

2nd INTERNATIONAL CONFERENCE ON COMPUTATIONAL MODELLING, SIMULATION AND OPTIMIZATION

June 23-25, 2023
Bali (Indonesia)



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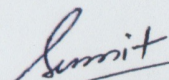
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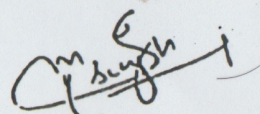
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This is to certify that Dr./Mr./Ms. **Iwan Binanto** from **Sanata Dharma University Yogyakarta, INDONESIA** has participated in the 2nd International Conference on Computational Modelling, Simulation and Optimization (ICCMSO-2023) during June 23-25, 2023 at Bali, INDONESIA.

He/She has presented a paper (Oral) entitled “**Handling of Unbalanced LC-MS Medicinal Plant Data using Near-Miss Undersampling Tested with Gaussian Naive Bayes and K-Nearest Neighbors**”


Dr. Sumit Tiwari
Programme Chair




Manish Kumar
Organizing Secretary



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Proceedings

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Computational Modelling, Simulation and
Optimization
ICCMSO 2023**

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**Bali, Indonesia
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Organized by

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Nitesh Prakash Yelve, *Indian Institute of Technology, Bombay, India*
Sunita Dhingra, *Maharshi Dayanand University Haryana, India*
Deepak Chhabra, *Maharshi Dayanand University Haryana, India*



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Message from the General Chair

ICCMSO 2023

I, Ashwani Kumar Dhingra, the General Chair of the ICCMSO-2023 welcome you all to the 2nd International Conference on Computational Modelling, Simulation and Optimisation (ICCMSO-2023) during 23 – 25 June 2023 at Bali (Indonesia). The conference will run in hybrid mode i.e online and onsite mode of the different technical sessions during the three days.

I am highly obliged and privileged to be the General Chair of the ICCMSO-2023 which is being organised by Innovative Research Foundation (IRF) in active association/collaboration with Sampoerna University Jakarta INDONESIA, National Institute of Technology Kurukshetra INDIA, National Institute of Technology Silchar INDIA & Andhra Loyola Institute of Engineering & Technology Andhra Pradesh INDIA.

It's a great achievement of the ICCMSO-2023 Bali that the delegates from the different parts of the world including INDIA, INDONESIA, MALAYSIA, SOUTH KOREA, HUNGARY and RUSSIA contributed in this International event. All the papers included in the conference schedule were selected after the peer review process with the total acceptance rate of around 40% which further enhance the quality.

I am thankful to our publication partner IEEE CS CPS for agreeing to publish the Conference proceedings. I would like to express my sincere gratitude to Keynote Speaker Prof. Anil Kumar, London Metropolitan University, Invited/Plenary Speaker(s) Prof. Reecha Madaan from Chitkara University Punjab INDIA, Dr. Mohammed Rizwan from Manipal University Jaipur INDIA, Session Chair(s) and finally the delegates for their active support and contribution in making this event a grand success.

I hope the delegates will surely excel their research capabilities through active participation and exchange of the novel ideas in the field of research during different technical sessions of the ICCMSO-2023 Bali.

Ashwani Kumar Dhingra, *Maharshi Dayanand University Haryana, India; Innovative Research Foundation*
ICCMSO 2023 General Chair

Message from the Conference Chairs

ICCMSO 2023

On behalf of the ICCMSO-2023 Organising Committee, We heartily welcome all the Guest(s), Speaker(s), Session Chair(s) and Delegates to the 2nd International Conference on Computational Modelling, Simulation and Optimisation (ICCMSO-2023) during 23 – 25 June 2023 at Bali INDONESIA which is being organised by Innovative Research Foundation (IRF) in association Sampoerna University Jakarta INDONESIA, National Institute of Technology Kurukshetra INDIA, National Institute of Technology Silchar INDIA & Andhra Loyola Institute of Engineering & Technology Andhra Pradesh INDIA. This conference allows both researchers and practitioners to present and share their on-going ideas, experiences, and research results in the application areas of Computational Modelling, Simulation and Optimisation. The technical program includes the careful selection of interesting and novel research papers/Abstracts for presentation during the three days conference.

In response to the call for papers, we received large number of submissions from the different parts of the world. All the papers were evaluated on the basis of their significance, novelty, and technical quality. After careful review, total of 59 submissions have been considered for the oral presentation during the three day conference and out of 59, the 47 papers were duly selected for publication in the IEEE proceeding. The contributions cover a wide range of topics including theory, methods, and applications related to the computational Modelling, simulation and Optimisation.

We would like to express our appreciation to the whole organising committee of the ICCMSO-2023 including the General Chair, Organising Secretaries, Programme Chair, Conference Editors, Program Committee, the finance chairs; the session chairs who presided over the sessions; and all the authors, attendees, and presenters who really made this conference possible and successful along with the secondary reviewers who contributed a great amount of their time and effort to evaluate the submissions to maintain high quality of the conference;

We hope the delegates will enjoy the conference and have a memorable experience at ICCMSO-2023 Bali INDONESIA.

Filscha Nurprihatin, *Sampoerna University, Indonesia*
Rajneesh Kaushal, *National Institute of Technology, Kurukshetra, India*
ICCMSO 2023 Conference Chairs

Message from the Program Chairs

ICCMSO 2023

We are glad to share that Innovative Research Foundation (IRF) in association of Sampoerna University Jakarta INDONESIA, National Institute of Technology Kurukshetra INDIA, National Institute of Technology Silchar INDIA & Andhra Loyola Institute of Engineering & Technology Andhra Pradesh INDIA is organizing 2nd International Conference on Computational Modelling, Simulation and Optimisation (ICCMSO-2023) during 23 – 25 June 2023 at Bali INDONESIA.

The basic aim of the ICCMSO-2023 is to provide a platform for researchers, engineers, academicians, and industry professionals from all over the world to present the research results, development and advanced activities in the field of Engineering and Computational Sciences. I hope that the present conference provides an opportunity for the delegates to exchange novel ideas and research findings in a face-to-face environment, establish business or research relationships, and find global partners for future collaboration.

Total of around 120 submissions were received from the authors of different parts of the continent and 59 submissions have been accepted and registered for inclusion in the conference schedule which includes 47 for the oral presentation and publication in the conference proceedings along with 12 for the oral presentations only in the different onsite/online technical sessions of this Conference.

We are in full belief that the deliberations will enrich academic wisdom of the participants to enable exploration of new domains of applications in ICCMSO-2023. I hope that the delegates will have an enjoyable experience at the conference.

Suresh Kumar, *Punjabi University Patiala, India*
Tika Endah Lestari, *Sampoerna University, Indonesia*
Sumit Tiwari, *Shiv Nadar Institution of Eminence, Uttar Pradesh, India*
Sri Susilawati Islam, *Sampoerna University, Indonesia*
ICCMSO 2023 Program Chairs

Message from the Organizing Secretaries

ICCMSO 2023

It gives us utmost pleasure to welcome you all to ICCMSO-2023 being held at Bali (Indonesia). Bali Indonesia is also known as the Land of the Gods, Bali appeals through its sheer natural beauty of looming volcanoes and lush terraced rice fields that exude peace and serenity. It is also famous for surfers' paradise.

One year ago when we were entrusted with the task of organising this conference we were very thrilled and excited. But down the road we faced many hurdles and problems. However, with the support of our team and advisers we will be able to sail through this journey and we are hopeful that we would be able to meet the expectations of our esteemed guests and delegates.

The Organising Committee has worked really hard to make this conference a huge success. The Scientific Technical programme covered a wide spectrum of topic including the Keynote, Plenary/Invited Speaker in the thrust areas of the advancement in Engineering, Science and Technology which provide the right mix to enlighten you all with the latest development in application areas of computational modelling, simulation and optimisation.

We hope that you will return with sweet memories of this Conference and wish to attend this event again.

We the members of Organising Committee of ICCMSO-2023 Bali INDONESIA wish all the delegates a successful, enjoyable & memorable Conference.

Manish Kumar, *BayWa r.e. (Thailand) Co. Ltd., Thailand*
Rajat Vashistha, *The University of Queensland, Australia*
Ravinder Kumar Sahdev, *Maharshi Dayanand University Haryana, India*
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Handling of unbalanced LC-MS medicinal plant data using Near-Miss Undersampling tested with Gaussian Naive Bayes and K-Nearest Neighbors

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Abstract— Imbalanced data refers to data with classes that have extreme majority and minority data. Such data can lead to inaccurate results. The dataset used in this study came from LC-MS data of medicinal plants that had previously been labeled using the web scraping method and unbalance. There are several resampling algorithms to balance the data. This study used near-miss undersampling with consideration for being more robust against overfitting. The balanced data was split for training and testing with a ratio of 70:30, which will be tested using Gaussian Naive Bayes and K-Nearest Neighbors classification algorithms. The results showed that Near Miss version 1 sampling with the Gaussian Naive Bayes algorithm provided better accuracy and faster execution time.

Keywords—imbalance data, LC-MS, classification, machine learning, undersampling

I. INTRODUCTION

Imbalanced data is data where one class has significantly more observations compared to the other, causing the majority class to be given priority over the minority class in machine learning algorithms. The majority-minority class ratio can reach 100:1, 1000:1, or even 10000:1. Further to binary-class data, this issue also affects multi-class data (more than two classes). The majority class is usually referred to as the positive label, and the minority class is known as the negative label [1]. This can lead to inaccurate results.

This problem is very interesting because it may be seen in many classification problems in the real world, such fraud, risk management, the identification of contaminants, and remote sensing [2]. In addition, it also arises in cancer diagnosis [3], computer network security [4–6], detecting hard drive failures [7], and other fields [8–11]. These studies used existing resampling algorithms [3–10, 12–13] with their own data. There are two algorithms used in that studies which are SMOTE and Near Miss Undersampling.

SMOTE works by increasing the observations of the minority class, which can lead to overfitting and other issues [5, 8, 9, 12, 13]. On the other hand, some advantages of the near-miss undersampling method include preventing overfitting, preserving information, addressing the problem of classifying

minority classes, being effective for large majority classes, increasing accuracy, reducing bias, and improving the representation of minority classes. However, near-miss undersampling also has some disadvantages, such as not ensuring that the samples left from the majority class are the most representative and may cause problems in the model's performance on new data [8, 10]. NearMiss version 1 selects the three closest examples from the majority class and skips over the ones with the least average distance to them.

As a result, the NearMiss version 1 samples selected are similar to certain minority occurrences. NearMiss v2 selects from the majority class instances with the smallest average distance to the three furthest minority classes.

In simple terms, NearMiss version 2 looks for majority samples that are similar to all minority situations. In NearMiss version 3, there are k-instances of the majority class surrounding each instance of the minority class. For each minority occurrence, a considerable number of the nearest majority samples are picked [14, 15].

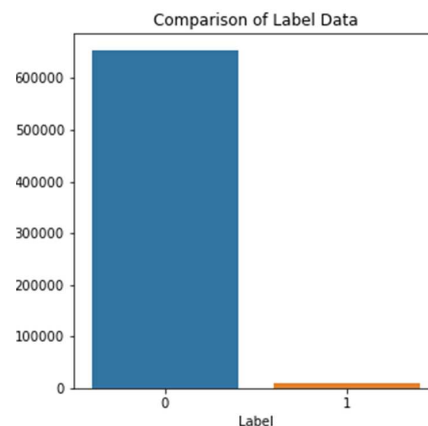


Fig. 1. Unbalanced LCMS data of medicinal plants

This study used a dataset from LC-MS data of medicinal plants that had been labeled using the webscraping technique in previous studies [16, 17]. This dataset consists of 663,228 rows with 7 columns. This dataset is prepared for supervised learning. The label used is a binary label. This dataset is unbalanced because there is a label "1," which is a minority, as shown in Fig. 1. This makes machine learning results inaccurate. This study will use the Near Miss Undersampling algorithm to handle data imbalances. As a test, supervised machine learning will be used using the Gaussian Nave Bayes and K-Nearest Neighbors algorithms. The use of these two algorithms is important because they are very affected by unbalanced data.

II. LITERATURE REVIEW

The data used in this research originated from the work of Sianipar et al. [18-22], who obtained their LC-MS data using tuber sections. The mutant plant outperformed the regular plant in this experiment. When processed using the data labeling employed in prior studies [16, 17], this data yields opposite outcomes. There are several methods for integrating the data. Using various data balancing techniques, Bagui et al. conclude that undersampling shortens training time and oversampling lengthens it; oversampling and undersampling both significantly improve recall when the data is highly unbalanced; and resampling has little effect if the data is not very balanced [5]. Uneven data, according to Haixiang et al., will impact classification results since it causes bias. The minority class can cause bias, which is known as noise [8]. Johnson et al. demonstrated this when investigating deep learning issues using unbalanced data [9]. Tanimoto et al. claimed that the Near Miss technique can improve classification by decreasing the majority sample size while retaining data information [10]. They show how the Near Miss technique enhances classification algorithm performance on unbalanced data sets including medical and network security datasets. [10]. The problem of psychological data, according to Rekha et al., is a complex and tough topic in machine learning. They concluded that there are numerous unsolved questions and numerous avenues for future research on how to address the problem of data inequality [11]. Several studies [23-26] compared the results of Naive Bayes and K-Nearest Neighbors classification techniques. Safri et al. used Nave Bayes with K-Nearest Neighbors to improve accuracy [26]. Nave Bayes is frequently employed due of its competitive accuracy and processing economy, according to Anand et al. [27]. Based on these considerations, this study will compare the two approaches using data that has been balanced by undersampling Near Misses.

The Naive Bayes [28] model is simple to develop and may be applied to a wide range of data sets. Naive Bayes can handle extremely complex classification procedures. Our hypothesis (h) in the classification job could be the class to be allocated to the new data instance (d) Based on our prior information, we can determine the probability of a hypothesis using Bayes' theorem. The following is an illustration of Bayes' theorem:

$$P(h|d) = (P(d|h) * P(h)) / p(d) \quad (1)$$

$P(h|d)$ represents the likelihood that hypothesis h will arise from data d. If hypothesis h is true, $P(d|h)$ reflects the chance that data d exists. $P(h)$ denotes the likelihood that hypothesis h is correct regardless of the data. The goal of our job, as we can see, is to estimate the future likelihood $P(h|d)$ given the prior probability $P(h)$ and the inputs $P(d)$ and $P(d|h)$. It is possible to compose:

$$MAP(h) = \max(P(h|d)) \quad (2)$$

or

$$MAP(h) = \max((P(d|h) * P(h)) / P(d)) \quad (3)$$

or

$$MAP(h) = \max(P(d|h) * P(h)) \quad (4)$$

Probabilities can be defined using $P(d)$, the normalized term. We may disregard it because it is a constant and only use it to normalize if we are only interested in the most likely hypothesis. If our training data has the same number of samples from each class, the probability ($P(h)$) for each class will be the same. We may remove this component because it is a constant in the equation, resulting in the formula (5).

$$MAP(h) = \max(P(d|h)) \quad (5)$$

$$d(x, y) = \sqrt{\sum_{i=1}^n (x_i - y_i)^2} \quad (6)$$

K-Nearest Neighbors has the simplest approach in statistical classification and is also the smartest technique ever discovered. The data feeder (Euclidean equation) will be trained into an algorithm in this way. Data sets can be gathered from classes that have been set up to be used as training data. The Euclidean equation is used to determine the distance between the test and training data points, where i denotes the attribute value and specifies the number of attribute dimensions [29].

III. METHOD

The dataset that has been obtained from previous research [16, 17] is visualized so that it is well seen that the dataset is unbalanced data, as shown in Fig. 1. This dataset is balanced with the Near Miss Undersampling algorithm versions 1 and 3. The data distribution is illustrated using the results. The data balance is then separated into training and testing data in a 70:30 ratio. Training data is tested with Gaussian Naive Bayes and K-Nearest Neighbors machine learning algorithms to obtain a model. This model is then tested with test data. This test will involve the confusion matrix to see accuracy, precision, recall, and F1-score. This research method is shown in Fig. 2. Near Miss version 2 was not used because it was not successful in obtaining sampling. This is due to the limited computer's memory used.

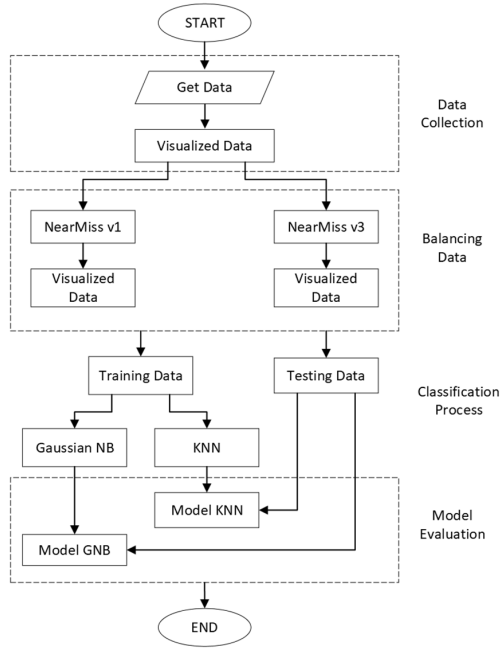


Fig. 2. Research Method

IV. RESULTS AND DISCUSSIONS

After balancing the data, the number of datasets decreases from 663,228 rows to 19,660 rows using the Near Miss version 1 and version 3 algorithms. Indeed, there is a reduction in the total amount of data needed to get balanced data. The visualization of the unbalanced data distribution is shown in Fig. 3. Fig. 4 shows a visualization of balanced data distribution using Near Miss version 1, while Fig. 5 shows a visualization of balanced data distribution using Near Miss version 3.

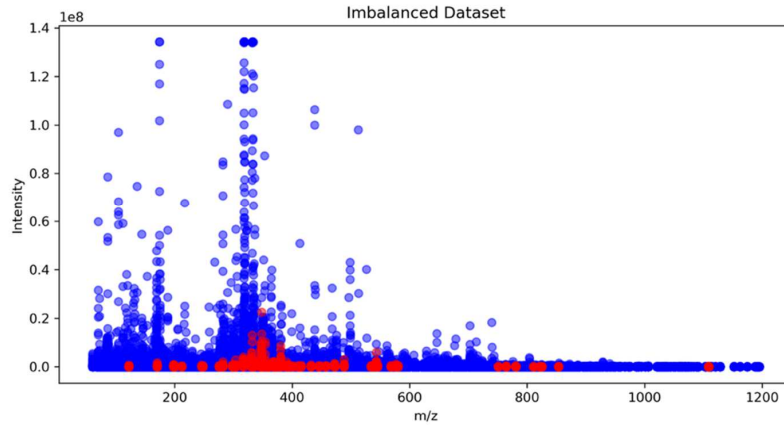


Fig. 3. Graph of unbalanced original data

Balanced data using Near Miss version 3 shows a more uniform distribution of majority and minority data than balanced data using Near Miss version 1. This shows that Near Miss version 3 seems to be better because the sample distribution becomes even.

Gaussian Naïve Bayes and K-Nearest Neighbors are then used to model the balanced data in order to determine the accuracy, precision, recall, and F1-score. The generated confusion matrix is used as the basis for calculating accuracy, precision, recall, and the F1-score.

TABLE I. RESULTS

| | Gaussian Naïve Bayes | | K-Nearest Neighbors | |
|--------------|----------------------|---------------------|---------------------|---------------------|
| | Near Miss version 1 | Near Miss version 3 | Near Miss version 1 | Near Miss version 3 |
| Accuracy | 0.961 | 0.578 | 0.938 | 0.710 |
| Precision | 0.996 | 0.559 | 1.00 | 0.723 |
| Recall | 0.925 | 0.705 | 0.875 | 0.673 |
| F1 Score | 0.959 | 0.623 | 0.933 | 0.697 |
| Process Time | 0.012 | 0.011 | 0.508 | 0.469 |

K-Nearest Neighbors uses optimal k, with value of 140, which is the square root of the amount of data that is already balanced. Table 1 shows the experimental outcomes.

From table 1 can be seen that the Near Miss version 1 tested with Gaussian Naïve Bayes has a better accuracy of 96% compared to that tested with K-Nearest Neighbors which is 93%. Likewise, the F1 Near Miss version 1 score with Gaussian Naïve Bayes is better than K-Nearest Neighbors. Process Time Gaussian Naïve Bayes is also faster, which is 0.012 seconds compared to K-Nearest Neighbors, which is 0.508 seconds. This is in accordance with the opinion of Anand et al that Naïve Bayes has computational efficiency [27].

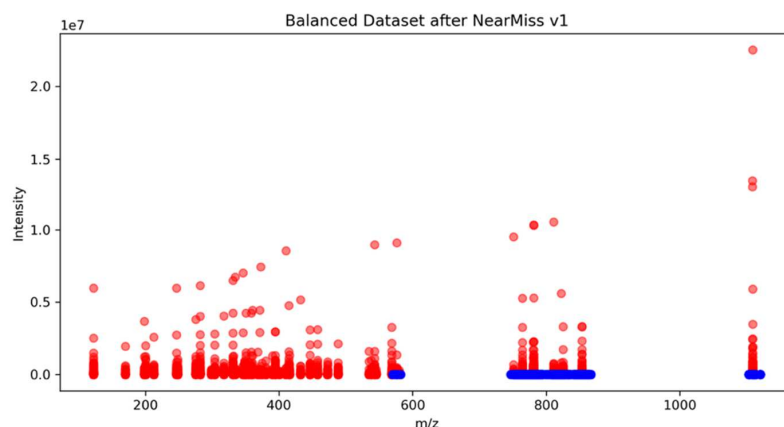


Fig. 4. Graph of balanced data with NearMiss version 1 prior to inclusion in both classification algorithms

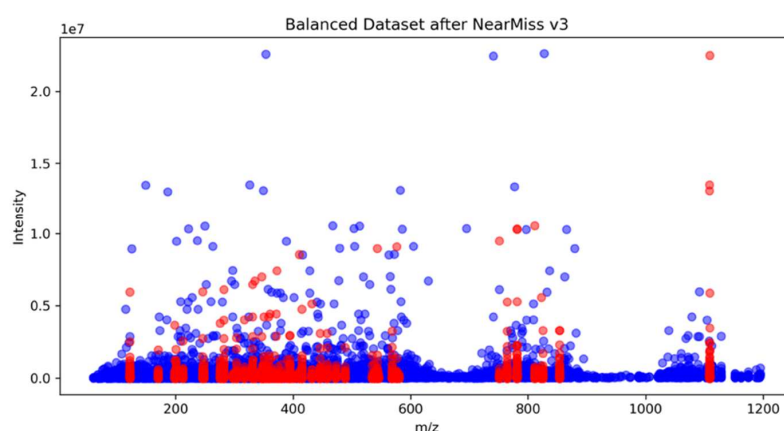


Fig. 5. Graph of balanced data with NearMiss version 3 prior to inclusion in both classification algorithms

V. CONCLUSIONS

The LC-MS data of medicinal plants is used in this investigation. It must be balanced because it is not currently balanced. The two methods that were selected are Near Miss versions 1 and 3, with the undersampling technique, which is more resistant to overfitting, being taken into consideration. Near Miss version 2 was not used because it failed to generate sampling. This is due to the limitations of the devices used.

For test the sampling, Gaussian Naive Bayes and K-Nearest Neighbors algorithms are used with consideration of their popularity and ease of use.

The results of this study indicate that Near Miss version 1 tested with Gaussian Naive Bayes is better in terms of accuracy and execution time than tested with K-Nearest Neighbors.

This research raises a new problem with Near Miss version 3, which has a more even distribution but poor accuracy, even though the execution time is faster. We'll be working on this in the future, along with conducting the experiment with different classification systems.

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