W5. Dealing with Imbalanced Data

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Week 5

Example: Credit Card Fraud Detection

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- Dataset Characteristics:
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  - Legitimate Transactions: 995,000 (99.5%)
  - Fraudulent Transactions: 5,000 (0.5%)
- The goal is to develop a machine learning model that accurately identifies fraudulent transactions.

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- **Challenges**:
  - **Model Bias**: Most classification algorithms will favor the majority class, leading to poor identification of fraudulent transactions.
  - **Evaluation Metrics**: Traditional accuracy is not an appropriate performance metric, as a model that predicts all transactions as legitimate would achieve a 99.5% accuracy rate, ignoring the critical fraudulent transactions.
  - **Over-fitting Minority Class**: Attempts to focus on the minority class can lead the model to over-fit the fraudulent transactions, reducing its generalization ability.

Approaches to Handle Imbalanced Data Set Problem

- **Choose proper evaluation metric**

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- **Synthetic Minority Oversampling Technique (SMOTE)**

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- The other metrics such as precision, i.e.,

$$\frac{TP}{TP+FP}$$

is the measure of how accurate the classifier's prediction of the positive class, while recall, i.e.,

$$\frac{TP}{TP+FN}$$

is the measure of the classifier's ability to identify the positive class.

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- Rather, for an imbalanced class dataset, F_1 score is a more appropriate metric. It is the harmonic mean of precision and recall:

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- In summary, F_1 score only increases if both the number and quality of prediction improves.

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  - Precision (Model A) $=$?
  - Recall (Model A) $=$?
  - F1 Score (Model A) $=$?
- Model B Metrics
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  - Recall (Model B) $=$?
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- Recall emphasizes the proportion of actual positives that were identified correctly. Model A has a higher recall than Model B, indicating it is better at capturing as many actual cases of the disease as possible.
- F1 Score provides a balance between precision and recall. It is particularly useful in imbalanced datasets because it considers both false positives and false negatives. In this scenario, despite Model B having a higher precision, its recall is significantly lower, resulting in a lower F1 score. Model A, despite having lower precision, has a balanced performance between precision and recall, leading to a higher F1 score.

An example to illustrate the choice of F1 – Conclusion

- The F1 score is a more appropriate metric than precision and recall individually in scenarios like this because it captures the balance between the two. This is crucial in imbalanced datasets where a model might have a high precision by predicting the majority class correctly but fails to capture the minority class effectively, or vice versa.

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- The F1 score is a more appropriate metric than precision and recall individually in scenarios like this because it captures the balance between the two. This is crucial in imbalanced datasets where a model might have a high precision by predicting the majority class correctly but fails to capture the minority class effectively, or vice versa.
- The F1 score helps to identify models that maintain a balance between identifying positive cases correctly and minimizing false positives, which is especially important in critical applications like medical diagnostics.

Resampling methods

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- Data centric AI vs Algorithm centric AI

Types of Resampling methods

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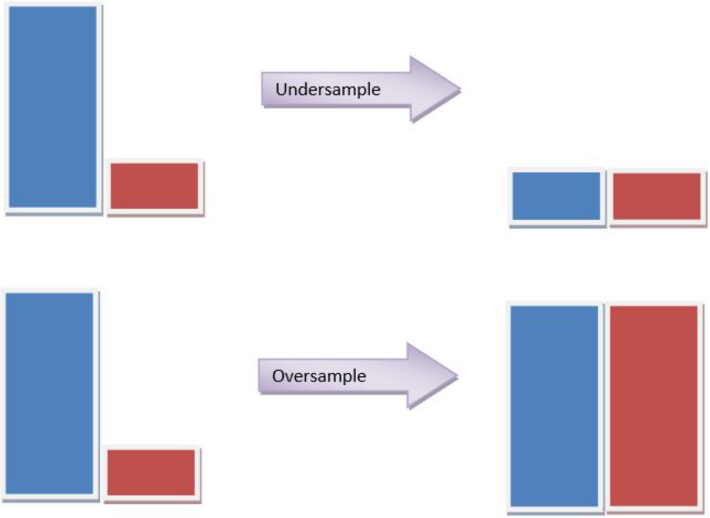
- **Oversampling the Minority Class**: It refers to the process of increasing the number of instances in the minority class(es) within a dataset to address the issue of class imbalance.
- **Undersampling the Majority Class**: It involves reducing the number of instances in the majority class(es) to achieve a more balanced class distribution in situations where one class significantly outnumbers the other(s).

Sktech map of oversampling and undersamping



Exercise: Manual Resampling Methods

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  - Negative instances: N1, N2, N3, N4, N5, N6, N7, N8
  - Positive instances: P1, P2
- **Task**: Your task is to manually apply undersampling and oversampling to make the dataset balanced.

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- **Undersampling**

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  - Goal: Reduce the number of instances in the majority class (Negative) to match the minority class (Positive).

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- **Undersampling**
  - Goal: Reduce the number of instances in the majority class (Negative) to match the minority class (Positive).
  - Instructions: Choose 2 instances randomly from the Negative class to keep. Your new dataset should have 2 Positive instances and 2 Negative instances.

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  - Selected Negative instances: N3, N7

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  - Selected Negative instances: N3, N7
  - New Dataset: N3, N7, P1, P2

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- **Oversampling**
  - Goal: Increase the number of instances in the minority class (Positive) to match the majority class (Negative).
  - Instructions: Duplicate instances from the Positive class until you have as many Positive instances as Negative. Your new dataset should have 8 Positive instances and 8 Negative instances.

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Exercise: Manual Resampling Methods

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  - New Dataset: N1, N2, N3, N4, N5, N6, N7, N8, P1, P1, P1, P1, P2, P2, P2, P2

Synthetic Minority Over-sampling Technique (SMOTE)

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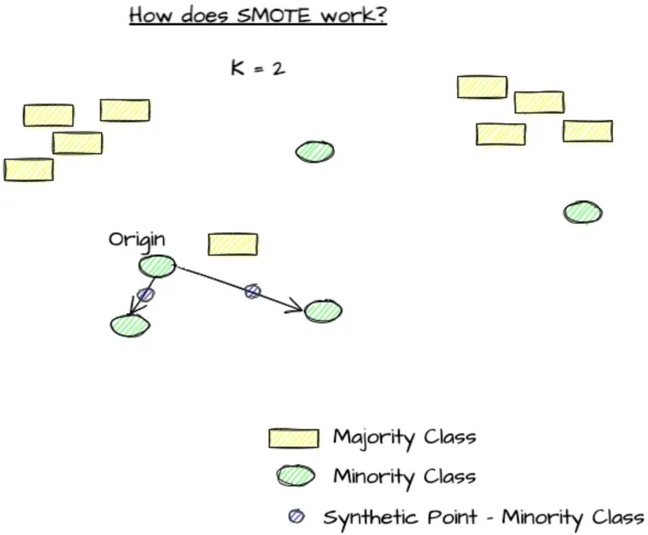
- A brief introduction to generative AI: GAN and Diffusion Models for unstructured data such as image; marginal based method for structured data such as tabules.

How does a basic SMOTE work ?



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- Repeat this process until you get the desired number of synthetic samples.

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- We need an improved version

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  - A point is called "Noise" if all its nearest neighbours belong to a different class (i.e. the majority).
  - On the other hand, "Border" points are those that have a mix of majority and minority class points as their nearest neighbours.

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- This relaxation helps select points that are at risk of mis-classification and new points closer to the boundary. Everything else is the same.
- But this solution is not a silver bullet. Restricting sampling from just border points and relaxing the neighbourhood selection criteria need not work in every scenario.

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- Do K-Means Clustering on the data. Select clusters that have a high proportion ($>50\%$ or user-defined) of minority class samples.
- Apply conventional SMOTE to these selected clusters. Each cluster will be assigned new synthetic points. The number of these generated points will depend on the sparsity of the minority class in the cluster; the more the sparsity, the more new points.

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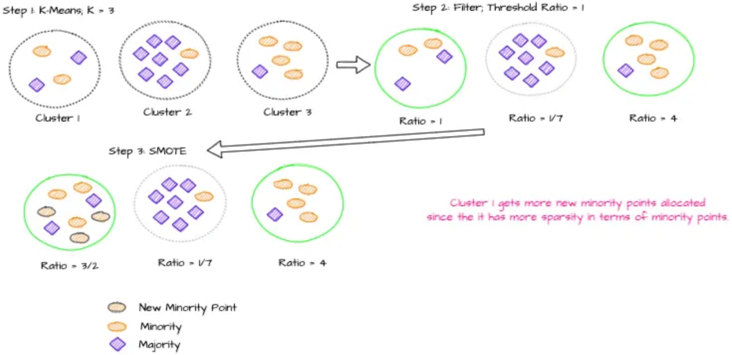
- Optimization: Iterates by re-assigning data points to the nearest centroid and recalculating centroids until centroids stabilize or a set number of iterations is reached.
- Evaluation: Uses metrics like the silhouette score or the elbow method to determine the optimal number of clusters.

K-Means SMOTE



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- In essence, this method helps create clusters of the minority class (that are not greatly influenced by other classes). This can ultimately benefit the ML model. However, it inherits the weaknesses of the K-Means algorithm — such as finding the right K, among others.

An example of SMOTE

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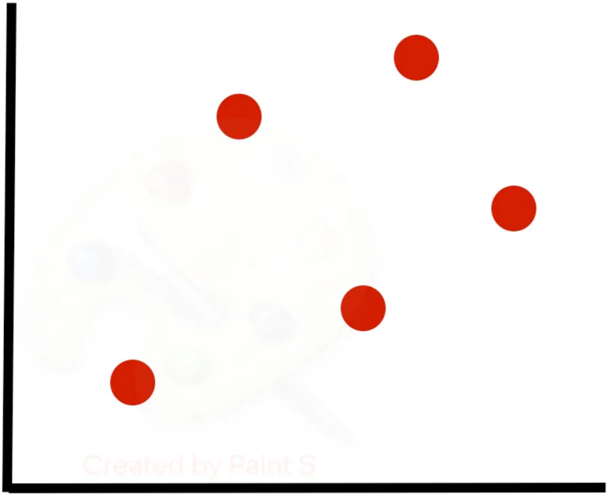
- We proceed to plot a subset of the rows belonging to the minority class.
- We're only considering 2 of the many features (one corresponds to X-axis; another to Y-axis).

An example of SMOTE



An example of SMOTE

- We consider the first row (or a random row), and compute its k nearest neighbors. We then select a random nearest neighbor out of the k nearest neighbors.

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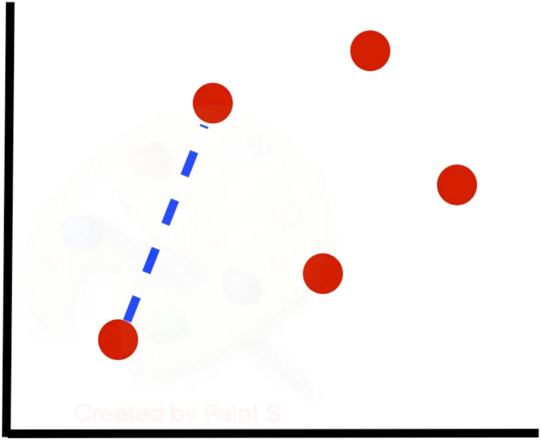

An example of SMOTE

- We compute the difference between the two points and multiply it by a random number between 0 and 1. This gives us a synthetic example along the line between the two points.

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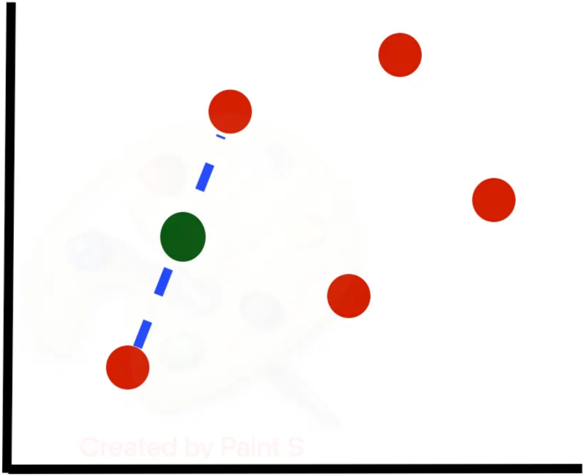
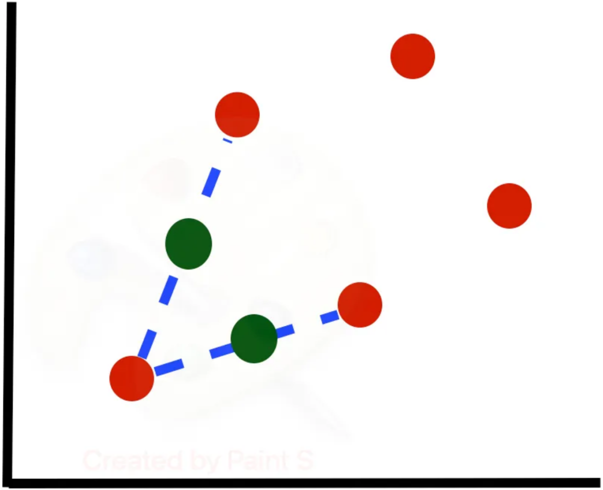


An example of SMOTE

- We repeat the process L times. Here, L represents the over-sampling rate. For example, the original minority class has 100 samples, while we aim to oversample to achieve 300 samples. Then, $L = 3$.
- In this case, only $300/100 = 3$ neighbors from the $k = 5$ nearest neighbors are chosen and one sample is generated in the direction of each.

An example of SMOTE



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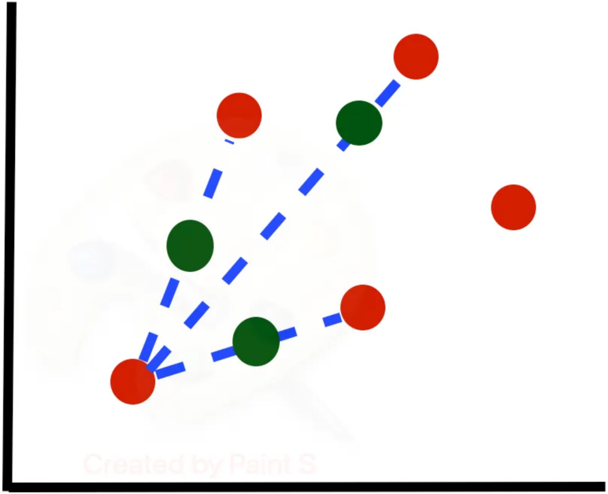
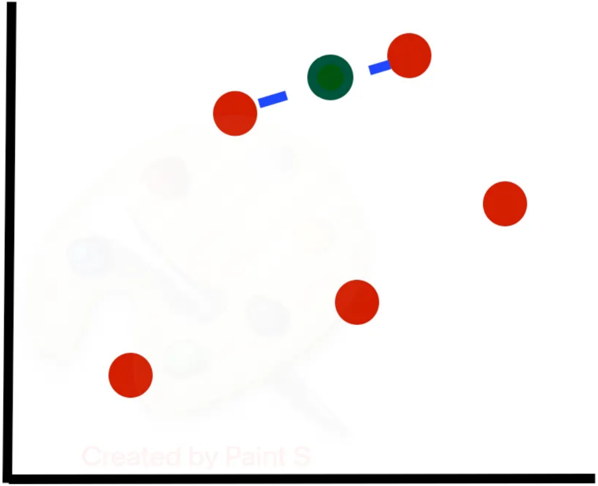


An example of SMOTE

- We then move on to the next row, compute its k nearest neighbors and select $300/100 = 3$ of its nearest neighbors at random to use in generating new synthetic examples.

An example of SMOTE



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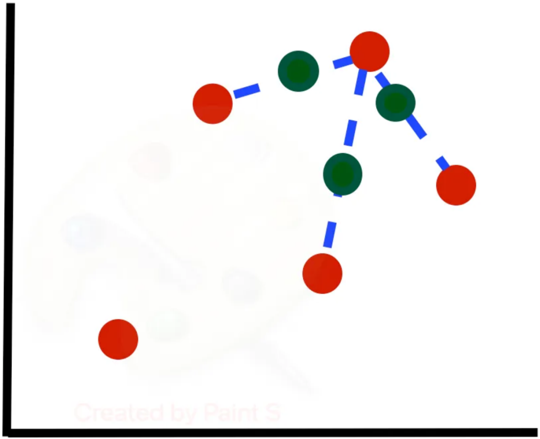

SMOTE in Python

- Let's walk through an example of using SMOTE in Python.
- We begin by importing the required libraries.

SMOTE in Python

```
from random import randrange, uniform
from sklearn.neighbors import NearestNeighbors
import numpy as np
import pandas as pd
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import train_test_split
from sklearn.metrics import confusion_matrix, recall_score
```

SMOTE in Python

- In this example, we will make use of the Credit Card Fraud Detection dataset on Kaggle to train a model to determine whether a given transaction is fraudulent. We read the CSV file and store its contents in a Pandas DataFrame as follows:

SMOTE in Python

```
df = pd.read_csv("creditcard.csv")
```

- Unfortunately, due to confidentiality issues, they cannot provide the original features. Features $V_1, V_2, \cdots, V_{28}$ are the principal components obtained with PCA, the only features which have not been transformed with PCA are 'Time' and 'Amount'.

What is PCA?

- Principal Component Analysis (PCA) is a statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components.
- Will give details in later lecture.

SMOTE in Python

```
df.head(5)
```

...	V21	V22	V23	V24	V25	V26	V27	V28	Amount	Class
...	-0.018307	0.277838	-0.110474	0.066928	0.128539	-0.189115	0.133558	-0.021053	149.62	0
...	-0.225775	-0.638672	0.101288	-0.339846	0.167170	0.125895	-0.008983	0.014724	2.69	0
...	0.247998	0.771679	0.909412	-0.689281	-0.327642	-0.139097	-0.055353	-0.059752	378.66	0
...	-0.108300	0.005274	-0.190321	-1.175575	0.647376	-0.221929	0.062723	0.061458	123.50	0
...	-0.009431	0.798278	-0.137458	0.141267	-0.206010	0.502292	0.219422	0.215153	69.99	0

SMOTE in Python

```
df['Class'].value_counts()
Out:
0    284315
1       492
Name: Class, dtype: int64
```

- As we can see, there are significantly more negative samples (class 0) than positive samples (class 1).

SMOTE in Python

- For simplicity, we remove the time dimension.

```
df = df.drop(['Time'], axis=1)
```

- We split the dataset into features and labels.

```
X = df.drop(['Class'], axis=1)
y = df['Class']
```

- In order to evaluate the performance of our model, we split the data into training and test sets.

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
```

SMOTE in Python

- Next, we initialize an instance of the RandomForestClassifier class.

```
rf = RandomForestClassifier(random_state=42)
```

- We fit our model to the training set.

```
rf.fit(X_train, y_train)
```

- Finally, we use our model to predict whether a transaction is fraudulent given what it has learnt.

```
y_pred = rf.predict(X_test)
```

SMOTE in Python

- Without implementing SMOTE, below is the confusion matrix that evaluates the model's performance. As we can see, our model classified 23 samples as non-fraudulent when, in fact, they were.

```
confusion_matrix(y_test, y_pred)
Out:
array([[56862,     2],
       [   23,    75]])
```

SMOTE using library

- The Python implementation of SMOTE actually comes in its own library (outside Scikit-Learn) which can be installed as follows:

```
pip install imbalanced-learn
```

- We can then import the SMOTE class.

```
from imblearn.over_sampling import SMOTE
```

- To avoid confusion, we read the csv file again.

```
df = pd.read_csv("creditcard.csv")
df = df.drop(['Time'], axis=1)
X = df.drop(['Class'], axis=1)
y = df['Class']
```

- We instantiate an instance of the SMOTE class. It's worth noting that, by default, it will ensure that there are an equal number of positive samples as negative samples.

```
sm = SMOTE(random_state=42, k_neighbors=5)
```

- We apply the SMOTE algorithm to the dataset as follows:

```
X_res, y_res = sm.fit_resample(X, y)
```

SMOTE using library

- Again, we split the dataset, train the model and predict whether the samples in the testing dataset should be considered fraudulent or not.

```
X_train, X_test, y_train, y_test = train_test_split(X_res, y_res, test_size=0.2, random_state
rf = RandomForestClassifier(random_state=42)
rf.fit(X_train, y_train)
y_pred = rf.predict(X_test)
```

- If we look at the confusion matrix, we can see that there are an equal number of positive samples as negative samples and the model didn't have any false negatives. The recall is 1.

```
confusion_matrix(y_test, y_pred)
Out:
array([[56737,    13],
       [    0, 56976]])
recall_score(y_test, y_pred)
Out: 1.0
```

Empirical comparison of different approaches to deal with imbalanced data

- Empirically compare undersampling, oversampling, and SMOTE methods for dealing with imbalanced data

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- Wongvorachan, T., He, S., and Bulut, O. A comparison of undersampling, oversampling, and smote methods for dealing with imbalanced classification in educational data mining. Information, 14(1):54, 2023.

Empirical comparison of different approaches to deal with imbalanced data

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- **Step 2: Apply Resampling Methods**
  - Undersampling: Randomly remove samples from the majority class to match the number of samples in the minority class.
  - Oversampling: Randomly duplicate samples in the minority class to match the number of samples in the majority class.
  - SMOTE: Generate synthetic samples for the minority class by interpolating between existing minority samples.

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  - F1-score provides a balance between precision and recall.
  - AUC represents the likelihood of your model distinguishing between classes.

The results in Educational Data Mining [Wongvoracha, et al 2023]

Table 4. Classification results for each resampling condition.

	Performance Metrics	Baseline Mean (SD)	ROS Mean (SD)	RUS Mean (SD)	SMOTE-NC + RUS Mean (SD)
Moderately Imbalanced	Accuracy	0.736 (0.009)	0.877 (0.006)	0.705 (0.014)	0.779 (0.011)
	Precision	0.773 (0.006)	0.926 (0.006)	0.724 (0.014)	0.796 (0.013)
	Recall	0.888 (0.007)	0.819 (0.010)	0.662 (0.024)	0.749 (0.018)
	ROC-AUC	0.763 (0.013)	0.968 (0.003)	0.763 (0.015)	0.868 (0.010)
	F1	0.827 (0.005)	0.870 (0.006)	0.692 (0.017)	0.772 (0.013)
Extremely Imbalanced	Accuracy	0.887 (0.004)	0.984 (0.002)	0.731 (0.021)	0.905 (0.006)
	Precision	0.665 (0.058)	0.971 (0.003)	0.736 (0.024)	0.911 (0.008)
	Recall	0.193 (0.028)	0.999 (0.001)	0.721 (0.031)	0.898 (0.008)
	ROC-AUC	0.801 (0.016)	0.999 (0.0003)	0.800 (0.020)	0.967 (0.002)
	F1	0.299 (0.038)	0.985 (0.002)	0.728 (0.022)	0.904 (0.006)

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- Oversampling can improve the model's ability to detect the minority class but might increase the risk of overfitting because of the duplication of minority class samples.
- SMOTE tends to offer a good balance by generating synthetic samples, potentially leading to improved model generalization without losing information or overly increasing the risk of overfitting.