New Developments for Addressing Class Imbalance Issue in Classification Tasks

Ph.D. Thesis Defense

Surani Matharaarachchi

November, 08 2024

Outline

Introduction

- The rapid advancement of science and technology has resulted in increasingly complex datasets
- Predictive Modeling
- Make data-driven decisions
- Challenges in Predictive Modeling: Class Imbalance Issue
  - Abnormal instances
  - Curse of dimensionality

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Class Imbalance Issue

- Occurs when the number of instances in different classes is significantly disproportionate.
- Examples:
  - Fraud Detection
  - Spam Detection
  - Medical Diagnosis
  - Churn Prediction
- Issues:
  - Leads to biased models
  - Decreases predictive accuracy
- Abnormal Instances

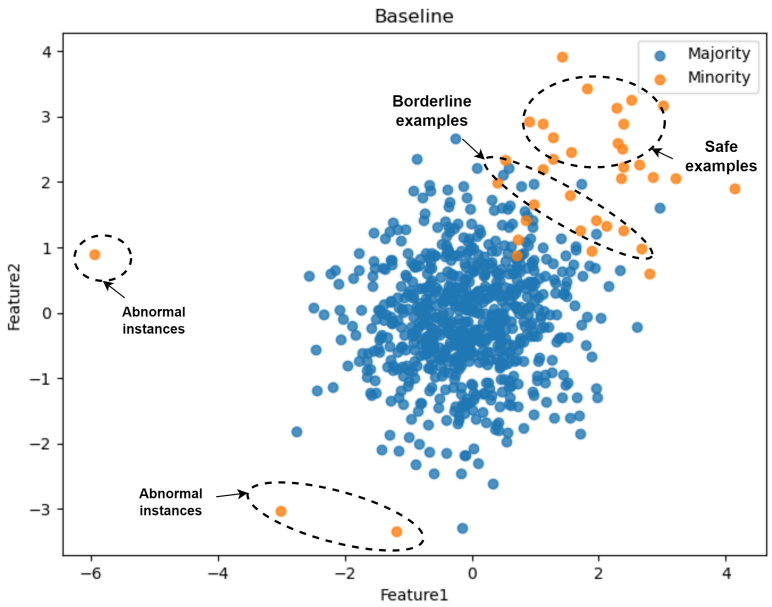

Figure: Class imbalance with outliers in minority class

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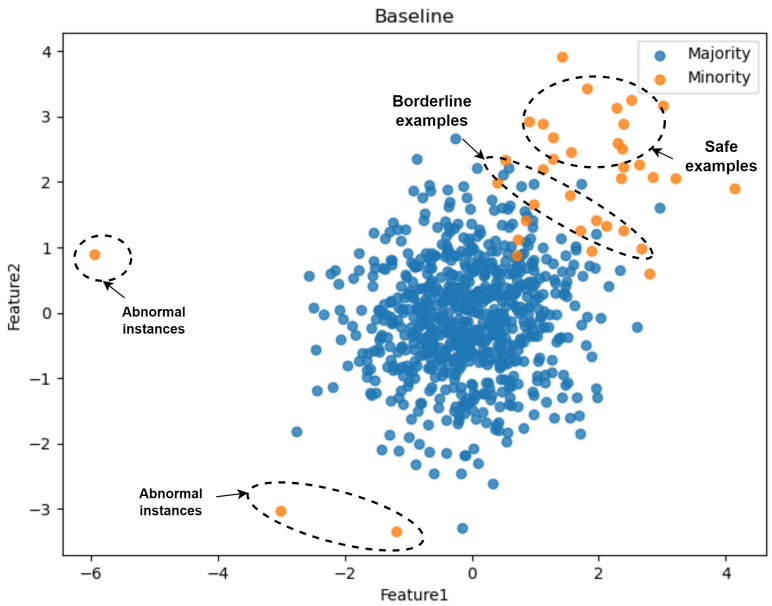

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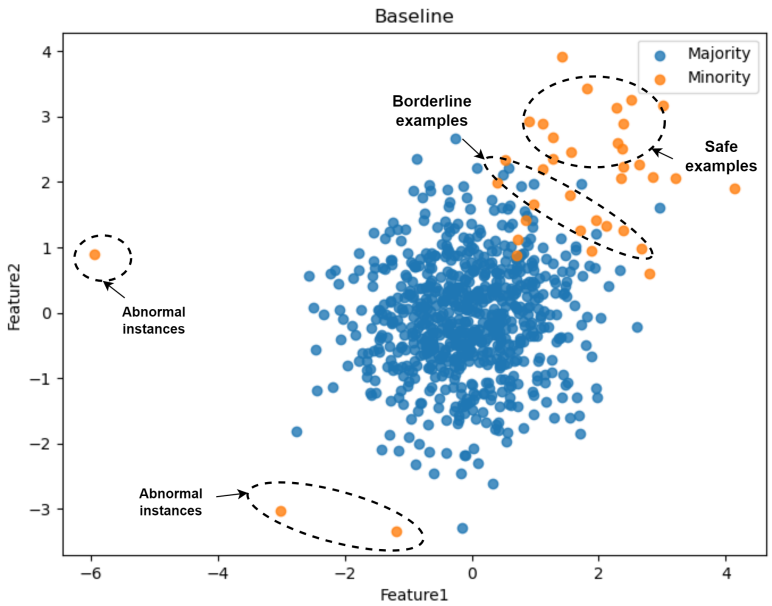

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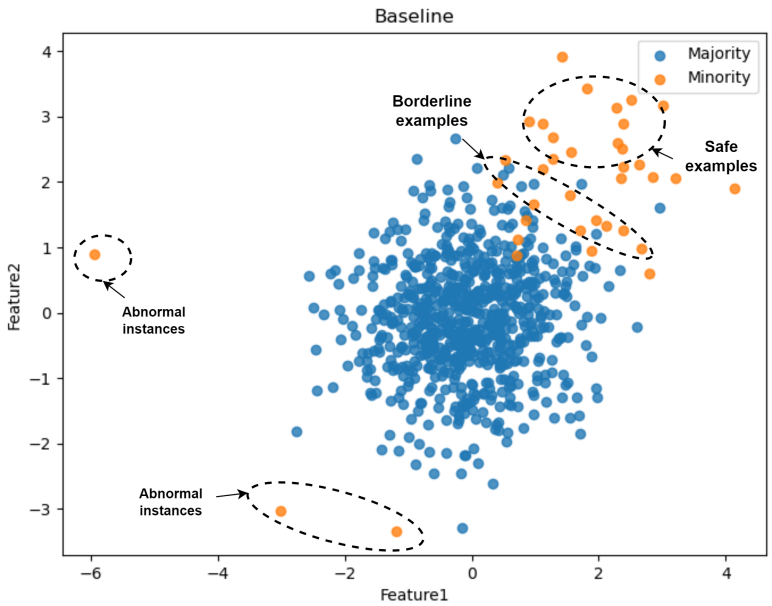

Figure: Class imbalance with outliers in minority class

Objectives

- Develop novel techniques for addressing class imbalance in classification tasks.
  - To investigate the impact of outliers within the minority class using popular existing methods.
  - To propose innovative strategies capable of mitigating the adverse effects of outliers on class imbalance data.
  - To further extend our approaches to address high-dimensionality issue.
  - To offer empirical evidence, supported by simulated and experimental results, that demonstrates the effectiveness of these proposed solutions in enhancing classification performance.

Thesis Contribution

- Challenges of Imbalanced Data: Identifying Long COVID Patients
  1. Discovering Long COVID Symptom Patterns: Association Rule Mining and Sentiment Analysis in Social Media Tweets (Published) [5]
  2. Long COVID Prediction in Manitoba Using Clinical Notes Data: A Machine Learning Approach (In Review) [6]
- Advancements for Imbalance Data Classification
  3. Enhancing SMOTE for Imbalanced Data with Abnormal Minority Instances Just Published!!! [9]
  4. Deep-ExtSMOTE: Integrating Autoencoders for Advanced Mitigation of Class Imbalance in High-Dimensional Data Classification (In Review) [4]

Third Manuscript

Enhancing SMOTE for Imbalanced Data with Abnormal Minority Instances [9]

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Enhancing SMOTE for imbalanced data with abnormal minority instances

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ABSTRACT

Imbalanced datasets are frequent in machine learning, where certain classes are markedly underrepresented compared to others. This imbalance often results in sub-optimal model performance, as classifiers tend to favour the majority class. A significant challenge arises when abnormal instances, such as outliers, exist within the minority class, diminishing the effectiveness of traditional re-sampling methods like the Synthetic Minority Over-sampling Technique (SMOTE). This manuscript addresses this critical issue by introducing four SMOTE extensions: Distance ExtSMOTE, Dirichlet ExtSMOTE, FCRP SMOTE, and BGMM SMOTE. These methods leverage a weighted average of neighbouring instances to enhance the quality of synthetic samples and mitigate the impact of outliers. Comprehensive experiments conducted on diverse simulated and real-world imbalanced datasets demonstrate that the proposed methods improve classification performance compared to the original SMOTE and its most competitive variants. Notably, we demonstrate that Dirichlet ExtSMOTE outperforms most other proposed and existing SMOTE variants in terms of achieving better F1 score, MCC, and PR-AUC. Our results underscore the effectiveness of these advanced SMOTE extensions in tackling class imbalance, particularly in the presence of abnormal instances, offering robust solutions for real-world applications.

Synthetic Minority Oversampling Technique (SMOTE)

- Resampling
- Balancing the Dataset:
  - Create new samples for the minority class.
- Technique:
  - Interpolate between randomly chosen minority class samples and their nearest neighbors.
  - $p_{new} = p_0 + \alpha(p_3 - p_0)$

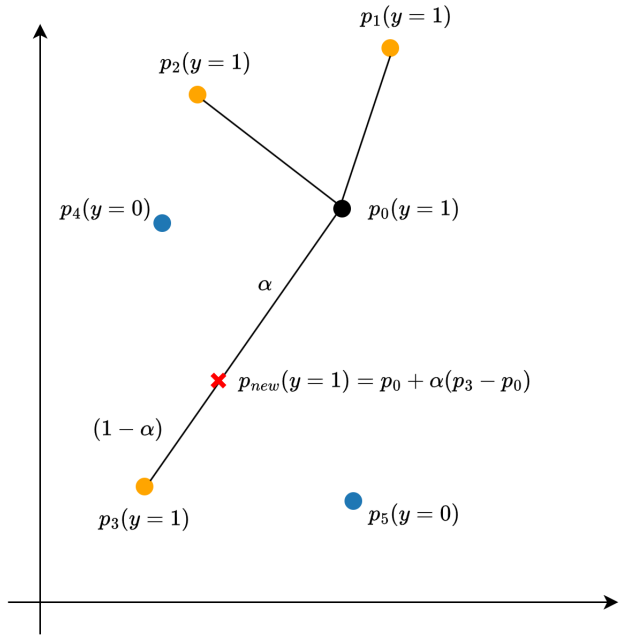

Figure: SMOTE data generation

Limitation with SMOTE

- Challenged by outliers within the minority class.

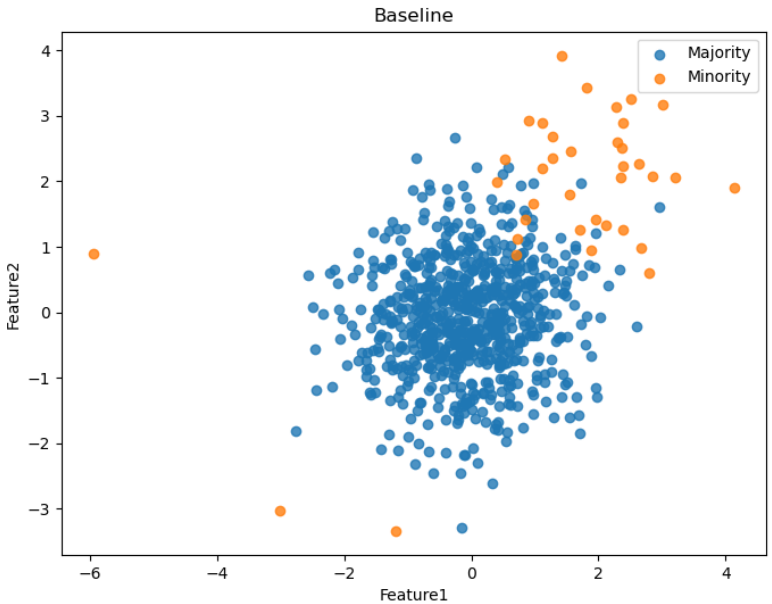

Figure: Original Data

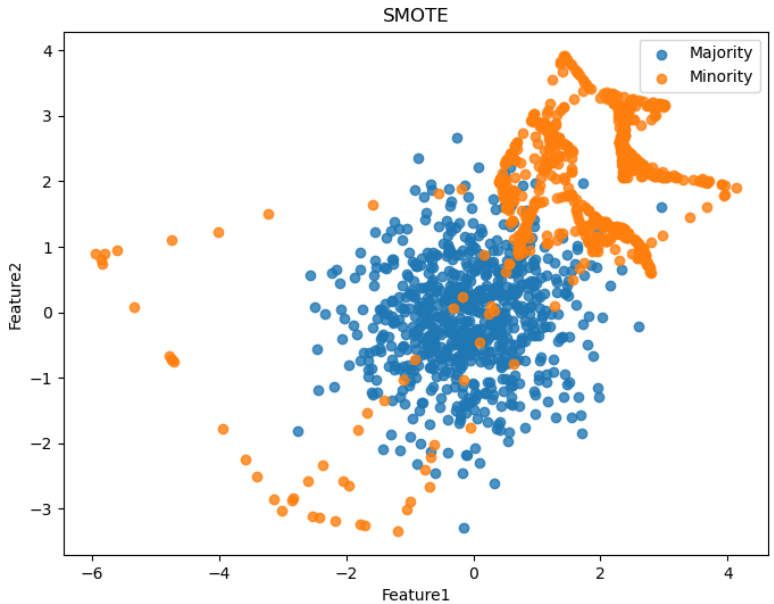

Figure: Re-sampled data with SMOTE

Proposed Solution

- Technique:
  - Use a weighted average of neighbouring instances.
  - $p_{new} = \frac{\sum_{j=1}^{k}(w_j \times p_j)}{\sum_{j=1}^{k} w_j}, j = 1, \ldots, k$
  - Improve robustness against outliers and noisy data.
  - Learn from a more extensive set of nearest neighbours.
- Challenge:
  - Selecting suitable weights to enhance resilience to outliers and noisy data.

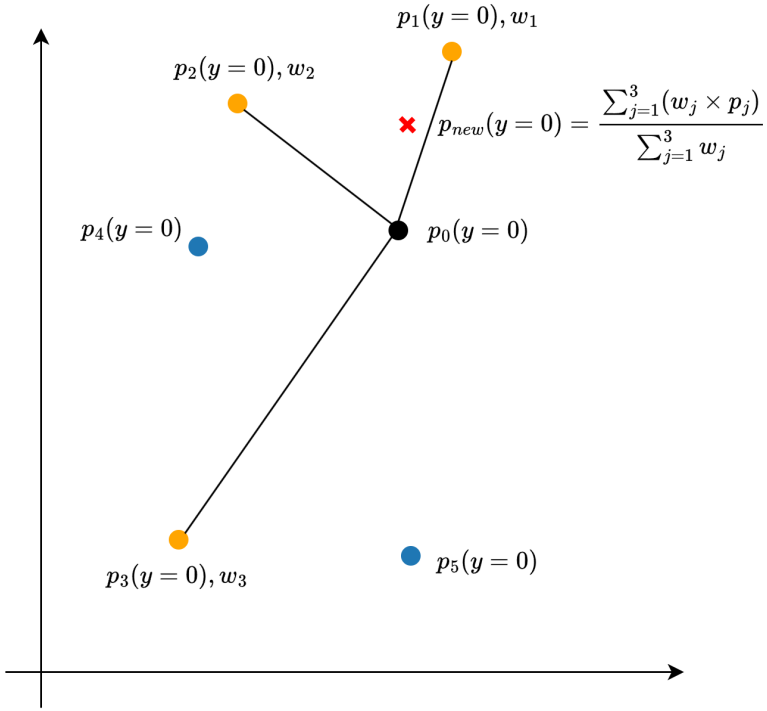

Figure: Proposed method data generation

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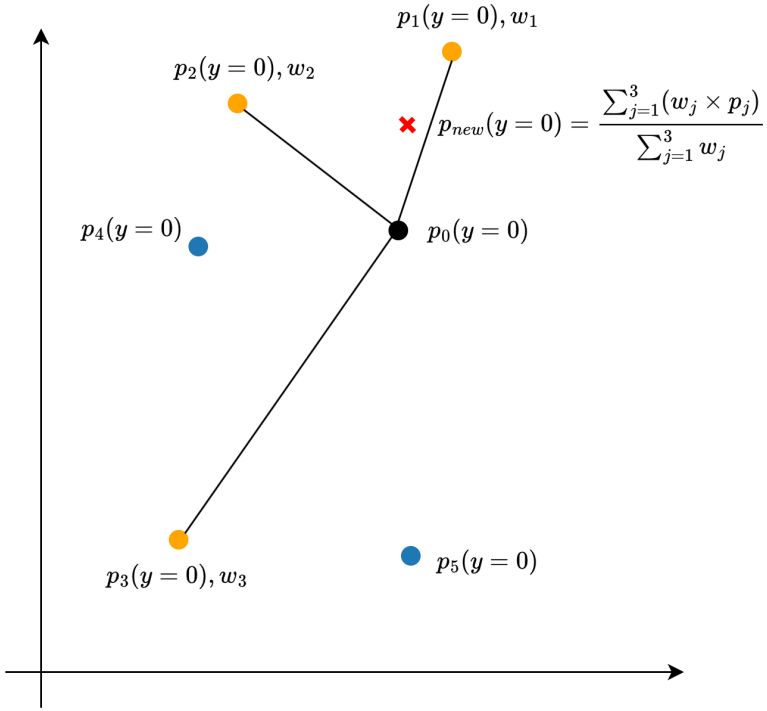

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How to Define Weights?

- Distance-based approach: Higher weights for closer instances in feature space.
- Use inverse distance to the median centroid of the minority class.
- Developing new SMOTE extensions:
  1. Distance extSMOTE
  2. Dirichlet extSMOTE [1]
  3. FCRP SMOTE - SMOTE with Chinese Restaurant Process Idea
  4. BGMM SMOTE - SMOTE with Bayesian Gaussian Mixture Model

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1. Distance extSMOTE

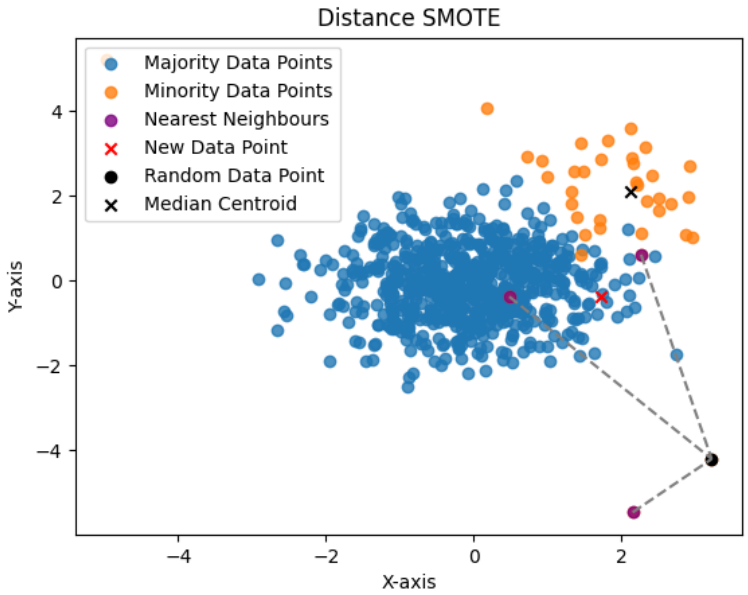
- $d_j \in \mathbb{R}$ is the Euclidean distance between the median centroid of the minority class and the nearest neighbours
- $w_j = d_{j,norm}^{-1} =$ Normalized inverse distance

Algorithm Distance ExtSMOTE

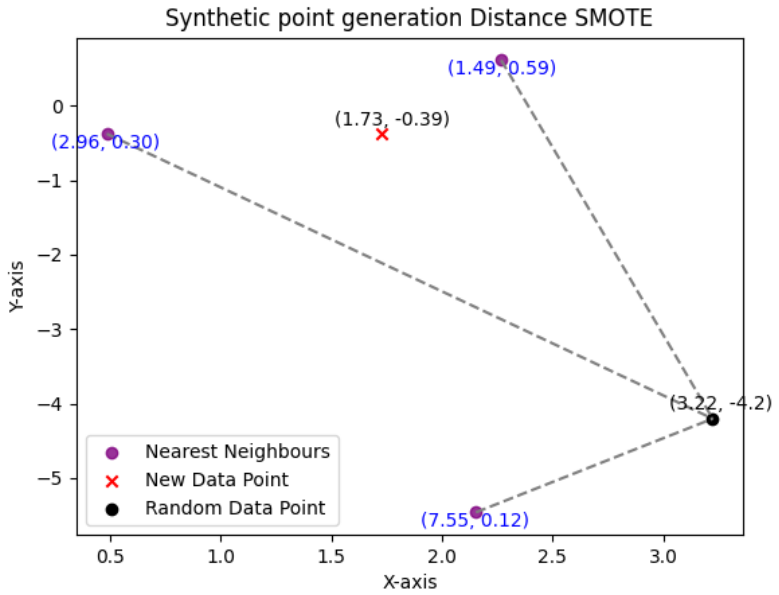
Require: $X \in \mathbb{R}^{n \times p}$ the features, $Y \in \{0,1\}^n$ the binary class label outputs.
Require: $k \in \mathbb{N}$ the number of neighbors to select for the k-Nearest Neighbors.
Ensure: Generated data $X_{new} \in \mathbb{R}^{q \times p}$ and $Y_{new} \in \{0,1\}^q$ with q points created.

1: Denote by S_1 the number of points labelled as the minority class and S_0 the number of points labelled as the majority class.
2: Initialize X_{new} and Y_{new} as empty vectors.
3: Obtain the median centroid (μ) of the minority class.
4: **while** $S_1 < S_0$ **do**
5: Filter $\mathcal{D} = \{X_i | Y_i = 1\}$, the set of points labeled as minority class 1.
6: Randomly choose $r \in \mathcal{D}$ and find the indices of its k nearest neighbors, $r_1, \ldots, r_k$.
7: Consider the inverse distances, from μ, to each nearest neighbour as weights, $w_j = d_j^{-1}$
8: $x^{new} \leftarrow \frac{\sum (w_j \times x_{r_j})}{\sum w_j}$ for all j from 1 to k.
9: $y^{new} \leftarrow 1$
10: $S_1 = S_1 + 1$
11: Append x^{new} to X_{new}, append y^{new} to Y_{new}
12: **end while**
13: return X_{new}, Y_{new}

1. Distance extSMOTE



(a) This scenario occurs when an outlier is chosen as a neighbouring point.



(b) The values within parentheses indicate (d_j, w_j).

Figure: An example of creating a sample - Distance extSMOTE

2. Dirichlet extSMOTE

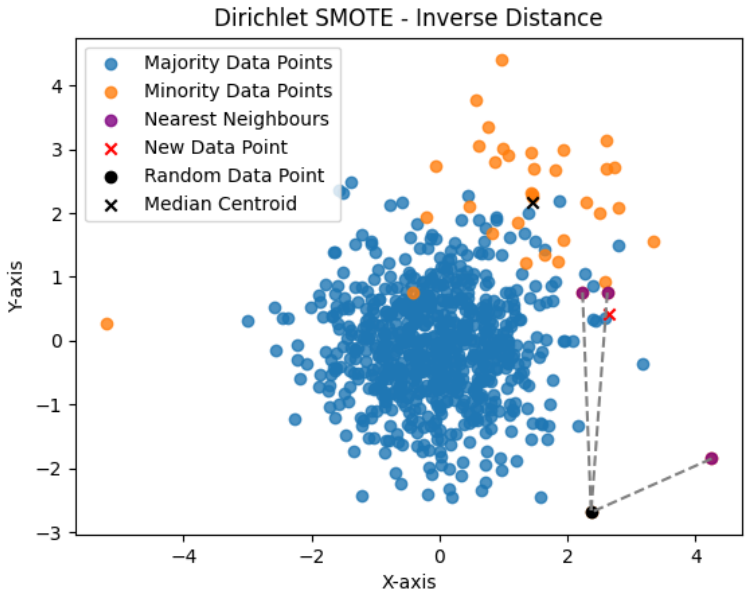
- The pdf of the Dirichlet distribution for a point $\boldsymbol{p}$ on the simplex:

$$w_j = P(\boldsymbol{p}|\alpha) \sim Dir(\alpha_1, \alpha_2, \ldots, \alpha_K) \stackrel{\text{def}}{=} \frac{\Gamma(\sum_j \alpha_j)}{\prod_j \Gamma(\alpha_j)} \prod_{j=1}^{K} p_j^{\alpha_j - 1} \quad (1)$$

Algorithm Dirichlet ExtSMOTE

if Type is 'Inverse distance (D)' **then**
  Calculate the distances, $\boldsymbol{D} = [d_1, \ldots, d_k]$ from μ to each nearest neighbour and obtain the reciprocal of each distance $\boldsymbol{D}^{-1} = [\frac{1}{d_1}, \ldots, \frac{1}{d_k}]$. Then $\boldsymbol{\alpha} = \boldsymbol{D}^{-1} \times m$
else if Type is 'Uniform Vector (UV)' **then**
  Generate a vector $\boldsymbol{\alpha} = \mathbf{1_k} \times m$, where $\mathbf{1_k} = [1, \ldots, 1]$
else if Type is 'Uniform Distribution (UD)' **then**
  Generate vector $\boldsymbol{U}$ of size k from $uniform(0, 1)$ distribution, then $\boldsymbol{\alpha} = \boldsymbol{U} \times m$.
end if
Use $\boldsymbol{\alpha}$ as parameters to the Dirichlet Distribution and generate random weights $w_j \sim Dir(\boldsymbol{\alpha})$
$x^{new} \leftarrow \sum w_j x_{r_j}$ for all j from 1 to k, as $\sum w_j = 1$
$y^{new} \leftarrow 1$
$S_1 = S_1 + 1$
Append x^{new} to X_{new}, append y^{new} to Y_{new}
return X_{new}, Y_{new}

2. Dirichlet extSMOTE (Inverse Distance)



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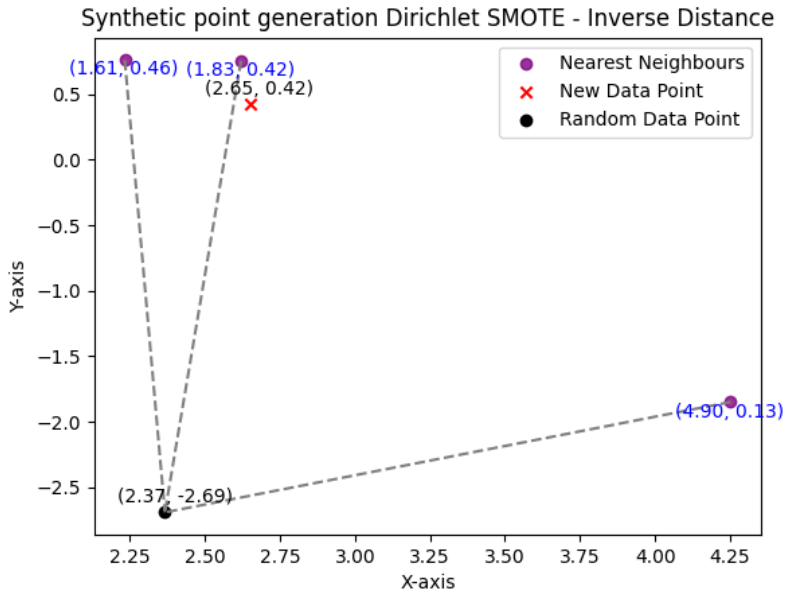

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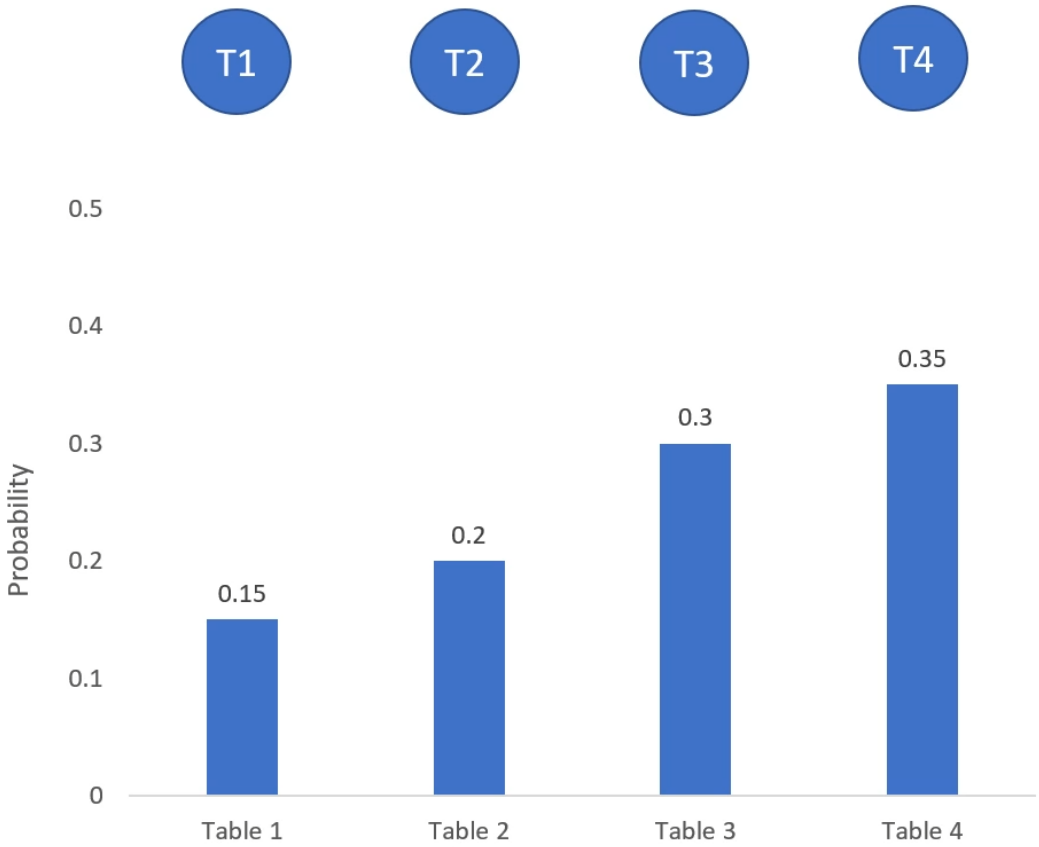
Figure: An example of creating a sample - Dirichlet extSMOTE

3. FCRP SMOTE



- Showcasing the weight selection of FCRP SMOTE using the Chinese restaurant process concept with finite number of tables with a parameter value $\alpha = 0.1$

3. FCRP SMOTE

Algorithm FCRP SMOTE

Require: $X \in \mathbb{R}^{n \times p}$ the features, $Y \in \{0,1\}^n$ the binary class label outputs.
Require: $k \in \mathbb{N}$ the number of neighbors to select for the k-Nearest Neighbors.
Require: $\alpha \in \mathbb{R}$, scalar parameter to update preferences.
Ensure: Generated data $X_{new} \in \mathbb{R}^{q \times p}$ and $Y_{new} \in \{0,1\}^q$ with q the number of points created.

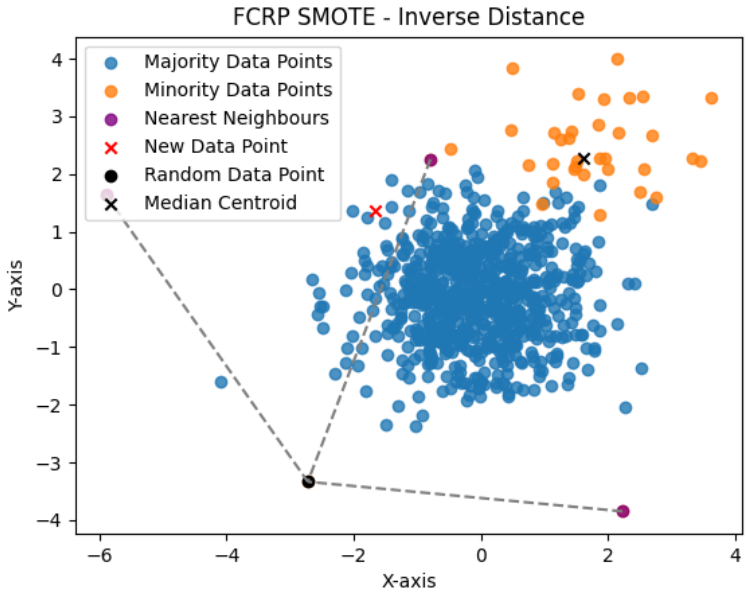
1: Denote by S_1 the number of points labelled as the minority class and S_0 the number of points labelled as the majority class.
2: Initialize X_{new} and Y_{new} as empty vectors.
3: Filter $\mathcal{D} = X_i | Y_i = 1$, the set of points labeled as minority class 1 and obtain the median centroid (c_m) of the minority cluster.
4: **while** $S1 < S_0$ **do**
5: Randomly choose $r \in \mathcal{D}$ and find the indices of its k nearest neighbors, $\{r_1, \ldots, r_k\}$.
6: Consider the normalized inverse distances, from c_m, to each nearest neighbour as initial preferences, $P = \boldsymbol{D}_{norm}^{-1}$ and choose first nearest neighbour with probability p_i, i from $1, \ldots, k$.
7: **for** N-1 **do**
8: Choose the next nearest neighbour with the following updated probabilities q_i,

$$q_i = \begin{cases} \frac{p_i + \alpha}{1+\alpha}, & \text{for previously chosen neighbour} \\ \frac{p_i}{1+\alpha}, & \text{for other neighbours} \end{cases}$$

9: $p_i = q_i$
10: **end for**
11: Obtain the final preferences for each nerighbour p_i as the weights w_j.
12: $x^{new} \leftarrow \sum (w_j \times x_{r_j})$ for all j from 1 to k and $y^{new} \leftarrow 1$
13: $S_1 = S_1 + 1$
14: Append x^{new} to X_{new}, append y^{new} to Y_{new}
15: **end while**
16: return X_{new}, Y_{new}

3. FCRP SMOTE

- Initial preferences $= d_{norm}^{-1}$
- $w_j =$ Final allocation probabilities



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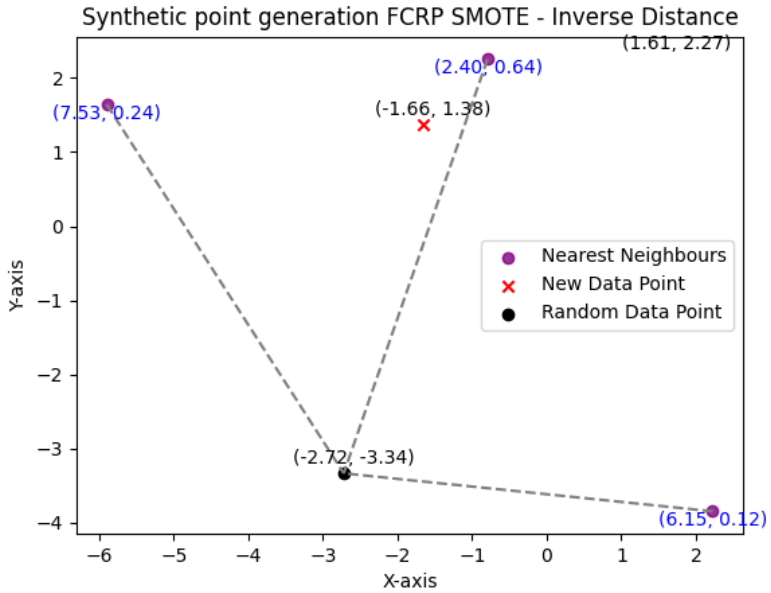


(b) The values within parentheses indicate (d_j, w_j).

Figure: An example of creating a sample - FCRP SMOTE

4. BGMM SMOTE

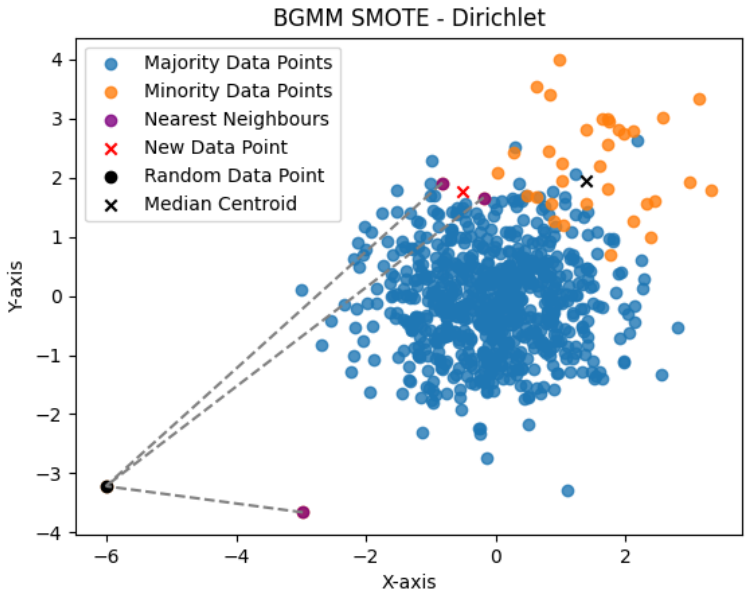
Bayesian Gaussian Mixture Models (BGMM)

- A probabilistic model used for clustering
- Cluster Assignment

1. Expectation Maximization:
   - Expectation (E-step): For each data point, the model calculates the probability of the point belonging to each cluster
   - Maximization (M-step): Update the parameters of the model by maximizing the expected log-likelihood
2. Cluster Assignment: Probabilistically assigns data points to clusters based on the calculated probabilities.
3. Soft Assignments: This does not definitively allocate a point to a single cluster.

4. BGMM SMOTE

- c_j = Cluster assignment of the j^{th} nearest neighbour
- w_j = Normalized cluster probability of the cluster which the median centroid belongs



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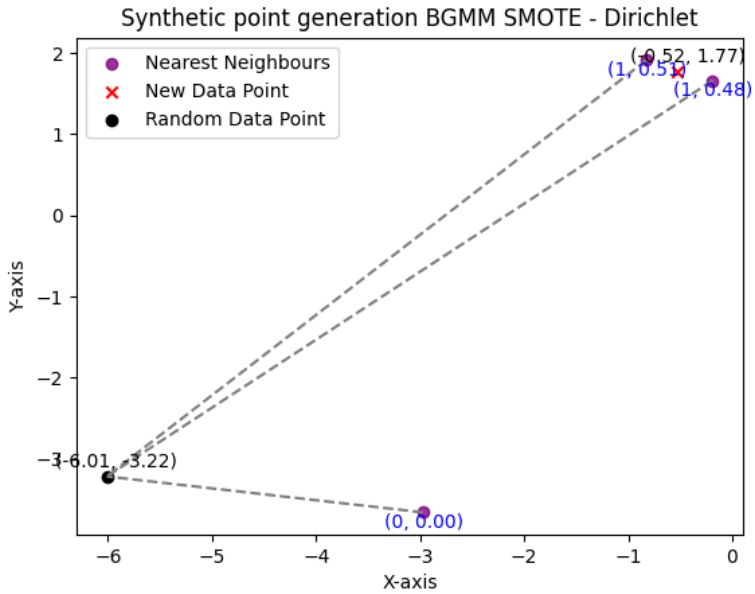


(b) The values within parentheses indicate (c_j, w_j).

Figure: An example of creating a sample - BGMM SMOTE (D)

Synthetic Data Generation

- $\boldsymbol{X}_{minority-outliers} \sim \mathcal{N}_{2\times 2}(\boldsymbol{\mu}_{2\times 1}^{(1)}, \boldsymbol{\Sigma}_{2\times 2}^{(1)})$
- $\boldsymbol{X}_{majority} \sim \mathcal{N}_{2\times 2}(\boldsymbol{\mu}_{2\times 1}^{(2)}, \boldsymbol{\Sigma}_{2\times 2}^{(2)})$
- $\boldsymbol{X}_{outliers} \sim \text{Uniform}([-10, 10]^2)$

$$\boldsymbol{\mu}_{2\times 1}^{(1)} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}_{2\times 1}, \boldsymbol{\Sigma}_{2\times 2}^{(1)} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}_{2\times 2}$$

$$\boldsymbol{\mu}_{2\times 1}^{(2)} = \begin{bmatrix} 3 \\ 4 \end{bmatrix}_{2\times 1}, \boldsymbol{\Sigma}_{2\times 2}^{(2)} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}_{2\times 2}$$

Synthetic Data Generation

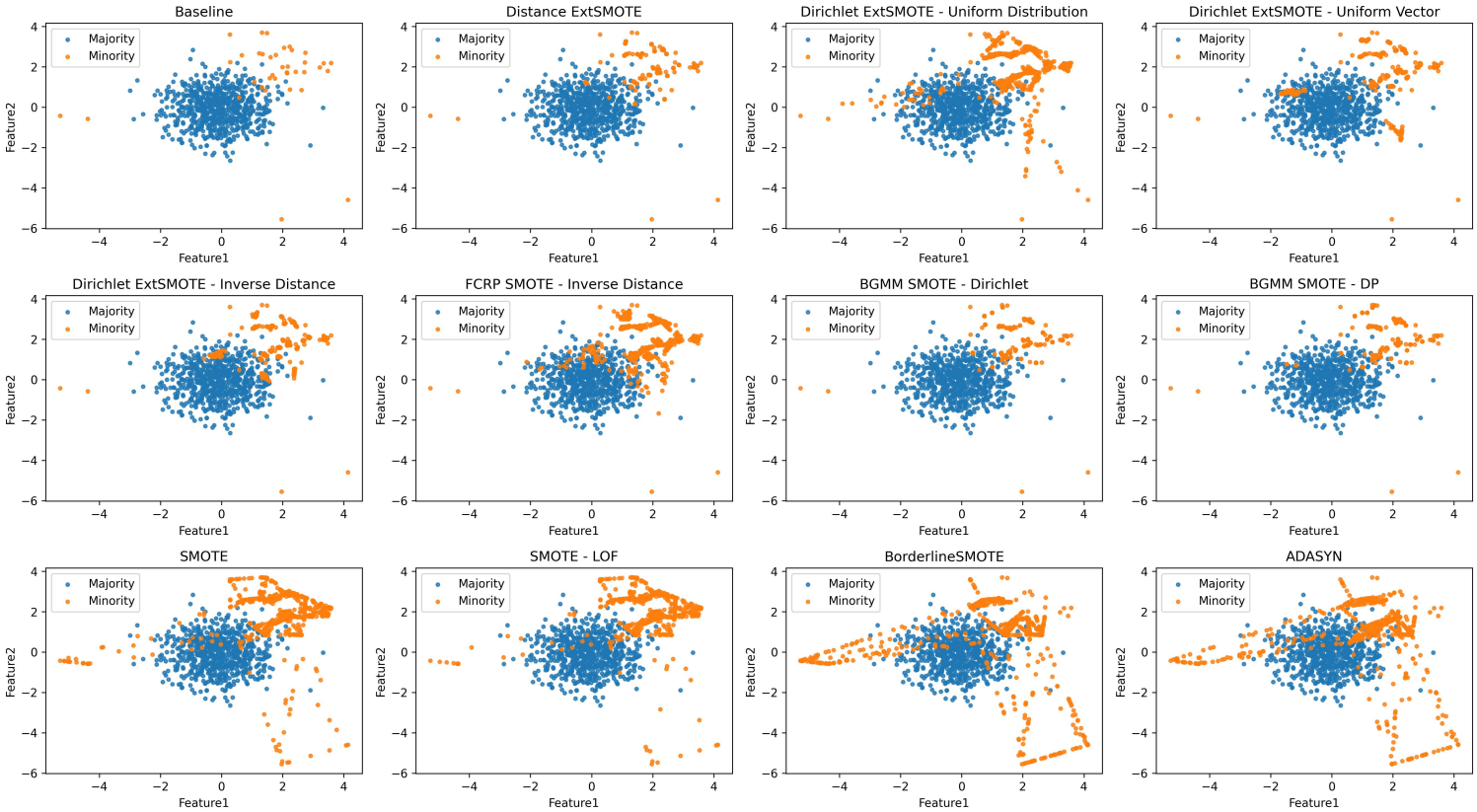
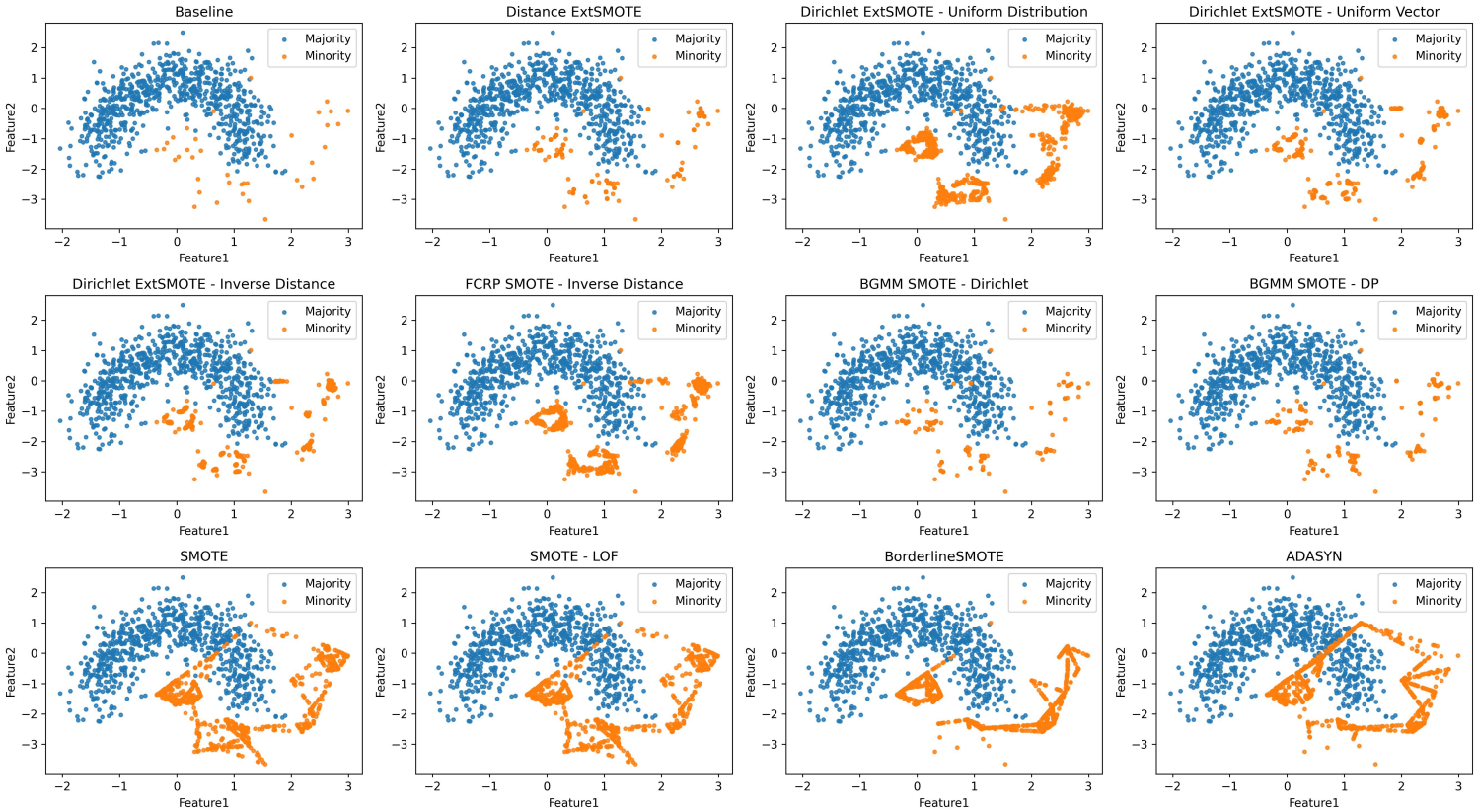


Figure: Comparison of resampled data

Simulation Results (Noisy Moons)



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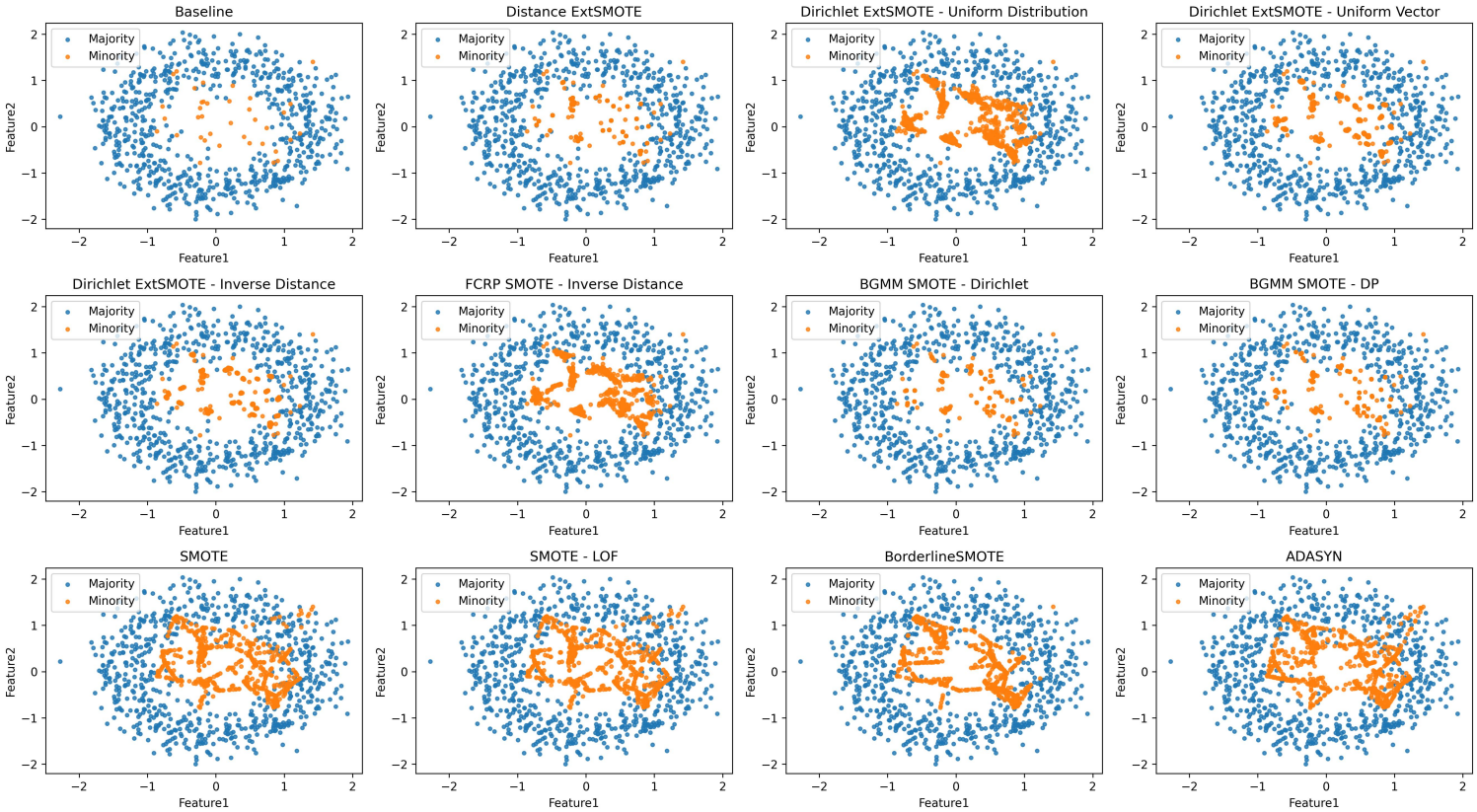
Simulation Results (Noisy Circles)



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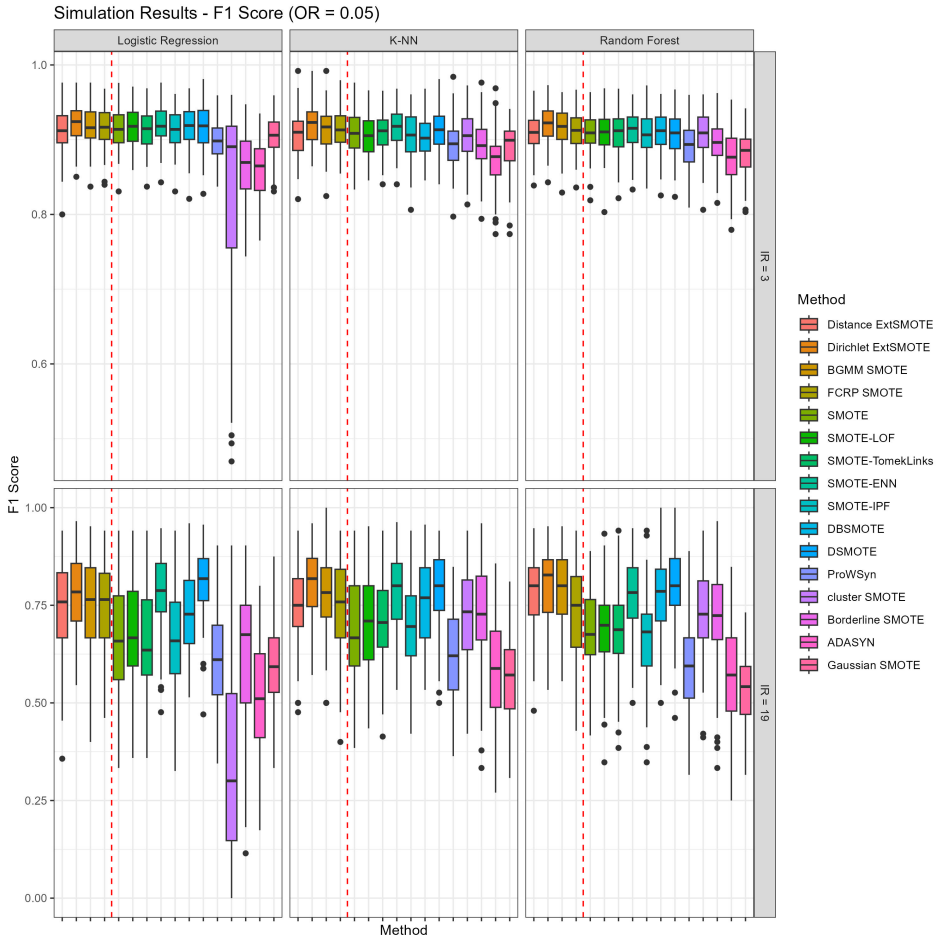

Figure: F1 Scores for 100 simulated datasets with 5-fold cross validation

Application Data

Table: Characteristics of the binary class datasets used in the computational study.

No	Dataset	Instances	Features	Minority class	Majority class	%Minority	%Majority	IR	Presence of LOF Outliers
1	yeast6	1484	8	EXC	Remaining classes	2.36	97.64	41.40	Yes
2	yeast5	1484	8	EXC, ERL	Remaining classes	2.70	97.30	36.10	Yes
3	yeast-1289vs7	947	8	VAC	NUC, CYT, ERL, POX	3.17	96.83	30.57	Yes
4	yeast4	1484	8	ME2	Remaining classes	3.44	96.56	28.10	Yes
5	yeast-2vs8	483	8	POX	CYT	4.14	95.86	23.15	Yes
6	glass12357vs6	214	9	6	Remaining classes	4.21	95.79	22.78	Yes
7	yeast-1458vs7	693	8	VAC	NUC, ME3, ME2, POX	4.33	95.67	22.10	Yes
8	oil	937	49	minority	majority	4.38	95.62	21.85	No
9	abalone9_18	731	7	9, 18	Remaining classes	5.75	94.25	16.40	Yes
10	glass12367vs5	214	9	5	Remaining classes	6.07	93.93	15.46	Yes
11	thyroid_sick	3772	52	sick	healthy	6.12	93.88	15.33	Yes
12	yeast-1vs7	459	8	VAC	NUC	6.54	93.46	14.30	Yes
13	us_crime	1994	100	>0.65	<=0.65	7.52	92.48	12.29	Yes
14	glass12vs5	159	9	5	1, 2	8.18	91.82	11.23	Yes
15	spectrometer	531	93	>=44	<44	8.47	91.53	10.80	Yes
16	landsat_satellite	6435	36	2	Remaining classes	9.73	90.27	9.28	Yes
17	mfeatmor0	2000	6	0, 1	Remaining classes	10.00	90.00	9.00	Yes
18	yeast3	1484	8	ME3	Remaining classes	10.98	89.02	8.10	Yes
19	mfeatmor01	2000	6	0	Remaining classes	20.00	80.00	4.00	Yes
20	glass123vs567	214	9	5, 6, 7	Remaining classes	23.83	76.17	3.20	Yes
21	parkinsons	195	22	1	0	24.62	75.38	3.06	Yes
22	habermans_survival	306	3	2	1	26.47	73.53	2.78	Yes
23	glass23567vs1	214	9	1	Remaining classes	32.71	67.29	2.06	Yes
24	breast_cancer	569	30	M	B	37.26	62.74	1.68	Yes
25	banknote	1372	4	1	Remaining classes	44.46	55.54	1.25	Yes

Application Results

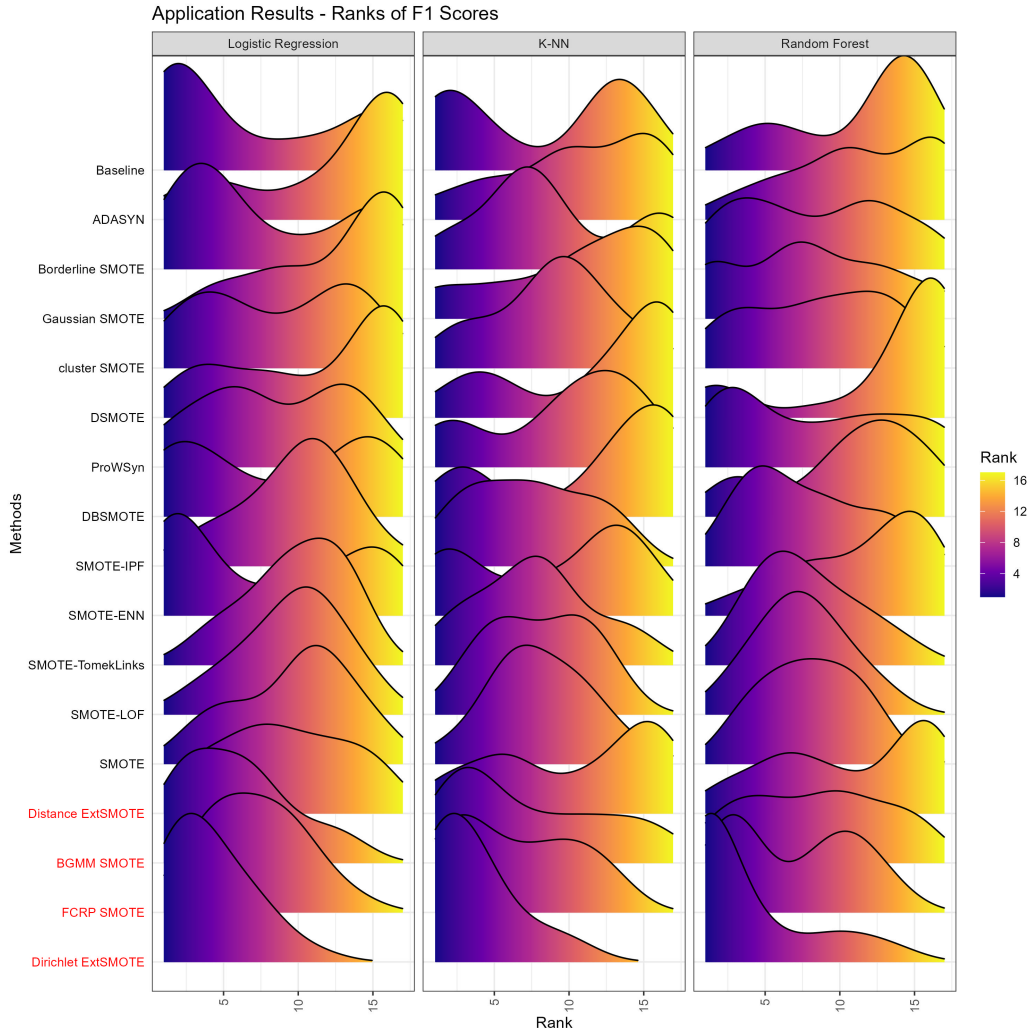

Figure: F1 Score Ranks for the datasets with 100 $\times$ 5-fold cross validation

Fourth Manuscript

Deep-ExtSMOTE: Integrating Autoencoders for Advanced Mitigation of Class Imbalance in High-Dimensional Data Classification [4]

High-Dimensional Data

- Curse of Dimensionality
  - A large number of features relative to the available data, “large p, small n” problem [3].
  - Challenges:
    - Data Sparsity
    - Increased Model Complexity and Overfitting
    - Computational Challenges
- Feature Reduction
  - A critical strategy to address the challenges of high dimensionality in class imbalance [2, 7, 8].

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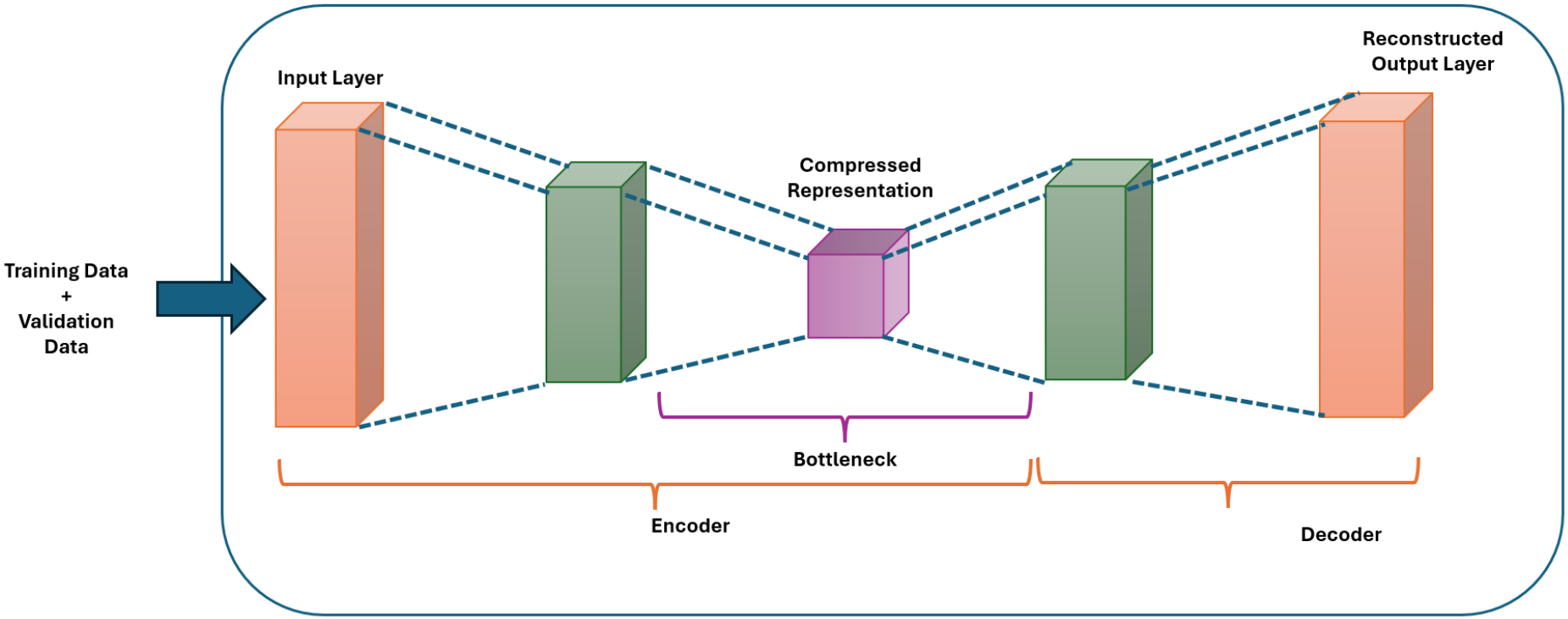
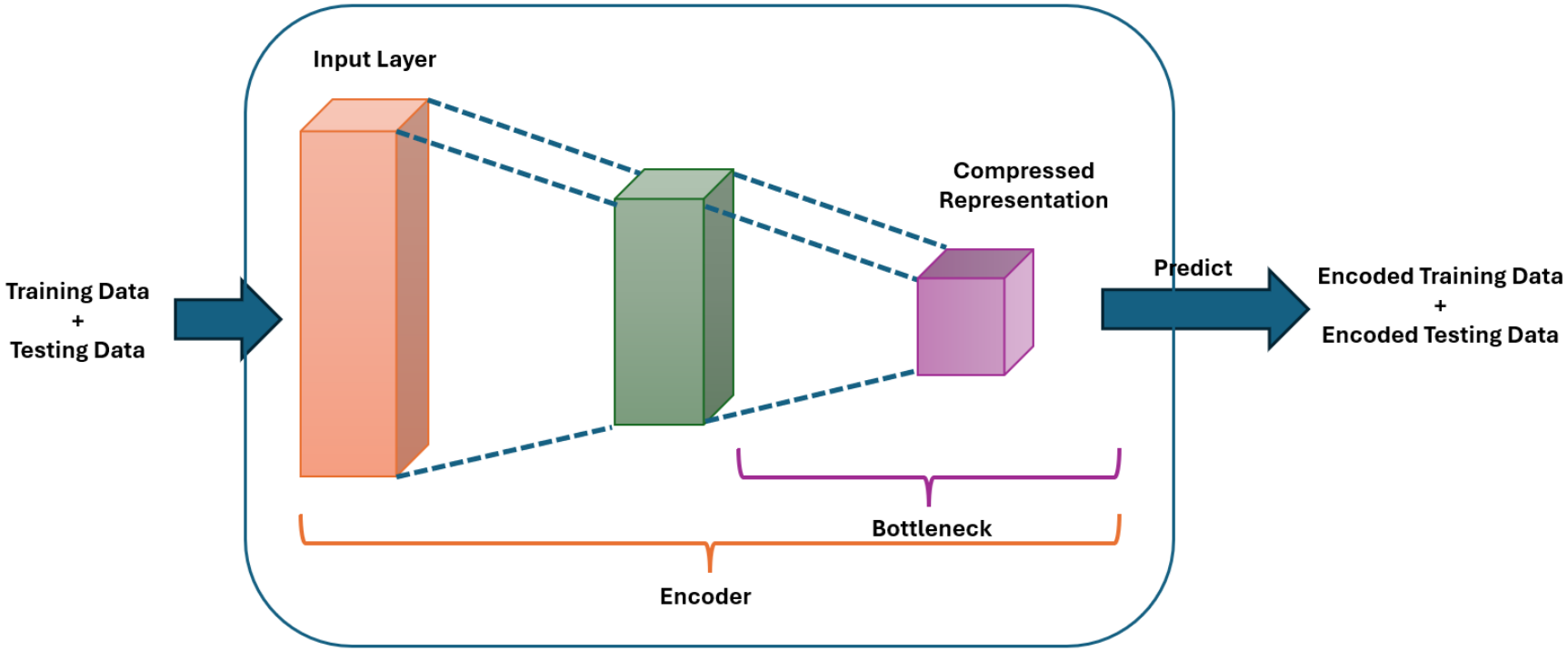
5. Deep-ExtSMOTE

- Autoencoder + Dirichlet ExtSMOTE
- Step 1: Train the Autoencoder



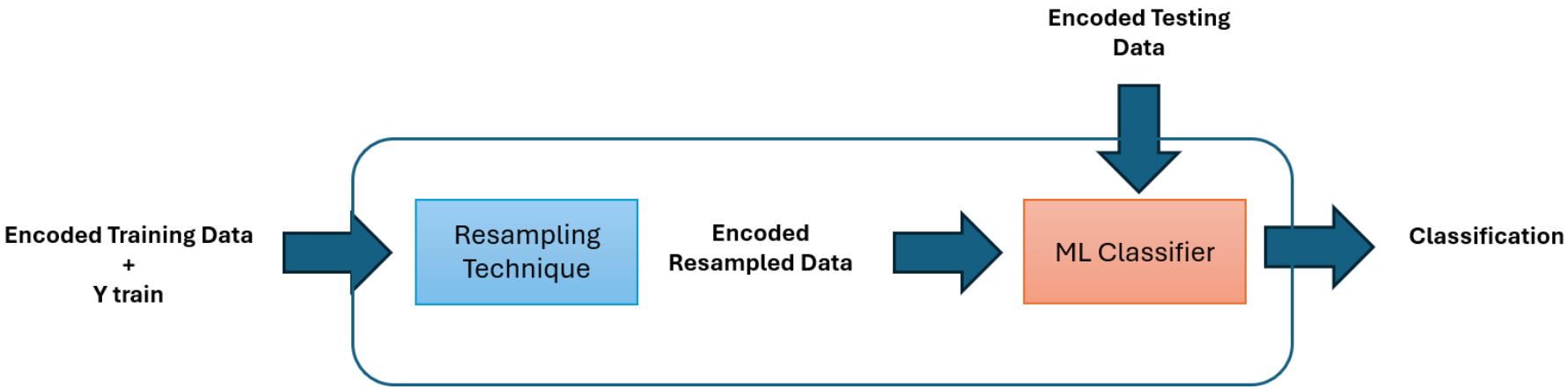
5. Deep-ExtSMOTE

- Step 2: Extract Encoded Representation



5. Deep-ExtSMOTE

- Step 3: Resampling and Classification



Simulation Results

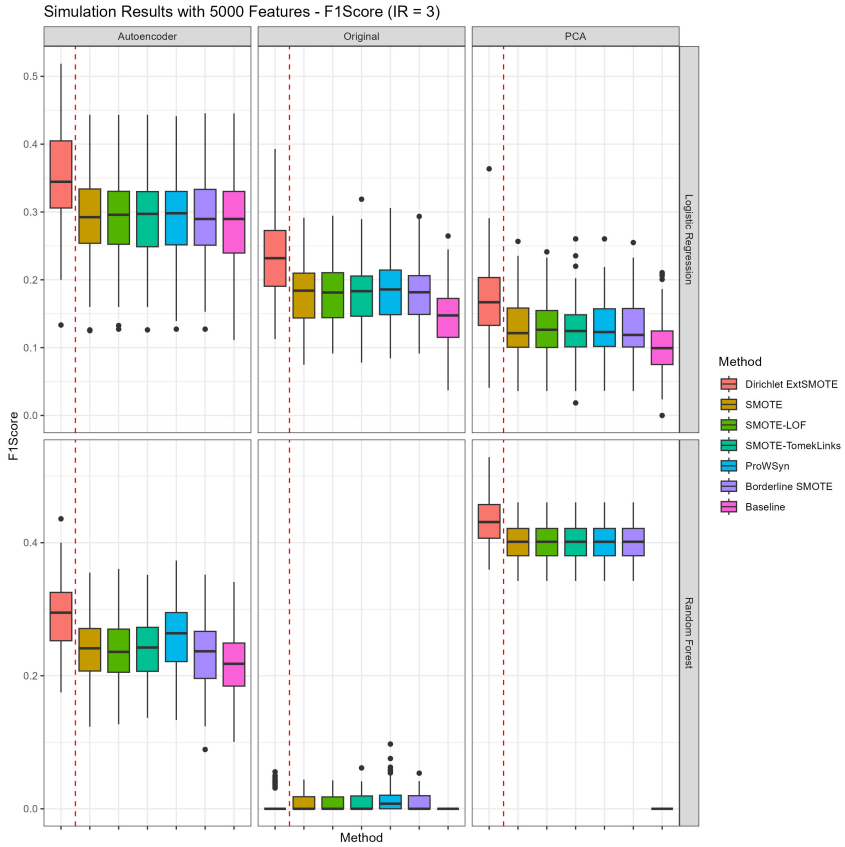


Figure: F1-Score distribution for 100 trials using simulated datasets with 1000 samples and 5000 features (2000 informative), with an imbalance ratio (IR) of 3.

Application Results

- Application 1: Isolet (Continuous Binary Classification)
  - Dataset includes 617 continuous features, representing processed characteristics of the audio signals.
  - Scenario 1: Original Isolet Dataset
    - Dataset includes 7797 samples, resulting in a feature-to-sample ratio of approximately 0.0791.
  - Scenario 2: Reduced Isolet Dataset
    - Selected a subset of 1000 samples from the original 7797 samples. This adjustment resulted in a feature-to-sample ratio of 0.617.

Application Results

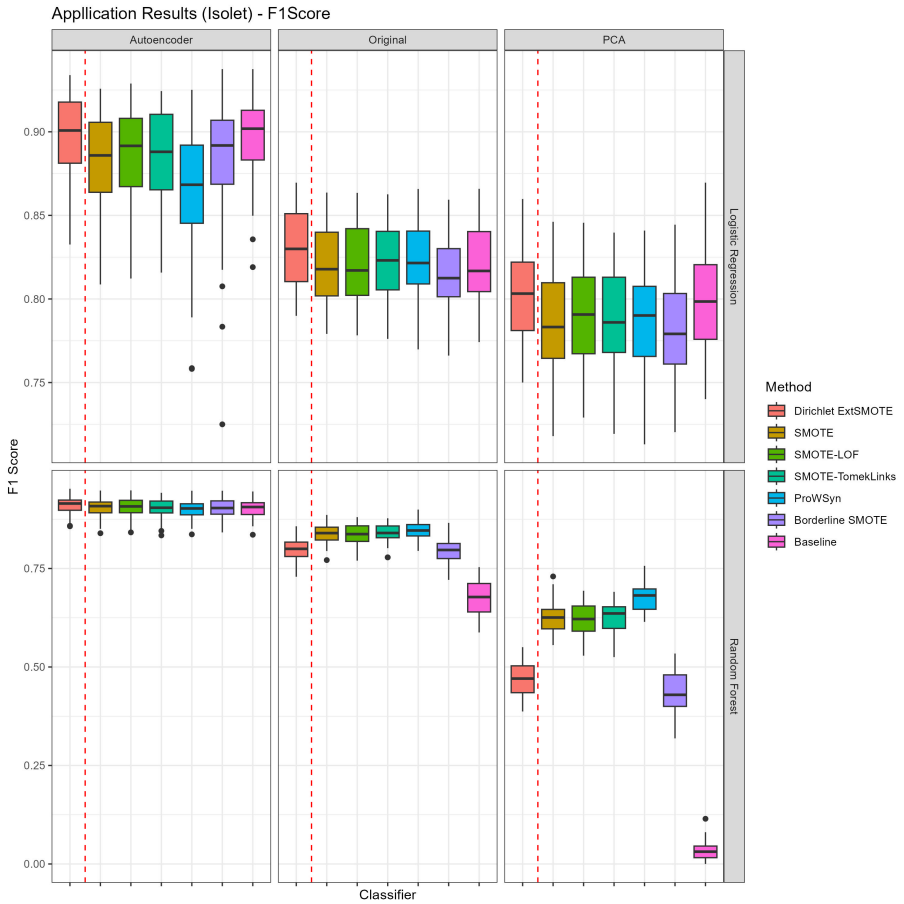


Figure: F1 Scores for the Isolet dataset across 50 training and test splits.

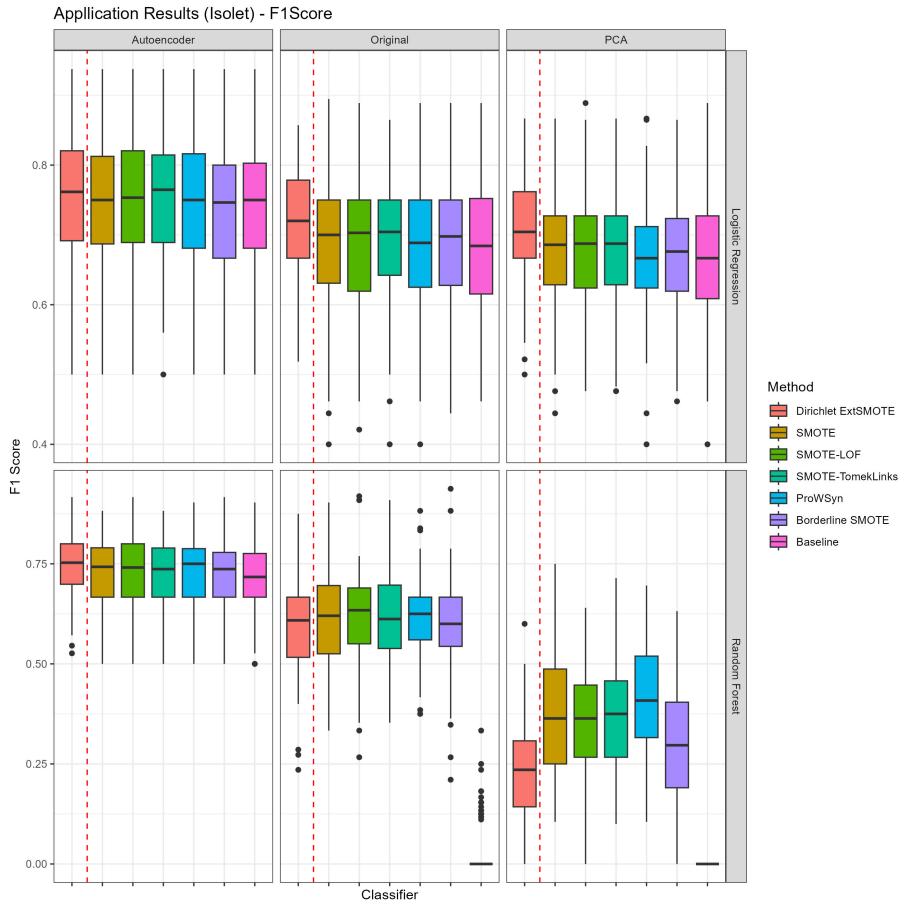


Figure: F1 Scores for the reduced Isolet dataset across 50 training and test splits.

Application Results

- Application 2: Chile (Categorical Binary Classification)
  - Predict the yield of 204 Chile pepper genotypes from multi-environment trials in New Mexico, USA.
  - Conduct experiment by starting with 2,500 features and increasing the number of features to 7,500.
  - Feature-to-sample ratio ranging from approximately 12.25 to 37.7.

Application Results

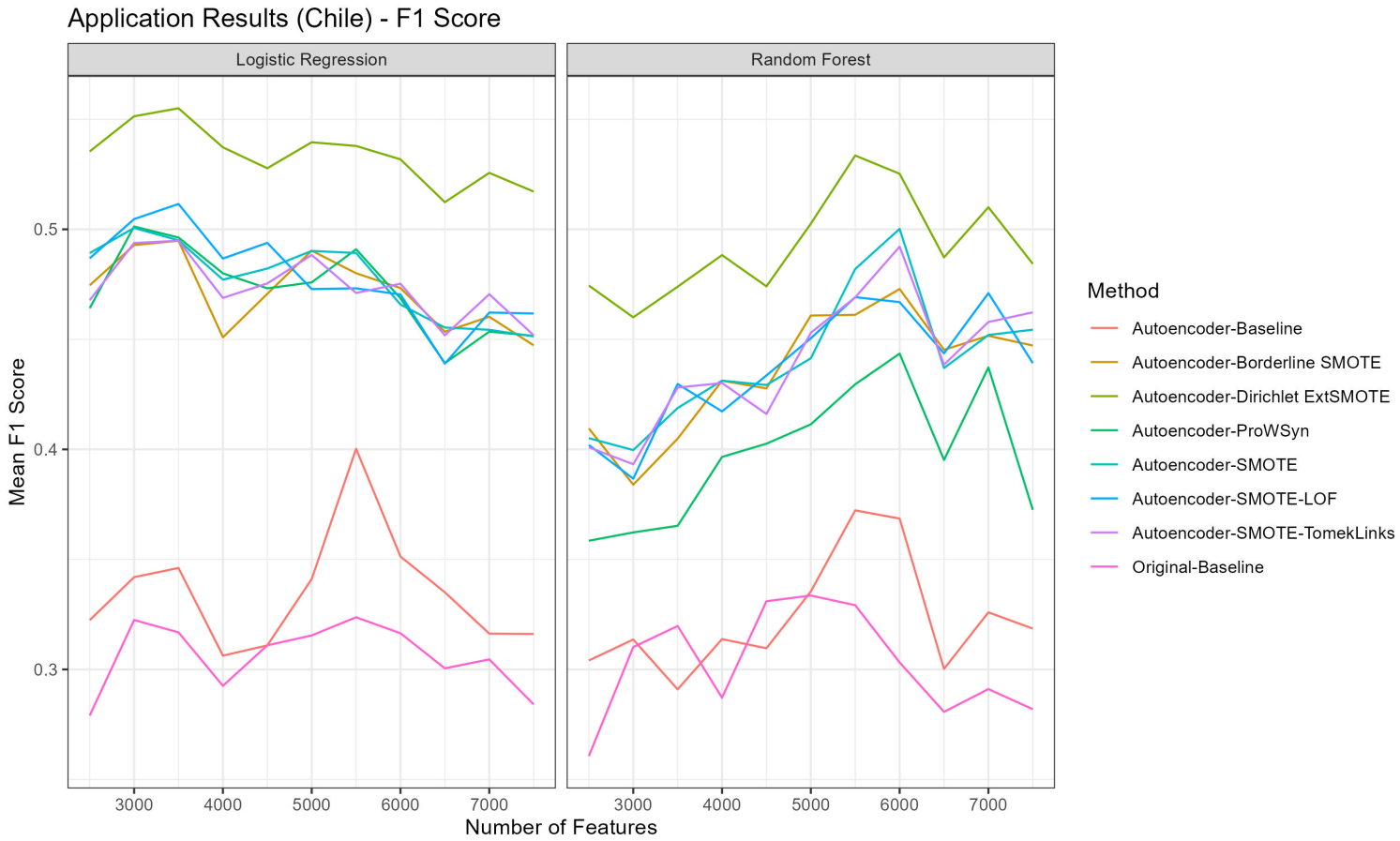


Figure: F1 score comparison with varying feature numbers.

Application Results

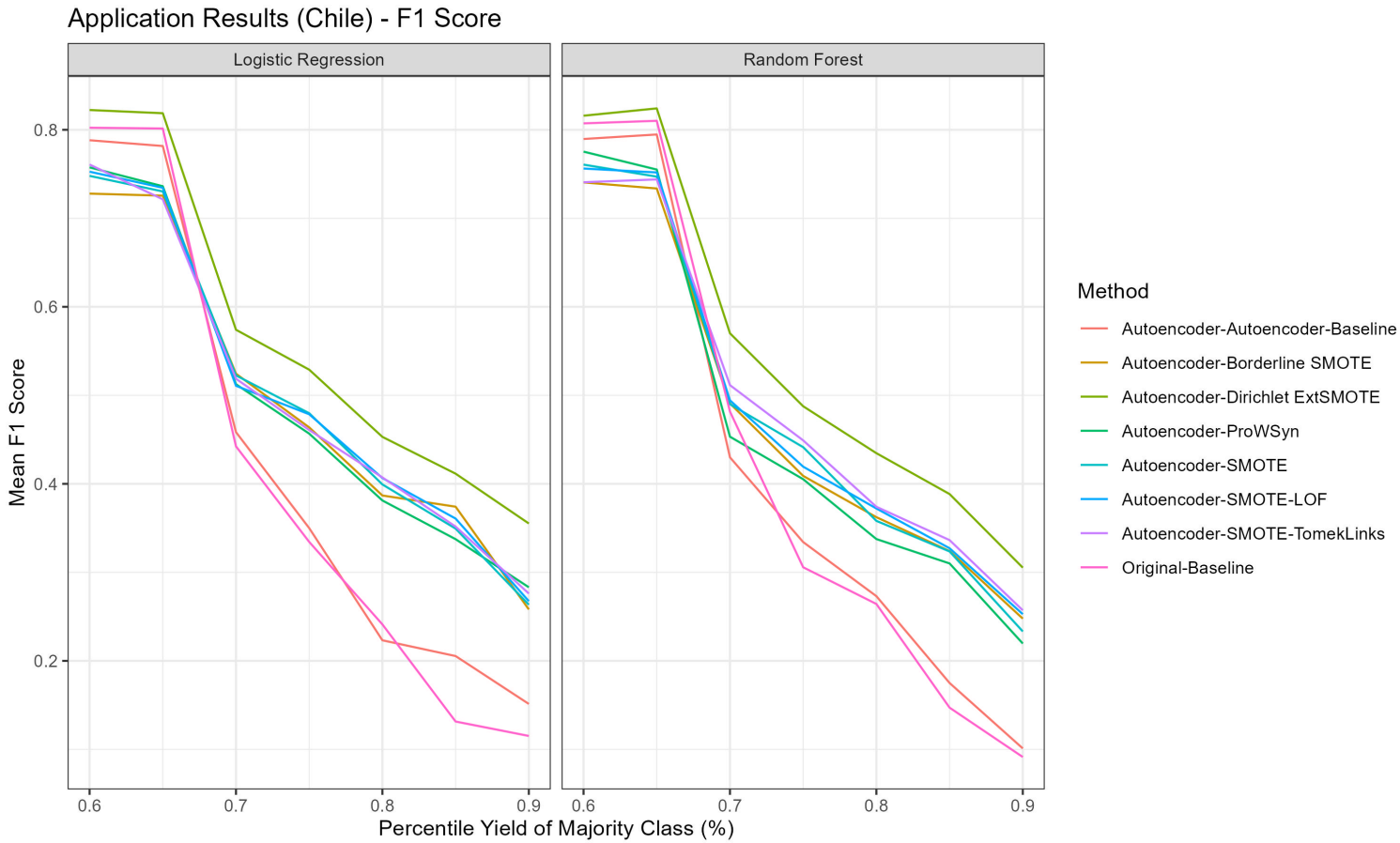


Figure: F1 score comparison with varying imbalance ratios.

Conclusion

- Class imbalance is a significant problem in classification.
- Novel methods advancing imbalanced classification within machine learning.
- Effectively incorporate measures to minimize outlier effects and curse of dimensionality.
- Create more **accurate and reliable predictive models.**
- Across diverse domains, including fraud detection, medical diagnosis, and churn prediction.
- All the computing were done using Python on Digital Research Alliance of Canada computing cluster.

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Thank You!

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Appendices

Manuscript 1: Discovering LCS Symptoms Patterns

Long COVID Syndrome (LCS)

- A condition in which individuals experience symptoms for weeks or months after recovering from COVID-19.
- Identifying the symptoms and medical conditions related to long COVID.
- Determining the patterns of symptoms and their associations.

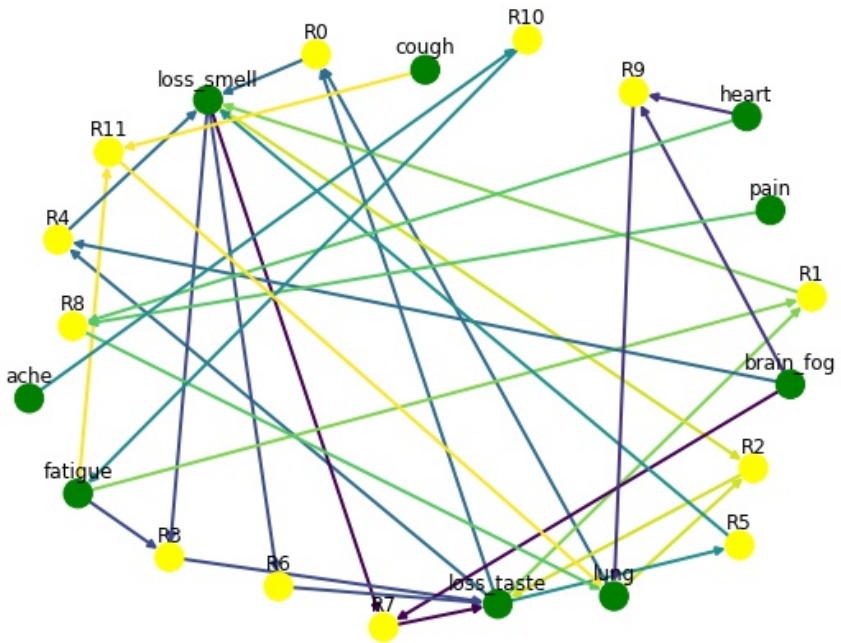


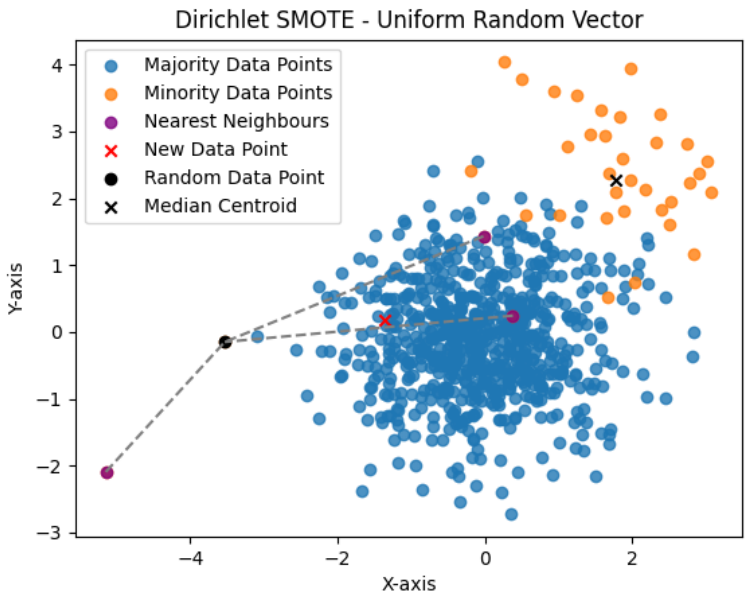
Figure: Association rules visualization. R: rule.

Manuscript 2: Predicting LCS patients in Manitoba

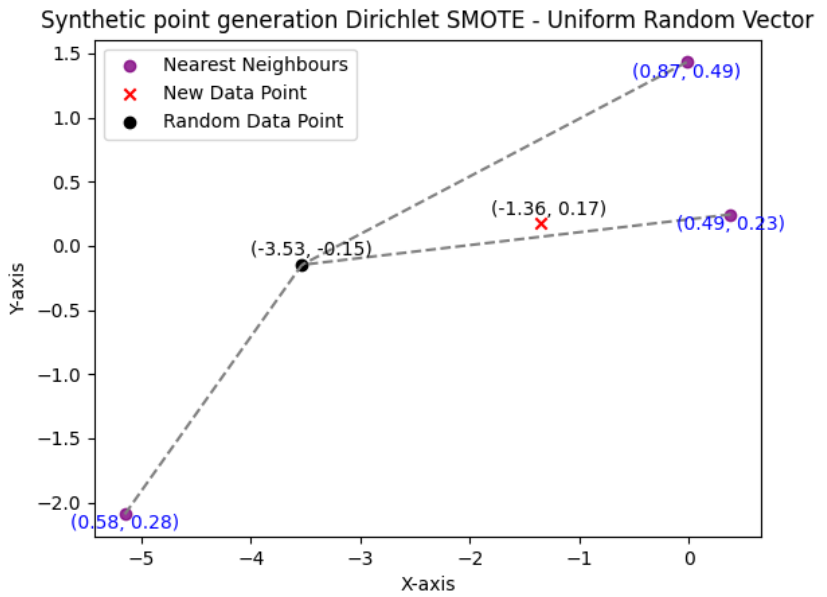
- Challenges in Predicting LCS Patients at Risk
  - The absence of a definitive diagnostic test for Long COVID Syndrome
- Identifying ‘known LCS’ group for classification
  - Use Natural Language Processing (NLP) methodologies.
  - Conduct word extraction processes.
  - Perform manual refinement techniques.
- Class imbalance issue (Ratio: 0.96:0.04)
  - Used rebalancing techniques
  - Random Over-Sampling and Random Under-Sampling
- Identified LCS group in Risk: 1124 (24.7%) LCS patients from the set of 4556 COVID-19 cases

Dirichlet extSMOTE (Uniform Random Vector)

- $w_j = Dir(\boldsymbol{\alpha})_j, \boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_k]$
- $\boldsymbol{\alpha} = m.\boldsymbol{u}, \boldsymbol{u} \sim Unif(0, 1)$
- $m \in \mathbb{N}$, is the multiplier for the concentration parameter.



(a) This scenario occurs when an outlier is chosen as a neighbouring point.

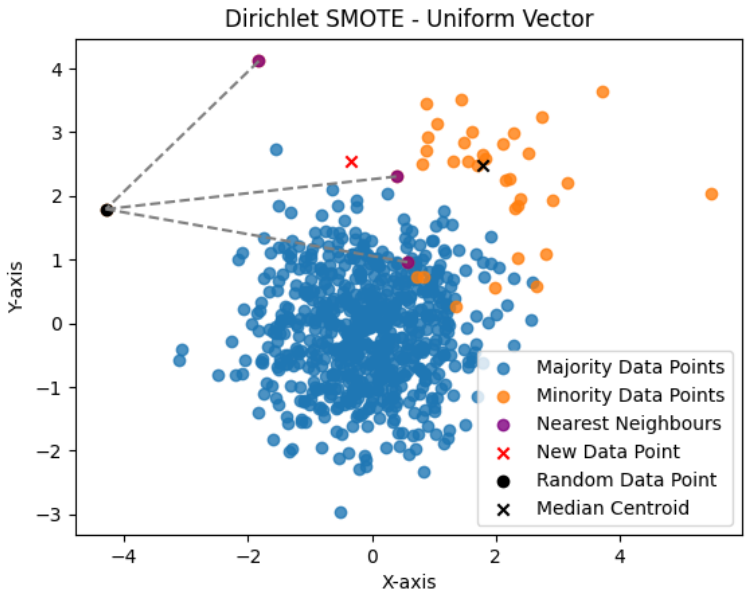


(b) The values within parentheses indicate (u_j, w_j).

Figure: An example of creating a sample - Dirichlet extSMOTE (Uniform Random Vector)

Dirichlet extSMOTE (Uniform Vector)

- $w_j = Dir(\alpha)_j$
- $\alpha = m.\mathbf{1_k}, \mathbf{1_k} = [1, \ldots, 1]$



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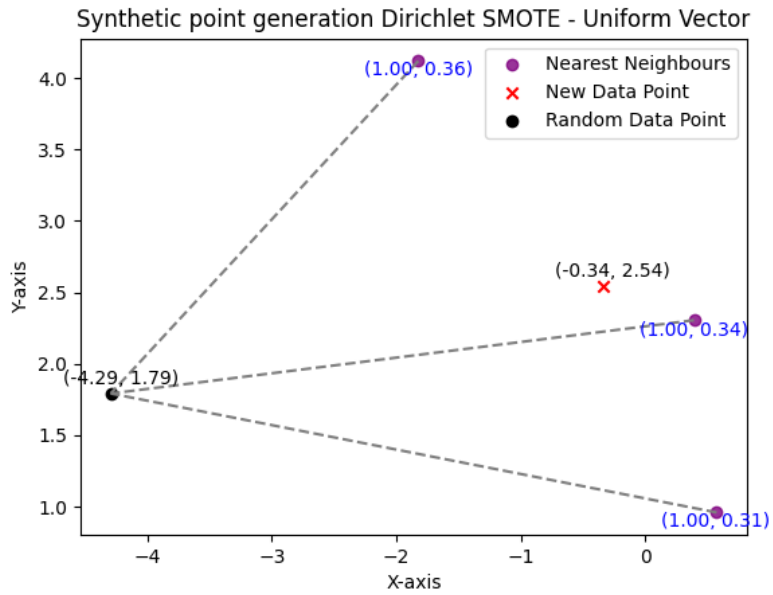

(b) The values within parentheses indicate $(1, w_j)$.

Figure: An example of creating a sample - Dirichlet extSMOTE

Simulation Results (Without Outliers)

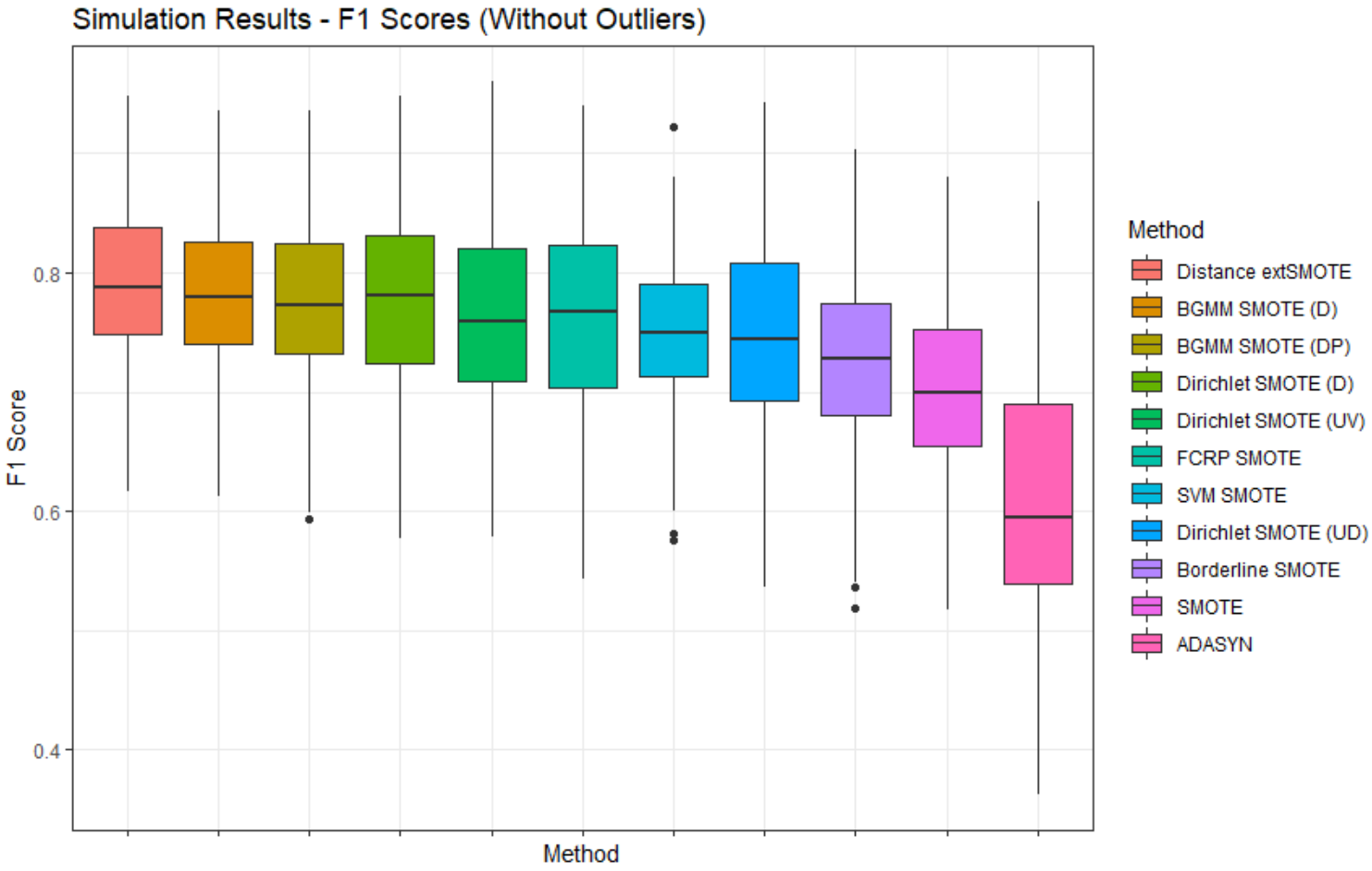

Figure: F1 Scores for 80 outlier free simulated datasets with 5-fold cross validation

Simulation Results (Without Outliers)

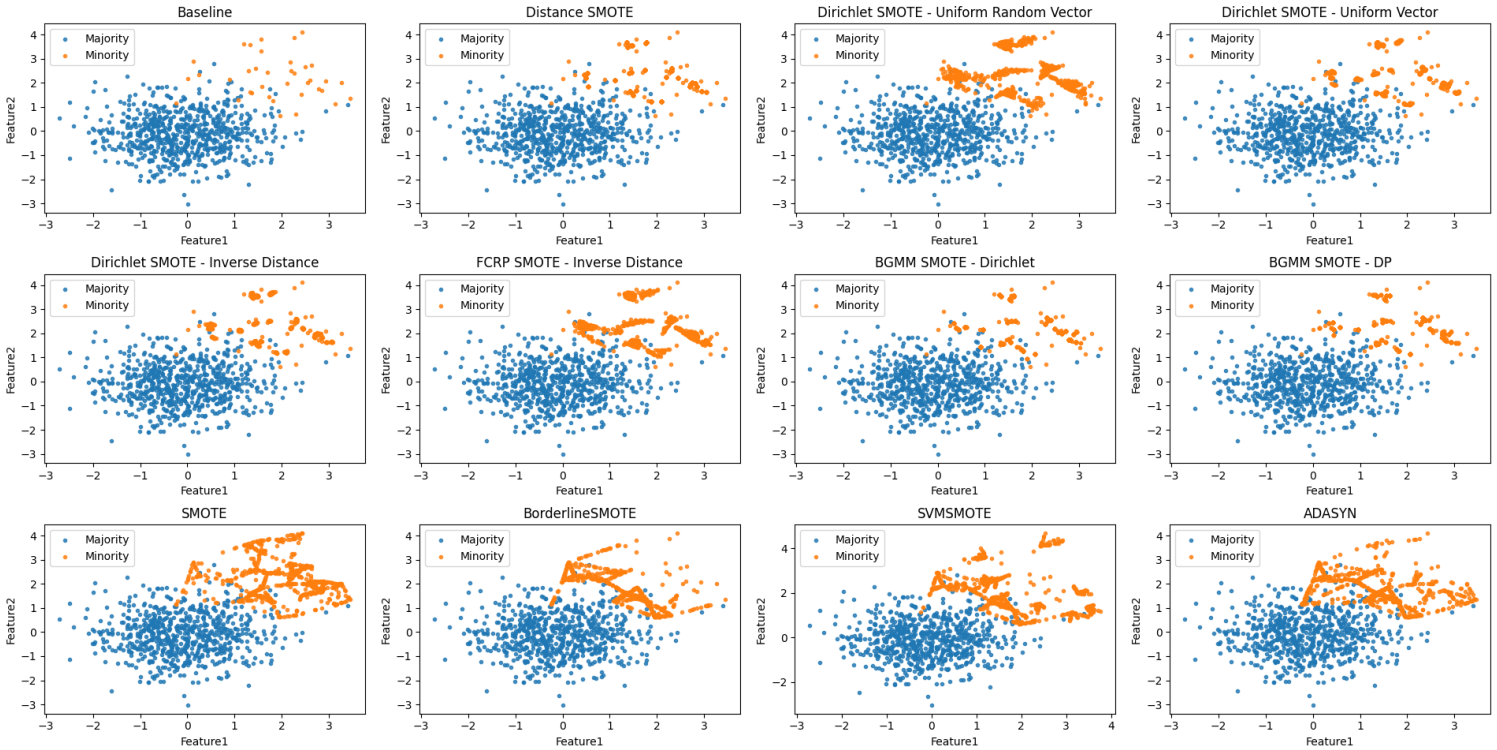

Figure: Comparison of resampled data

Manuscript 4: Simulation Results

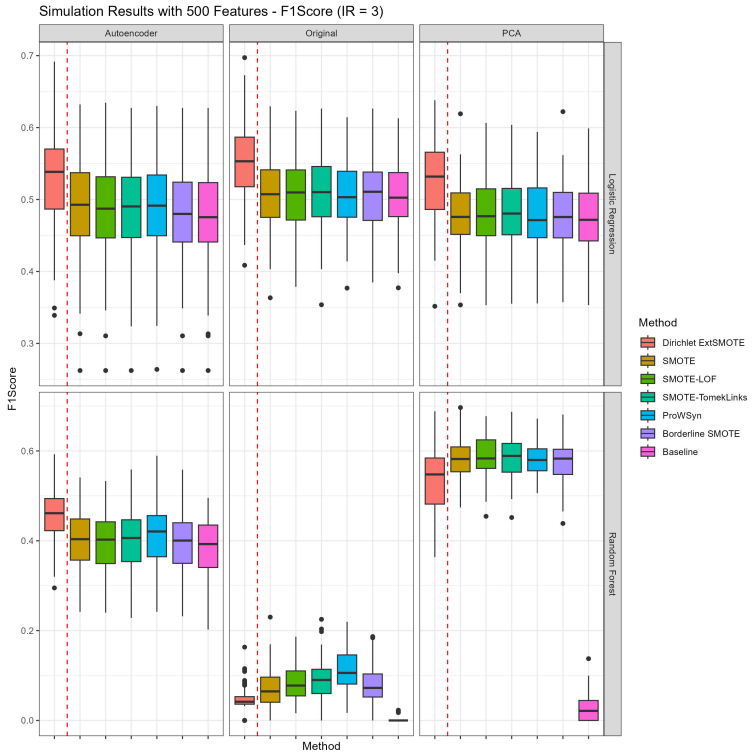

Figure: F1-Score distribution for 100 trials using simulated datasets with 1000 samples and 500 features (all informative), with an imbalance ratio (IR) of 3.

Advantages of using proposed methods

Method	Key Property	Advantages
Distance ExtSMOTE	- Proximity based approach	- Captures the local density variations preserves the underline structure of the minority class.
Dirichlet ExtSMOTE	- Probabilistic weight assignment	- Flexibility and control over variability and randomness. - Reduce the risk of overfitting. - Helps balance the bias-variance tradeoff. - Produces a more diverse set of synthetic samples. - Better approximates the true underline distribution.
FCRP SMOTE	- Bayesian non-parametric approach which introduces adaptive weighting through iterative probability adjustment.	- Enhances the diversity of synthetic examples, and better captures the true distribution and local density variations of the minority class. - Balances the bias-variance tradeoff.
BGMM SMOTE	- Uses the probabilistic clustering capabilities of BGMMs.	- Ensures that the synthetic instances are created in high-density region of the minority class. - Preserves the underline structure and relationships among data points.

When to use & Limitations

Method	When to use	Advantages
Distance ExtSMOTE	- Datasets with moderate complexity and large sample size where minority class has a relatively dense and well-defined structure.	- The deterministic nature can result less diverse synthetic samples.
Dirichlet ExtSMOTE	- Datasets where managing variability and uncertainty is crucial and the minority class has a complex, variable structure.	- May struggle with extremely sparse datasets.
FCRP SMOTE	- Datatsets with evolving patterns and high complexity and applications which require adaptive sampling that reflect the nuanced distribution of the minority class.	- Can be computationally intensive. - Might struggle to perform meaningful clusters with extremely sparse datasets.
BGMM SMOTE	- Datasets with significant class overlap and complex distributions where the minority class can be effectively modeled using Gaussian mixtures and, where capturing the probabilistic distribution of the data is crucial. - Ideal for applications requiring detailed and accurate representation of the minority class distribution.	- Computational complexity. - Model may struggle when the minority instances are sparse or do not perform clear clusters.