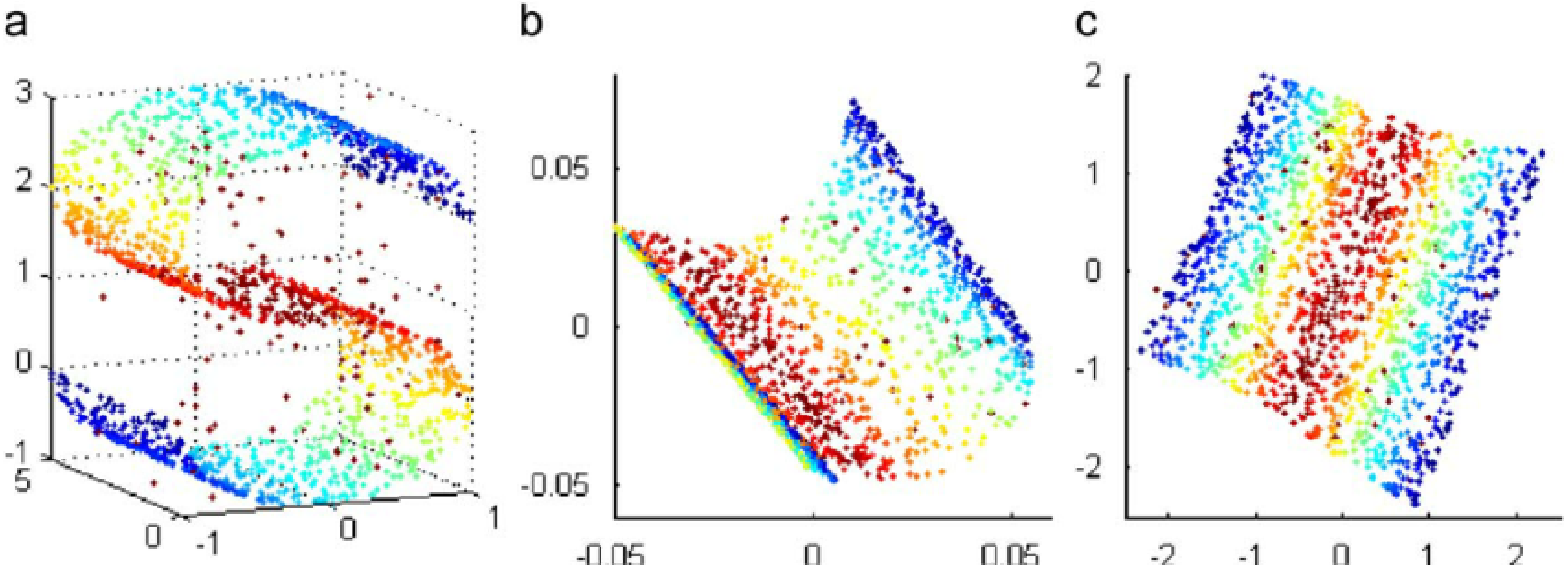
Definition

"Dimensionality reduction is the process of reducing the number of variables under consideration by obtaining a set of principal variables."



Why?

Pro's

- Reduce overfitting
- Obtain independent features
- Lower computational intensity
- Enable visualization

Con's

- Compression => Loss of information => loss of performance

Types

Feature selection (B ? A)

- Selecting a **subset** of existing features, based on predictive power
- **Non-trivial problem:** Looking for the best "team of features", not individually best features!

Feature extraction (B ? A)

- Transforming and combining existing features into new ones.
- Linear or non-linear **projections**.

Common algorithms

Linear (faster, deterministic)

- Principal Component Analysis (PCA)

```
from sklearn.decomposition \
  import PCA
```

- Latent Dirichlet Allocation

```
from sklearn.decomposition \
  import LatentDirichletAllocation
```

Non-linear (slower, non-deterministic)

- Isomap

```
from sklearn.manifold import Isomap
```

- t-distributed Stochastic Neighbor Embedding (t-SNE)

```
from sklearn.manifold import TSNE
```

Principal Component Analysis (PCA)

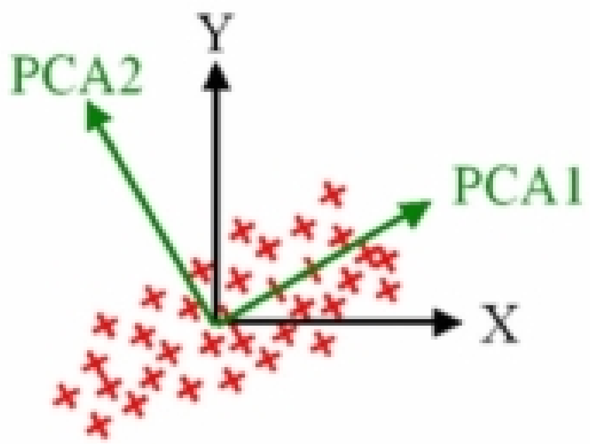
Family: Linear methods.

Intuition:

- **Principal components** are directions of highest variability in data.
- **Reduction =** keeping only top #N principal components.

Assumption: Normal distribution of data.

Caveat: Very sensitive to outliers.



Code example:

```
from sklearn.decomposition import PCA

pca = PCA(n_dimensions=3)

X_reduced = pca.fit_transform(X)
```

Use it wisely!

Clustering

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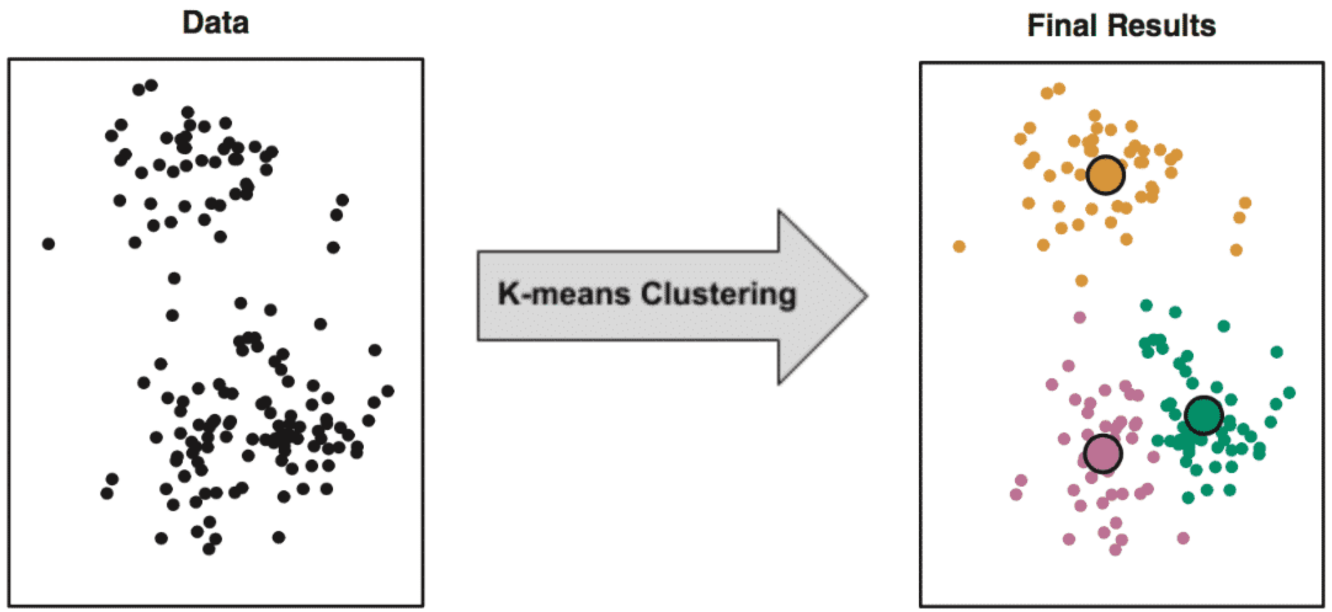
What is clustering?



Cluster = Group of entities or events sharing similar attributes.

Clustering (AI) = The process of applying Machine Learning algorithms for automatic discovery of clusters.

Popular clustering algorithms

KMeans clustering

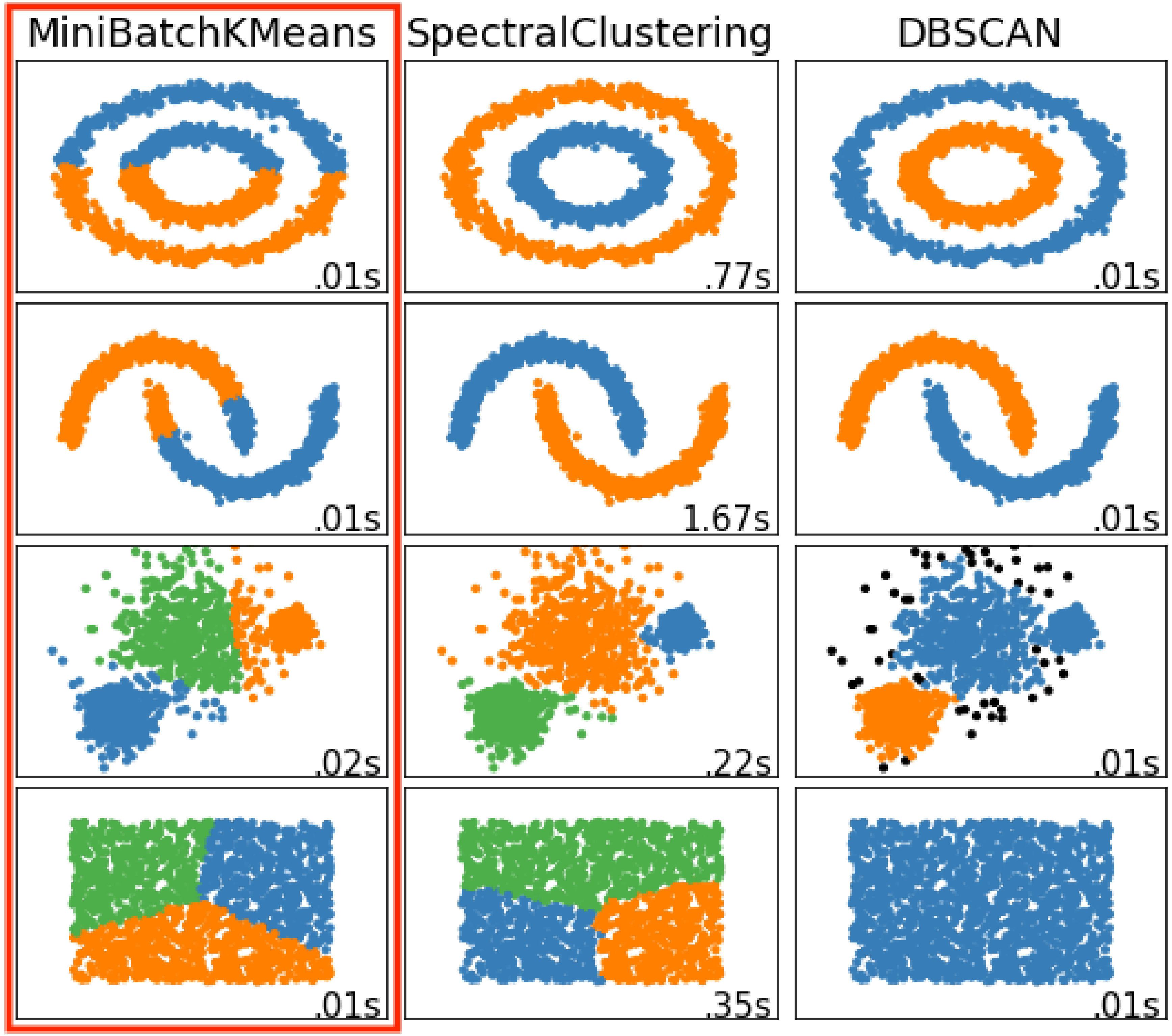
```
from sklearn.cluster import KMeans
```

Spectral clustering

```
from sklearn.cluster import SpectralClustering
```

DBSCAN

```
from sklearn.cluster import DBSCAN
```


MiniBatchKMeans
SpectralClustering
DBSCAN
.01s
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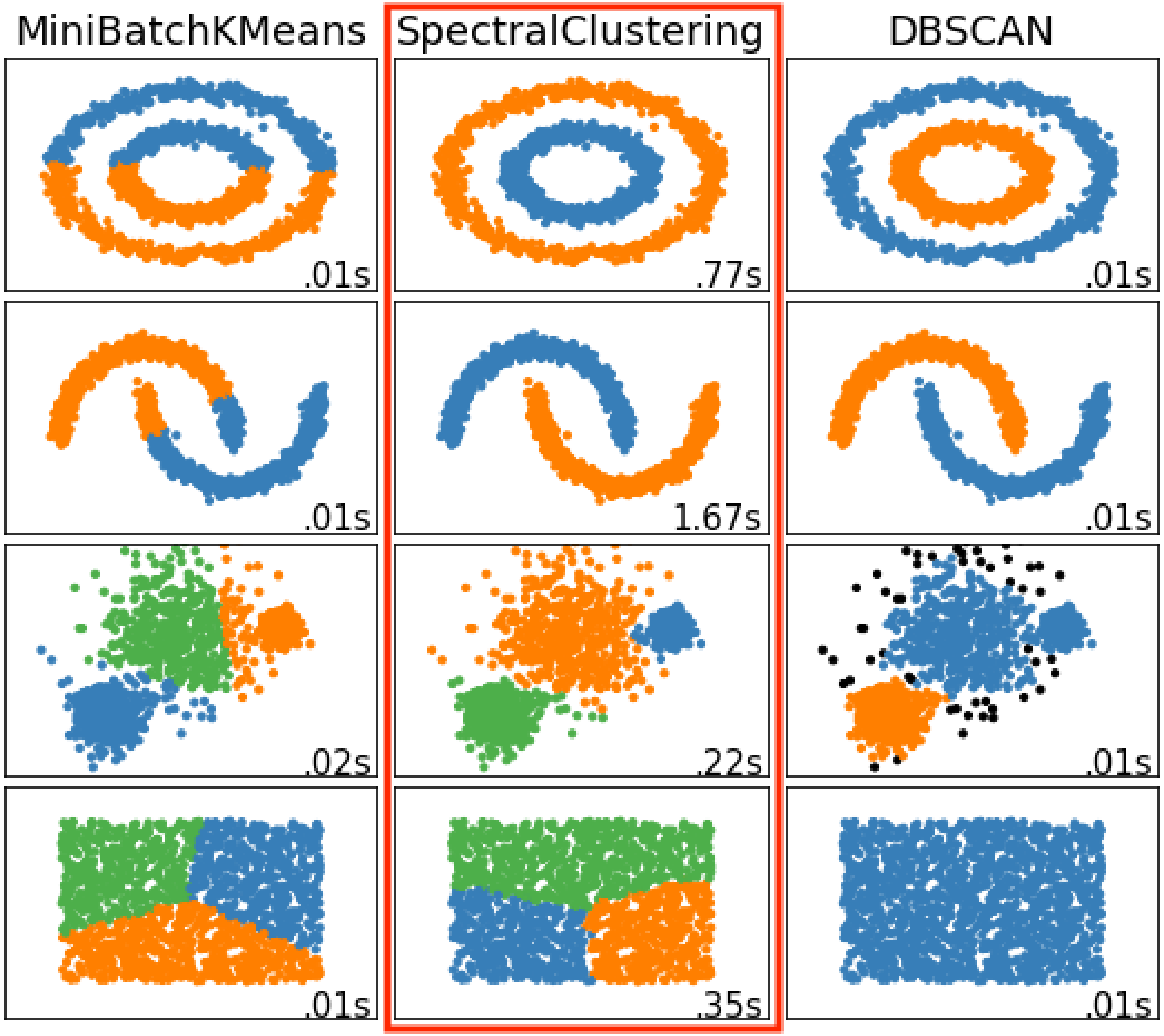
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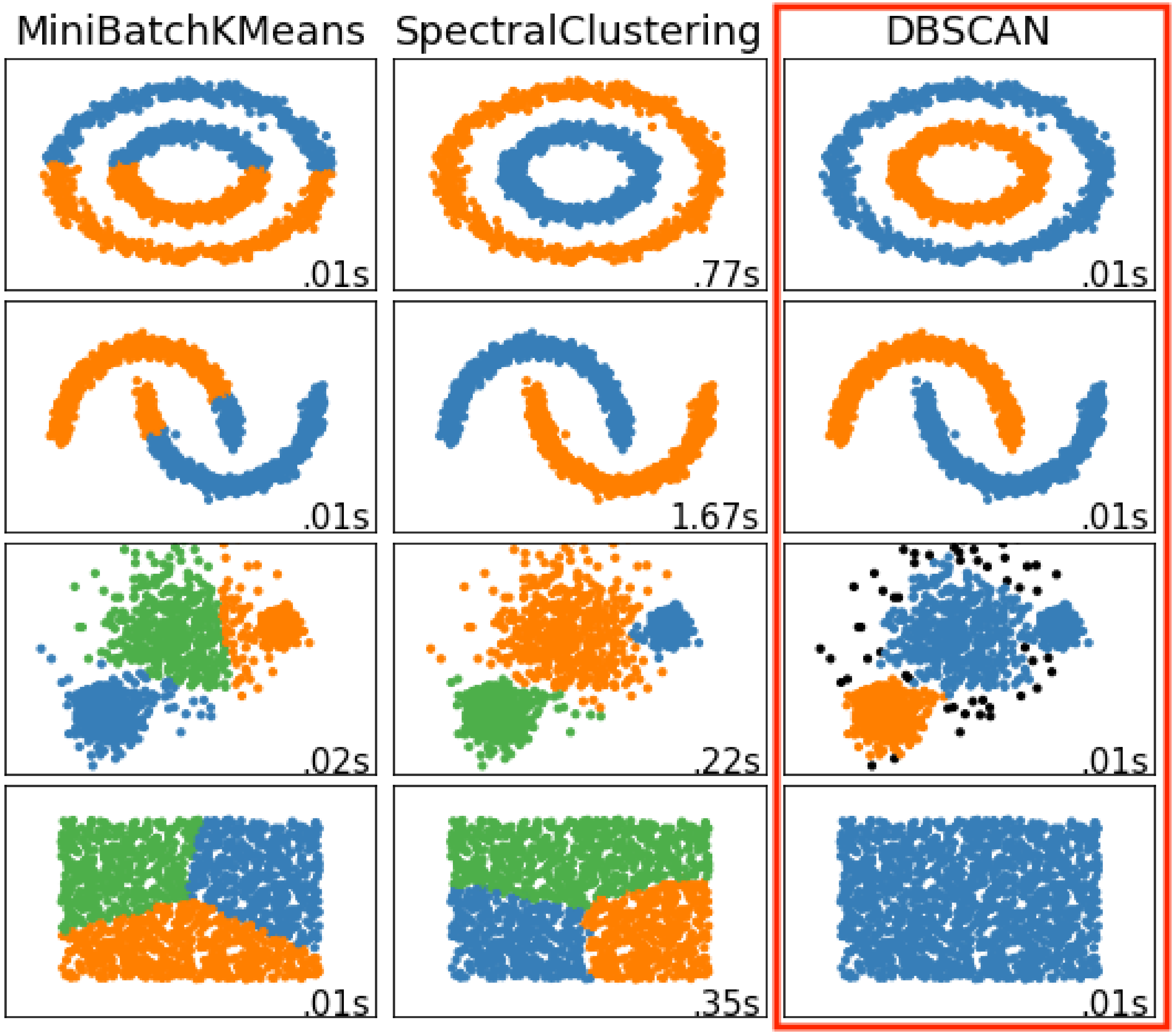
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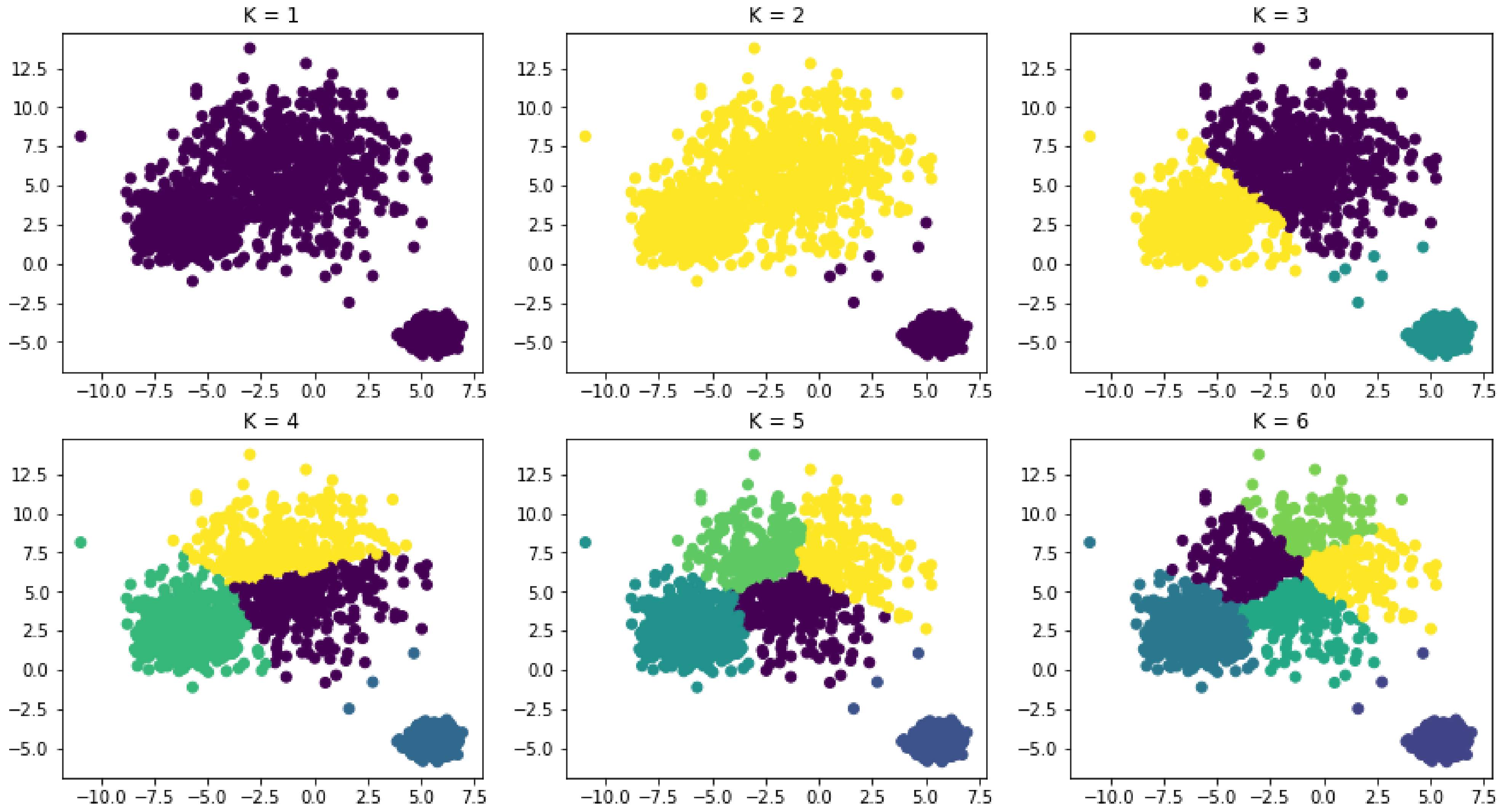
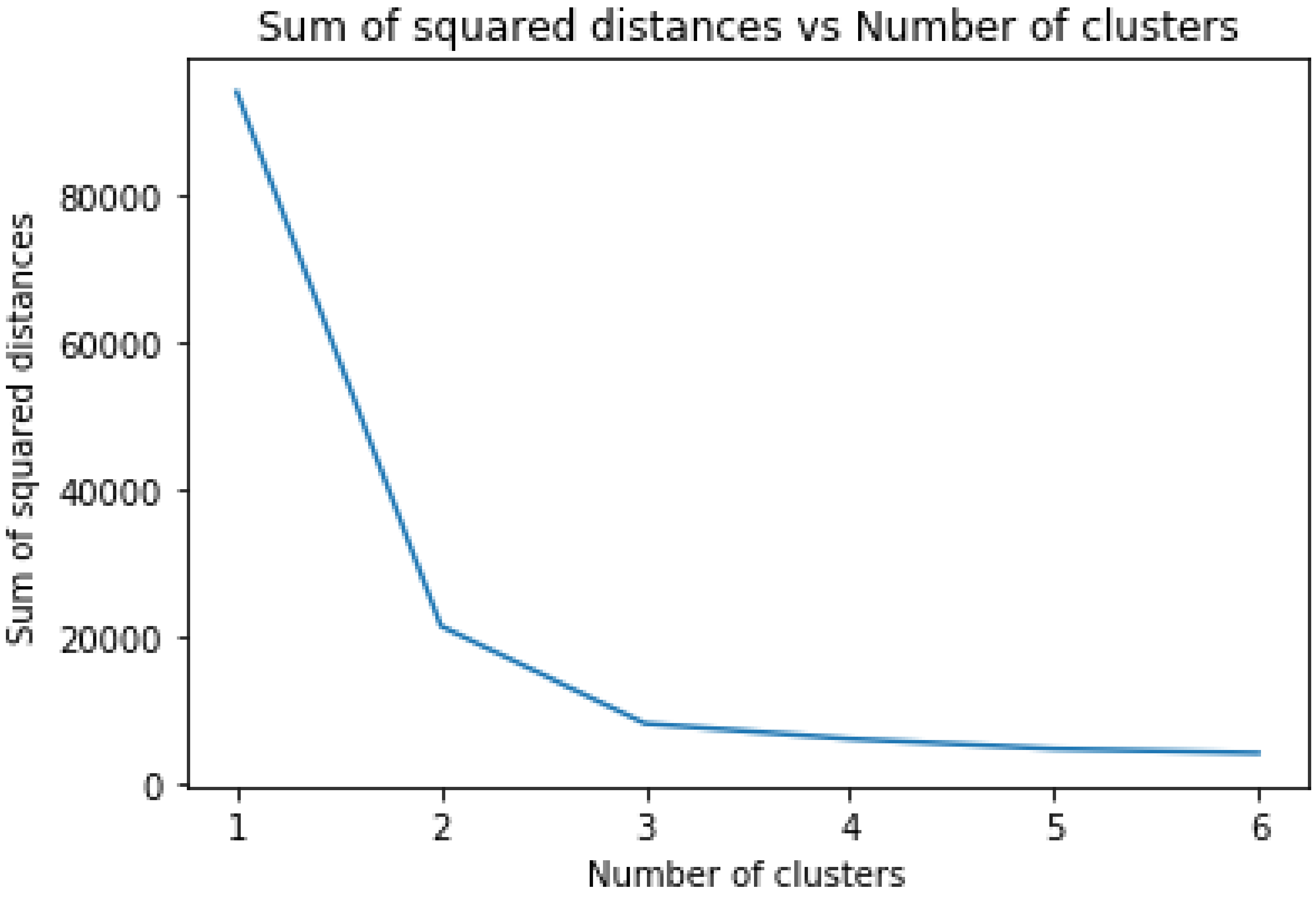
How many clusters do I have?



–> Elbow method!

How many clusters do I have?



Cluster analysis and tuning

Unsupervised (no "ground truth", no expectations)

- Variance Ratio Criterion: `sklearn.metrics.calinski_harabaz_score`
  - *"What is the average distance of each point to the center of the cluster AND what is the distance between the clusters?"*
- Silhouette score: `sklearn.metrics.silhouette_score`
  - *"How close is each point to its own cluster VS how close it is to the others?"*

Supervised ("ground truth"/expectations provided)

- Mutual information (MI) criterion: `sklearn.metrics.mutual_info_score`
- Homogeneity score: `sklearn.metrics.homogeneity_score`

Explore, experiment and tune!

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Anomaly detection

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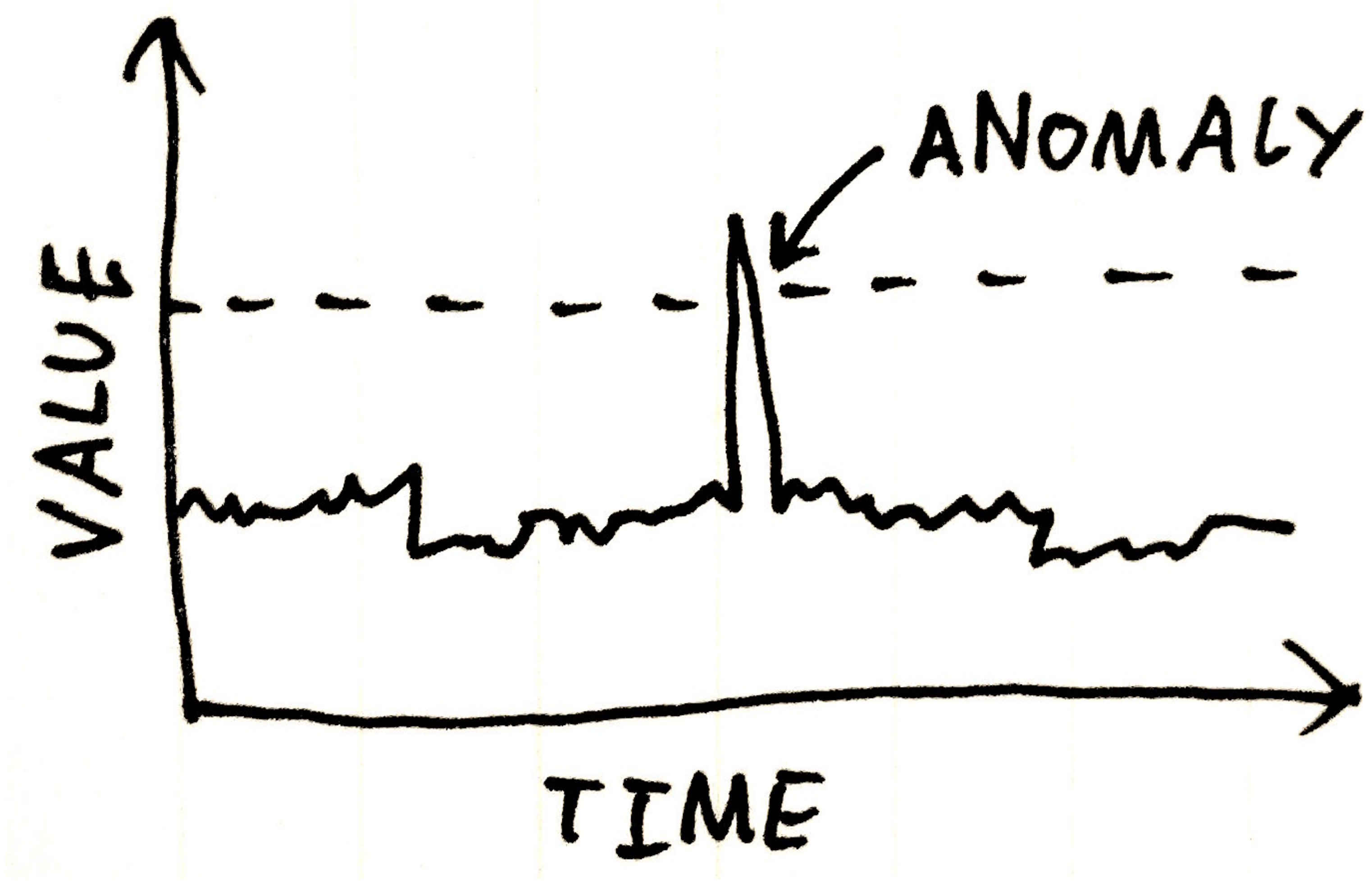
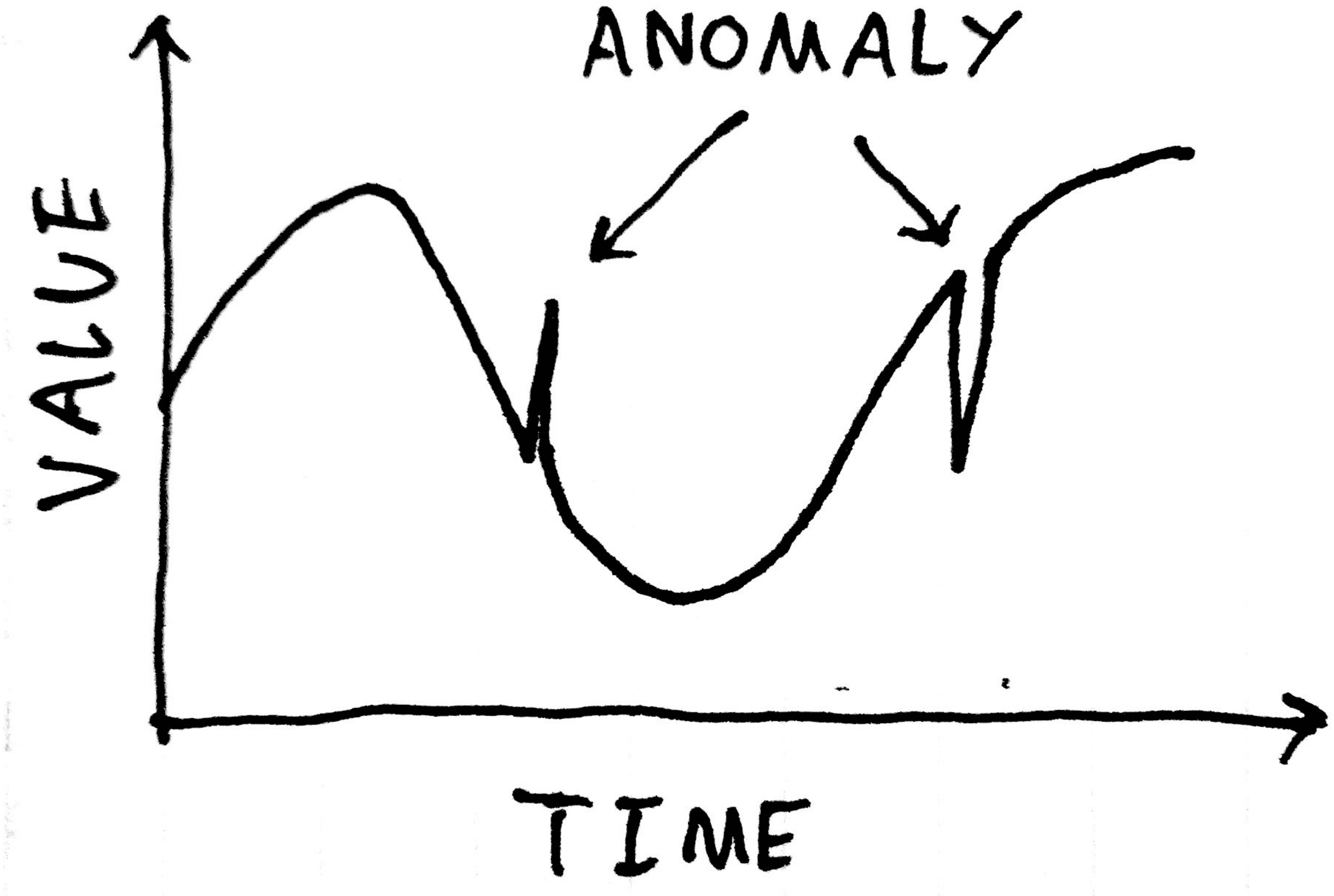
Definition and use cases

- Detecting unusual entities or events.
- Hard to define what's odd, but possible to define what's normal.
- **Use cases**
  - Credit card fraud detection
  - Network security monitoring
  - Heart-rate monitoring

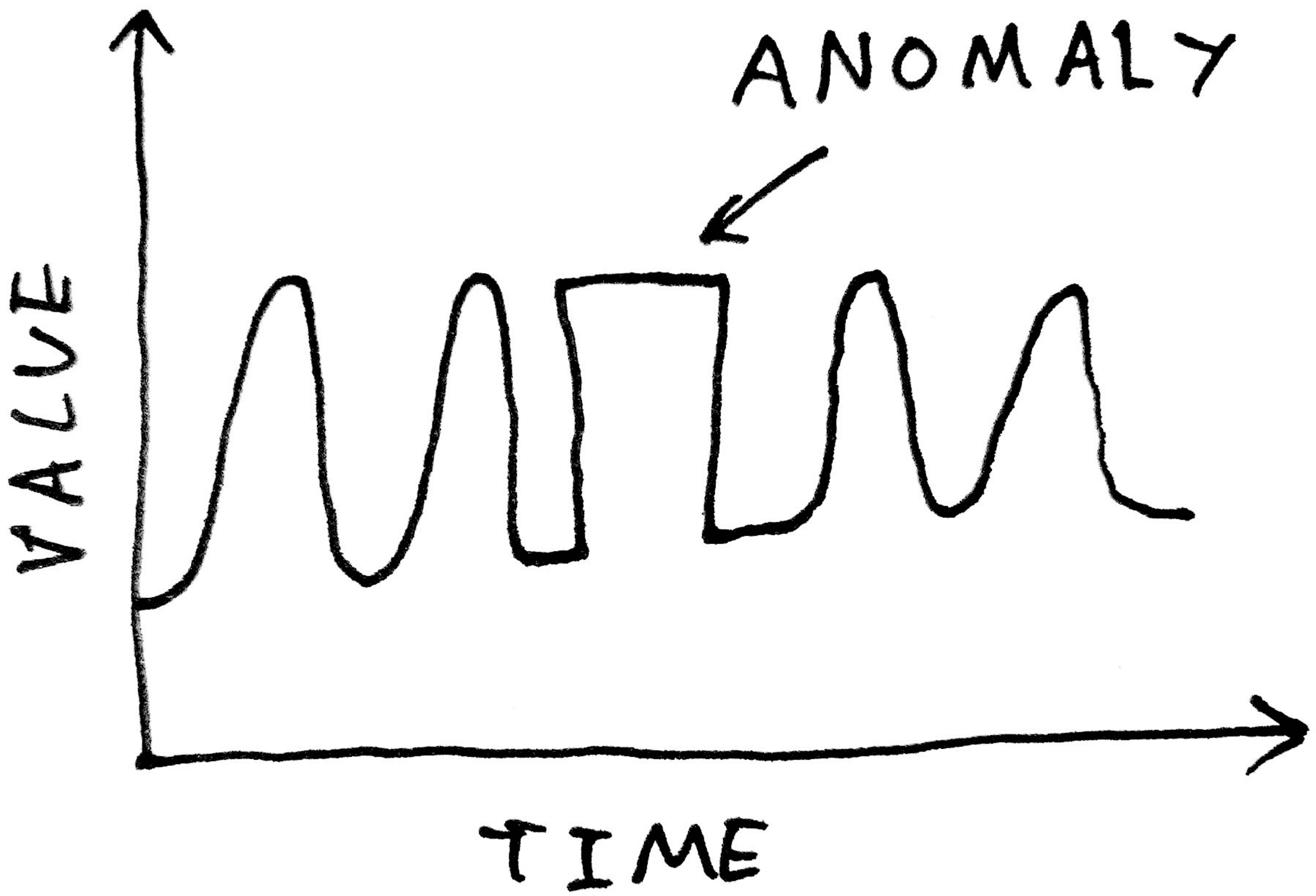
Approaches: Thresholding



Approaches: Rate of change



Approaches: Shape monitoring



Algorithms

Robust covariance (assumes normal distribution)

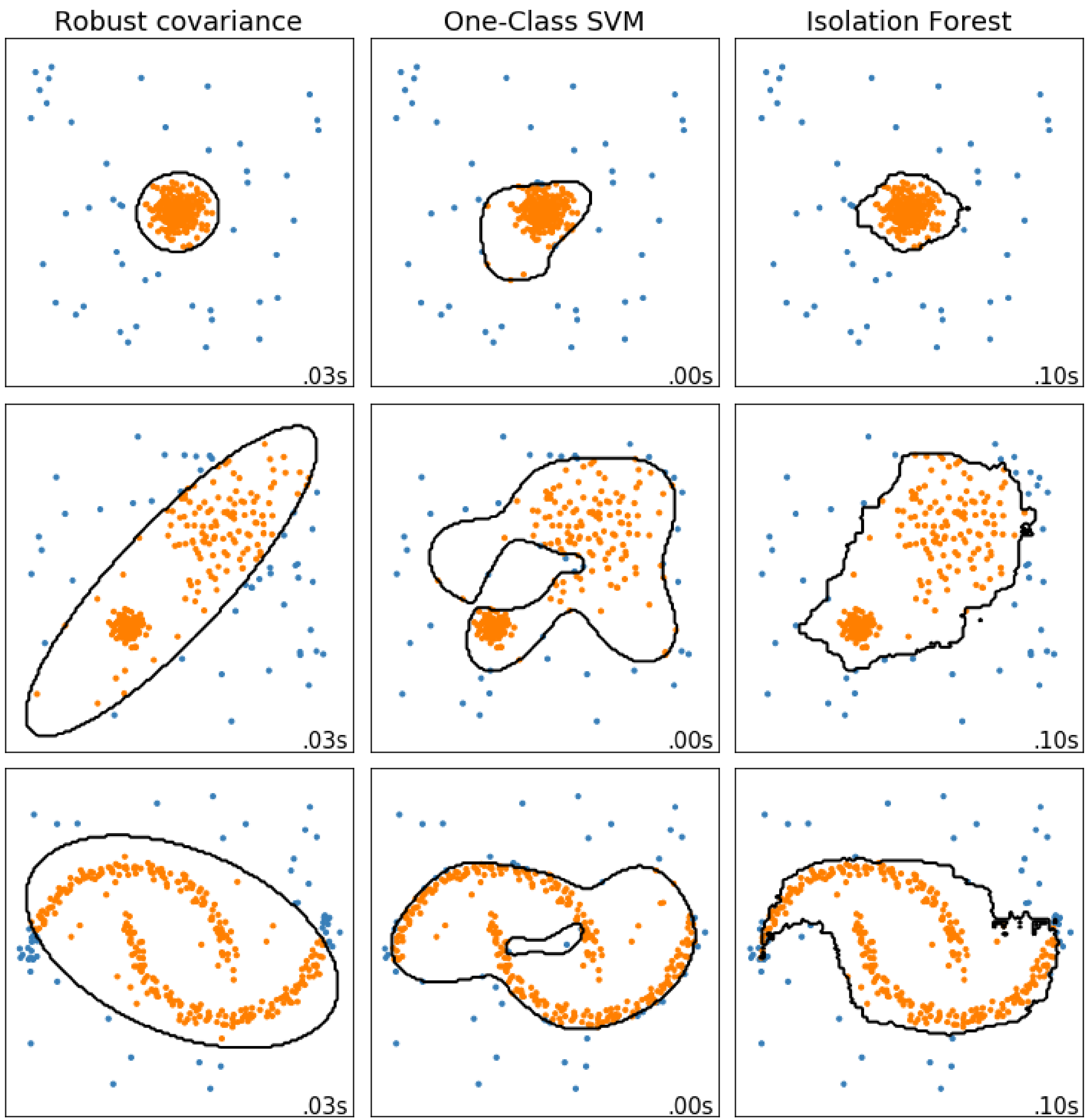
```
from sklearn.covariance import EllipticEnvelope
```

Isolation Forest (powerful, but more computationally demanding)

```
from sklearn.ensemble import IsolationForest
```

One-Class SVM (sensitive to outliers, many false negatives)

```
from sklearn.svm import OneClassSVM
```


Robust covariance
One-Class SVM
Isolation Forest
.03s
.00s
.10s
.03s
.00s
.10s
.03s
.00s
.10s

Training and testing

Example: Isolation Forest

```python
from sklearn.ensemble import IsolationForest

algorithm = IsolationForest()

# Fit the model
algorithm.fit(X)

# Apply the model and detect the outliers
results = algorithm.predict(X)
```

Evaluation

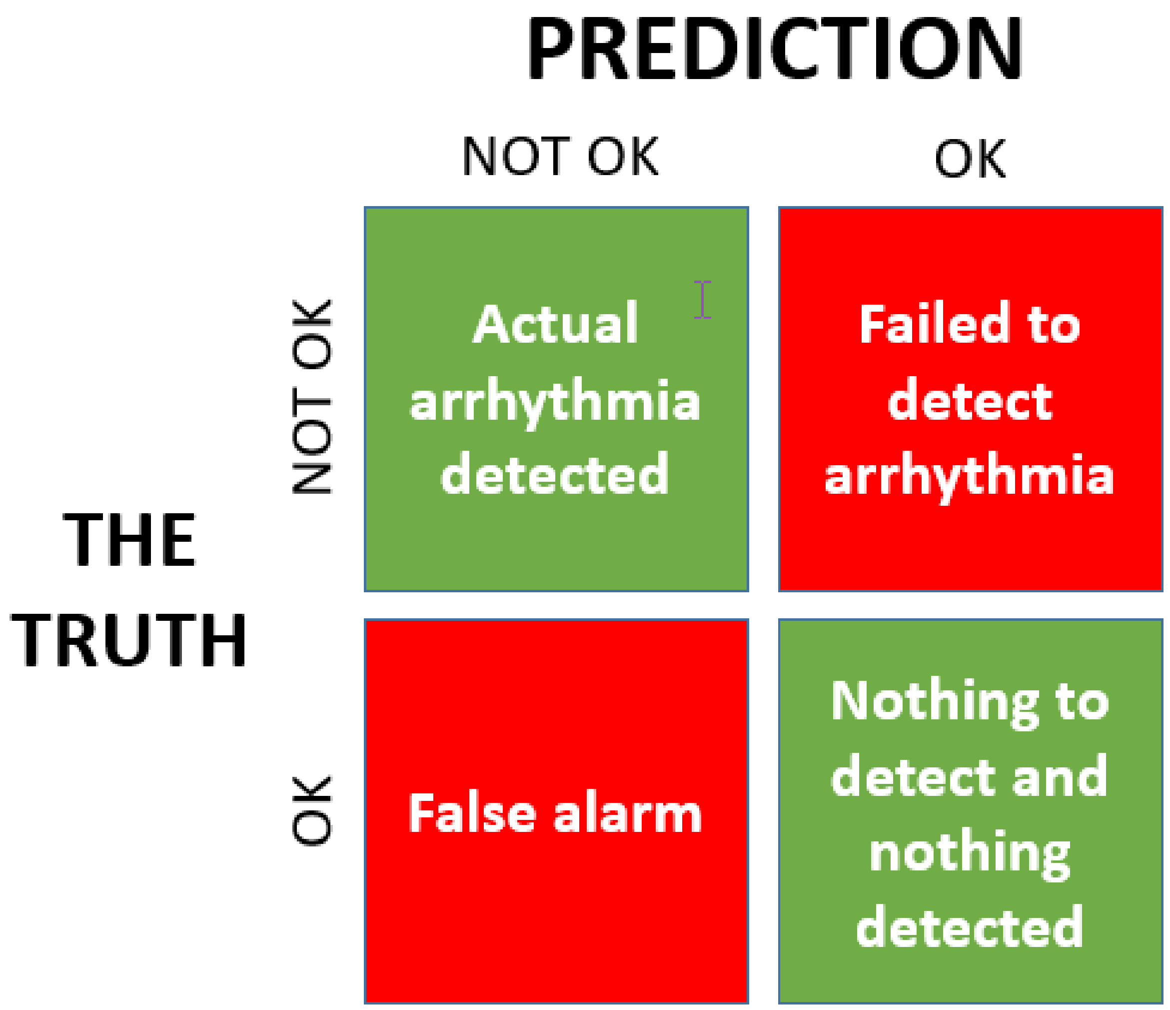
```
from sklearn.metrics \
import (confusion_matrix,
        precision_score,
        recall_score)

confusion_matrix(y_true, y_predicted)
```

Precision = How many of the anomalies I have detected are TRUE anomalies?

Recall = How many of the TRUE anomalies I have managed to detect?

Example: Arrhythmia detection



Want to learn more?

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Selecting the right model

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Model-to-problem fit

Type of Learning

- **Target variable defined & known? => Supervised.**
  - Classification?
  - Regression
- **No target variable, exploration? => Unsupervised.**
  - Dimensionality Reduction?
  - Clustering?
  - Anomaly Detection?

Defining the priorities

Interpretable models

- Linear regression (Linear, Logistic, Lasso, Ridge)
- Decision Trees

Well performing models

- Tree ensembles (Random Forests, Gradient Boosted Trees)
- Support Vector Machines
- Artificial Neural Networks

> **Simplicity first!**

Using multiple metrics

Satisfying metrics

- Cut-off criteria that every candidate model needs to meet.
- Multiple satisfying metrics possible (e.g. minimum accuracy, maximum execution time, etc)

Optimizing metrics

- Illustrates the ultimate business priority (e.g. "minimize false positives", "maximize recall")
- "There can be only one"

Final model:

- Passes the bar on all satisfying metrics and has the best score on the optimization metric.

Interpretation

Global

- *"What are the general decision-making rules of this model?"*
- Common approaches:
  - Decision tree visualization
  - Feature importance plot

Local

- *"Why was this specific example classified in this way?"*
- LIME algorithm (Local Interpretable Model-Agnostic Explanations)

Model selection and interpretation

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