Fair-Net: A Network Architecture for Reducing Performance Disparity between Identifiable Sub-populations

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Abstract: In real world datasets, particular groups are under-represented, much rarer than others, and machine learning classifiers will often preform worse on under-represented populations. This problem is aggravated across many domains where datasets are class imbalanced, with a minority class far rarer than the majority class. Naive approaches to handle under-representation and class imbalance include training sub-population specific classifiers that handle class imbalance or training a global classifier that overlooks sub-population disparities and aims to achieve high overall accuracy by handling class imbalance. In this study, we find that these approaches are vulnerable in class imbalanced datasets with minority sub-populations. We introduced Fair-Net, a branched multitask neural network architecture that improves both classification accuracy and probability calibration across identifiable sub-populations in class imbalanced datasets. Fair-Nets is a straightforward extension to the output layer and error function of a network, so can be incorporated in far more complex architectures. Empirical studies with three real world benchmark datasets demonstrate that Fair-Net improves classification and calibration performance, substantially reducing performance disparity between gender and racial sub-populations.

1 INTRODUCTION

Machine learning systems are widely used in a variety of tasks such as computer vision (LeCun et al., 2010), natural language processing (Mikolov et al., 2013), graphs (Matlock et al., 2019) as well as identifying causes and interventions for diseases (Datta et al., 2020; Barnette et al., 2020; Datta et al., 2021a). Decision-making systems, based on neural network architectures, are widely used in many critical tasks such as criminal justice (Završnik, 2021), granting loans (Turiel and Aste, 2020), skin cancer detection (Esteva et al., 2017) and face recognition (Merler et al., 2019). However, there have been growing concerns regarding the performance disparities of these decision making systems across many sensitive domains where there are under-represented subpopulations in the underlying training dataset or application domain.

Under-representation is when samples from a particular sub-population such as those based on gender or race are rare. Under these circumstances, classifiers tend to exhibit disparate performance, with greater accuracy on the majority sub-populations than the minority sub-populations. A previous case study by Buolamwini et al. (Buolamwini and Gebru, 2018) known as "Gender Shades" highlighted noticeable performance disparities in facial recognition systems between male and female sub-populations for classification tasks. Even though these classification systems achieved more than 90% global classification accuracy for gender detection, classification accuracy was much higher in light skinned individuals than darkskinned ones.

Numerous studies have been conducted that highlight the problem of under-representation in datasets (Kearns et al., 2019; Kim et al., 2019; Hardt et al., 2016; Verma and Rubin, 2018). The problem of under-representation is even more challenging in presence of class imbalance. Class imbalance occurs when samples from one class are far more rare than the other. Classifiers are usually biased towards the majority class, thereby performing poorly on the minority class. Since machine learning classifiers are commonly used in decision-making systems, they should simultaneously be accurate as

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well as produce well calibrated probabilities. Predictions from a binary classifier are said to be wellcalibrated if the outcomes predicted to occur with a probability p occur p fraction of the time. Since classifiers minimize error on training, it is often a common practise to assign high costs on misclassifications on the minority class so as to maximize the classification performance on the minority class but overlooking the calibration performance. Common parametric and non-parametric approaches such as Platt scaling (Platt, 1999), isotonic regression (Zadrozny and Elkan, 2002) and Bayesian binning into quantiles (BBQ) (Pakdaman Naeini et al., 2015) are often used to post-process classifiers' outputs for probability calibration. However, previous research (Huang et al., 2020) has shown that the common parametric and non-parametric calibration techniques are often unstable on class imbalanced datasets. Even though, a classifier is trained and post-processed to maximize classification and calibration accuracy for class imbalanced datasets, there may still be significant performance drops across under-represented subpopulations present in the dataset population.

Little work has been done to develop neural network architecture that jointly learns classification and calibration in under-represented sub-populations while handling the skewed distribution of the minority and majority samples in class imbalanced datasets. Recently, the Cal-Net neural network architecture (Datta et al., 2021b) demonstrated simultaneous improvement in classification and calibration performance on class imbalanced datasets. Here, we aim to build on this architecture to improve predictive performance across multiple sub-populations with Fair-Net: a neural network architecture that simultaneously optimizes classification and calibration performances across identifiable sub-populations in the dataset population. Empirically, we find that Fair-Net achieves the best classification and calibration performances across diverse sub-populations of interest.

2 RELATED WORK

Prior research works and methodologies that have been proposed to handle class imbalance and probability calibration while improving classification performance across under-represented sub-populations in datasets.

Previous research studies have proposed parametric and non-parametric post-processing probability calibration techniques such as Platt scaling (Platt, 1999), isotonic regression (Zadrozny and Elkan, 2002), histogram binning (Zadrozny and Elkan, 2001) and bayesian binning into quantiles (BBQ) (Pakdaman Naeini et al., 2015). The post-processing calibration techniques utilize a holdout validation dataset for re-scaling the base classifiers' outputs to improve calibration performance thereby reducing the effective number of sampling for training the base classifier. In datasets where the number of samples is low, this may often lead to under-trained classifiers.

Class imbalance is a widespread challenge in machine learning and previous studies have proposed several strategies to mitigate this problem. Sampling is a common approach to mitigate class imbalance. Common sampling strategies include oversampling (Ling and Li, 1998), where samples from the minority class is re-sampled randomly to eliminate the skewness from the data distribution. Similarly, under-sampling (Kubat and Matwin, 1997) eliminates samples from the majority class randomly to match the distribution of the minority class. Methods such as synthetic minority over-sampling technique (SMOTE) (Chawla et al., 2002) has been proposed that removes the skewness from the imbalanced data distributions by generating synthetic minority class samples. Cost-sensitive learning (Domingos, 1999; Elkan, 2001) and sample weighting(Ting, 1998) are commonly used to assign high weights to samples from the minority class by modifying the objective function. Even though sampling strategies are widely used for managing class imbalance, there are well-known pitfalls such as overfitting (Holte et al., 1989) due to over-sampling as well as information loss (Tang et al., 2009) and inducing bias in calibration due to under-sampling (Dal Pozzolo et al., 2015).

A naive approach to address challenges in predictive modeling across sub-populations of interest in a dataset is to train a separate classifier on each sub-population of interest while simultaneously using previously proposed strategies to handle class imbalance. We have included this approach as a baseline in our study. We find that this approach performs poorly in minority sub-populations where only a small number of samples are available to train sub-population specific classifiers. To overcome this shortcoming, branched neural network architectures can be used where each branch is trained on different sub-populations so as to improve the predictive performance for that specific sub-population. In our ablation studies, we have showed that this approach does not simultaneously achieve the best classification and calibration performances in minority sub-populations in class imbalanced datasets. Previous research studies have proposed methodologies (Kearns et al., 2019; Kim et al., 2019) to improve classification accuracy across sub-populations as well as various definitions of fairness such as equalized odds and equal opportunity (Hardt et al., 2016), demographic parity (Verma and Rubin, 2018) etc. Our definition of fairness is different from parity based notions (Hardt et al., 2016; Verma and Rubin, 2018). Instead, we increase fairness by reducing disparity in classification and calibration performance across sub-populations. Disparity is defined as the variance of performance across identifiable sub-populations of interest in class imbalanced datasets.

3 MATERIALS & METHODS

3.1 The Fair-Net Architecture

The Fair-Net architecture expands the Cal-Net architecture, which aimed to improve calibration on imbalanced datasets (Datta et al., 2021b). Like the Cal-Net architecture, the Fair-Net architecture transforms the binary classification problem into a multi-task problem using two outputs (Figure 1). The primary output (Y) is tuned to produce well-scaled probabilities, whereas the secondary output (Y') is utilized only during the training phase to maximize the classification performance by upweighting samples from the minority class to be equally prevalent as samples from the majority class.

Mirroring Cal-Net, the primary (Y) and secondary (Y') outputs in Fair-Nets, computed using logistic activation functions, are computed from a hidden layer (H) with a single node. This structure ensures that the neural network architecture enforces a monotonic relationship between the primary and the secondary outputs. Both the outputs are monotonic functions of a single number H so they are monotonic transformations of each other.

We have introduced two broad variants of Fair-Nets: "Fair-Net Branched" and "Fair-Net Un-Branched". In the first variant, "Fair-Net Branched" trains a different "branch" consisting of a primary output (Y) and a secondary output (Y'), computed using a single hidden node H, for each sub-population of interest. The primary output (Y) in a "branch" is tuned to produce well-calibrated probabilities, whereas the secondary output (Y') is tuned to maximize classification performance by upweighting samples from the minority class in the sub-population to be equally prevalent as samples from the majority class for that sub-population. This modification requires six trainable parameters in total, with three weights and three biases for each sub-population of interest. Thus, each branch is tuned to maximize the classification and cal-



Figure 1: Different variants of Fair-Nets. Fair-Net Branched trains a different branch for each sub-population, whereas Fair-Net Un-Branched computes the total loss by summing over losses for each sub-population of interest.

ibration performances for each sub-population of interest at the cost of more trainable parameters.

In the second variant, "Fair-Net Un-Branched," a single "branch" consisting of a primary output (Y) and a secondary output (Y'), computed from a single hidden node H, is tuned to maximize the classification and calibration performance across all the subpopulations of interest. Unlike the variant "Fair-Net Branched", the variant "Fair-Net Un-Branched" does not result in additional trainable parameters for each sub-population of interest.

3.2 Loss Components

All the variants of Fair-Nets make use of the same loss components used by Cal-Net (Datta et al., 2021b).

The primary output, $Y = \{y_{g,i}\}$, indexed by instance, *i*, in sub-population, *g*, for both "Fair-Net Branched" and "Fair-Net Un-Branched" utilize a logistic activation function. The loss component for each sub-population, *g*, are computed based on this output and the target class labels $T = \{t_{g,i}\}$.

The first loss component, $L_{X,g}$, is the binary cross entropy error between Y and T for sub-population g. The instances in the majority class for each subpopulation contribute more to the loss in class imbalanced datasets.

The second loss component, $L_{B,g}$, computes the balanced cross-entropy loss for each sub-population, g, between T and Y'. Instances from the minor-

ity class for each sub-population is upweighted to be equally prevalent as samples from the majority class for that sub-population. In all the variants of Fair-Nets, the majority (negatives) class samples in subpopulation g are weighted as $N_g/2n_g$ and the minority (positives) class samples are weighted as $N_g/2p_g$ where N_g is the number of samples in sub-population g and p_g and n_g are the number of samples in the minority (positives) and majority (negatives) classes, respectively. This weighting scheme ensures that for each sub-population g, the minority and majority classes are weighed equally.

The total loss function (L) for Fair-Net Branched and Fair-Net Un-Branched is computed as,

$$L = \sum_{g \in G} \lambda_g \cdot [L_{X,g} + L_{B,g}], \tag{1}$$

where G is the set of all sub-populations of interest and λ_g is a hyper-parameter that can be tuned to assign higher mis-classification costs for sub-population g. In all our experiments, $\lambda_g = 1$ for all sub-populations.

We also use the histogram loss from Cal-Net (Datta et al., 2021b) on the primary output Y for generating well scaled-probabilities. In a well-calibrated probabilistic model for binary classification tasks, the proportion of positive examples in each bin of a reliability diagram should match the average of the predictions for the bin, which is usually close to the midpoint of the bin. Hence, the histogram loss, $L_{H,g}$ for each sub-population g is computed as the RMSE between the proportion positives and the midpoints of the bin.

The total loss function (L) for Fair-Net Branched [histogram loss] and Fair-Net Un-Branched [histogram loss] is computed as,

$$L = \sum_{g \in G} \lambda_g \cdot [L_{X,g} + L_{B,g} + \lambda_{H,g} L_{H,g}]$$
(2)

where $L_{H,g}$ is the histogram loss for sub-population g and $\lambda_{H,g}$ is a hyper-parameter that can be used to tune $L_{H,g}$. Other formulations of the histogram loss may be effective, but exploring them is left for future work. Empirical analyses show that all the loss components are necessary to optimize classification and calibration across under-represented sub-populations in class imbalanced scenarios.

3.3 Datasets

For our experiments, we used three datasets namely (Table 1): (1) Propublica COMPAS dataset (Kirchner and Angwin, 2017) (2) UCI credit card default dataset (Yeh and hui Lien, 2009) and (3) UCI adult census dataset (Kohavi, 1996).

- Propublica COMPAS dataset: We used a smaller subset of the propublica COMPAS dataset (Kirchner and Angwin, 2017) consisting of 6172 instances with 5 features. A binary target variable indicated if an individual would re-offend within the next two years. We used the gender variable to consider two sub-populations namely: Female (F) and Not Female (NF). The imbalance ratios of the target variable in F and NF sub-populations were 1.8 and 1.08 respectively.
- UCI credit card default dataset: The credit card default dataset (Yeh and hui Lien, 2009) from UCI (Dua and Graff, 2020) repository consists of 30,000 instances with 23 features. The binary target variable indicated whether an individual would incur a default payment or not. We have considered two sub-populations based on gender namely: Male (M) and Female(F). The imbalance ratios for the target variable for M and F sub-populations are 3.14 and 3.81 respectively.
- UCI Adult Census dataset: The adult census dataset (Kohavi, 1996) from UCI (Dua and Graff, 2020) repository consists of 48,842 instances with 14 features and a binary target variable that indicated if an individual earned more than \$50,000 or not. After removing samples with missing values, 45,222 samples were used for the analyses. We have considered 8 sub-populations based on gender and race namely: Male (M), Female (F), Black (B), White (W), Black Male (BM), Black Female (BF), White Male (WM) and White Female (WF).

3.4 Training and Evaluation Protocol

We evaluated the variants of Fair-Nets and baseline models for probability calibration performance and classification accuracy using a stratified train, validation and test split. For each dataset, we kept a stratified split of the dataset as a test set(20 - 25% of the dataset) such that the percentages of sub-populations and the imbalance ratios for each sub-population are preserved across train, validation and test sets. Since most of these datasets have a low number of samples for the minority sub-populations, this strategy ensured that sufficient minority samples are present in all the splits. For our experiments, we trained the variants of Fair-Nets with a single hidden layer of 5 units with exponential linear unit (ELU) activation and L2 regularization.

3.5 Baselines

As a baseline for comparison with different variants of Fair-Nets, we trained neural network (NN) architectures with one ELU activated hidden layer consisting of 10 hidden units. We used balanced cross entropy loss to train these neural network architectures such that the samples from the minority class are upweighted to be equally prevalent as samples from the majority class. Balanced cross entropy loss usually improves the classification performance in class imbalanced datasets (Johnson and Khoshgoftaar, 2019). Also, we trained neural network architectures using the same architecture (one hidden layer with 10 ELU activated hidden units) for each sub-population of interest using balanced cross-entropy losses. Finally, we trained Cal-Net architectures with one hidden layer consisting of 5 hidden units with ELU activation. For our case studies, all the variants of Fair-Nets usually had less number of trainable parameters than the baseline NN [balanced xent] and subpopulation specific baselines.

3.6 Assessment Metrics

We evaluate the predictive performance of Fair-Nets and the associated baselines on different subpopulations by reporting the maximum F-measure and area under the receiver operating characteristic (ROC AUC). Previous research work (Davis and Goadrich, 2006) has shown that ROC AUC is often unreliable in class imbalanced datasets. On the contrary, F-measure is a commonly used metric to summarize classification performance in class imbalanced datasets. We highlight the imbalance ratio (IR), calculated as $\frac{n_0}{n_1}$, where n_1 is the number of minority (positives) samples and n_0 is the number of majority (negatives) samples across different sub-populations of interest in the datasets. In order to summarize the calibration performance of Fair-Nets and the associated baselines, we have reported the expected calibration error (ECE) (Pakdaman Naeini et al., 2015; Küppers et al., 2020) and utilized reliability diagrams (DeGroot and Fienberg, 1983). A classifier that achieves higher F-measure and higher AUROC along with lower ECE across different sub-populations of interest is preferred.

Table 1: Class Imbalance statistics for real world datasets.

Dataset	Size	% +ve	IR
COMPAS	6172	45.5	1.2
Credit default	30000	22.12	3.52
Census income	45222	24.78	3

4 RESULTS & DISCUSSION

4.1 Propublica COMPAS Dataset

Fair-Net variants outperformed the baselines on the Propublica COMPAS dataset in classification and calibration performances both on the overall population as well as on the different sub-populations of interest (Figure 2). For the F sub-population, the IR for the target variable was 1.8, which was higher than that of the overall sub-population. Fair-Net variants outperformed the baselines on the F sub-population in predictive performance by achieving the highest F-measure while simultaneously achieving the lowest ECE, thereby improving the calibration performance. Both the variants of Fair-Net Branched outperformed the variants of Fair-Net Un-Branched in classification performance owing to a greater number of available trainable parameters. For both Fair-Nets Branched and Fair-Nets Un-Branched variants, the inclusion of the histogram loss helped in improving calibration performance by reducing ECE. This highlights the potential benefit of incorporating histogram loss to further improve the calibration performance across sub-populations. Sub-population specific baseline models, trained exclusively for each sub-population of interest, usually exhibited poor predictive performance due to the availability of a lower number of samples in the training dataset. As empirically shown, all the variants of Fair-Nets improved predictive performance in the under-represented F sub-population with a high IR than the overall population.

4.2 UCI Credit Card Default Dataset

All the variants of Fair-Nets outperformed the baselines in classification and calibration performance on the overall population while simultaneously improving predictive performances across M and F subpopulations (Figure 2). We observed similar trends in this case study as well where both the variants of Fair-Net Branched outperformed the variants of Fair-Net Un-Branched at the cost of more trainable parameters. Both the variants of Fair-Nets with histogram loss outperformed the corresponding variants without histogram loss in calibration performance by achieving lower ECE scores. All the variants of Fair-Nets improved the predictive performance in the underrepresented M sub-population in the dataset.



Figure 2: On the benchmark datasets, variants of Fair-Net achieved the best predictive performance in terms of F-measure, ROC-AUC and ECE across different sub-populations of interest.

Table 2: Comparing performance of Fair-Net with published results in the literature such as Multi-accuracy (Kim et al., 2019) on similar, but not identical, test dataset.



Figure 3: Variants of Fair-Net achieved the best predictive performance (high F-measure and ROC AUC alongside low ECE) with lowest variance across identifiable sub-populations of interest for the adult census dataset (Kohavi, 1996). L_H refers to the histogram loss.

4.3 UCI Adult Census Dataset

Similar to the prior two case studies, variants of Fair-Nets achieved the best classification and calibration performance across different sub-populations in the adult census dataset (Kohavi, 1996). Eight subpopulations were considered in this case study: Male (M), Female (F), Black (B), White (W), Black Male (BM), Black Female (BF), White Male (WM) and White Female (WF). Out of all these sub-populations, B, BM and BF sub-populations were the most underrepresented, accounting for less than 10% of the overall population. Furthermore, the IR values across B, BM and BF sub-populations are 6.8, 4.26 and 14.7 respectively. Empirical results (Figure 2) showed that the variants of Fair-Nets outperformed the baselines across all the eight sub-populations as well as on the overall population in classification and calibration performances. Moreover, the improvements in classification performance for the variants of Fair-Nets were noticeable in the B, BM and BF subpopulations, where, all the variants of Fair-Nets outperformed the baselines by achieving higher Fmeasure and ROC AUC and lower ECE. The baseline neural network, trained using balanced cross entropy loss for the overall population, achieved similar classification performance to Fair-Nets in the majority sub-populations but incurred drops in Fmeasure in the under-represented sub-populations such as B, BM and BF. The sub-population specific baseline models, trained exclusively on different sub-populations, performed poorly in the underrepresented sub-populations with high class imbalances owing to a shortage in training samples. On the contrary, branched variants of Fair-Net achieved significantly higher predictive performance by adding six trainable parameters (three weight variables and three bias variables) for each sub-population of interest, whereas the un-branched variants of Fair-Nets did not add any additional trainable parameters for different sub-populations of interest. The branched variants of Fair-Net outperformed the un-branched variants in predictive performance due to the availability of more trainable parameters in the neural network architecture. Furthermore, the average classification and calibration performances of Fair-Net variants across different sub-populations are higher than the baselines with low standard deviation (Figure 3). This suggests that Fair-Nets do not incur any substantial performance drops in under-represented subpopulations with high class imbalance ratios. Finally, the classification error (%) across different subpopulations for the Fair-Net variants are comparable with prior published work by Kim et al. (Kim

et al., 2019). We observed that Fair-Net Branched achieved lower classification error (Table 2), suggesting that Fair-Nets achieve the best predictive accuracy in the under-represented sub-populations for the adult census dataset. However, we note that classification error(%) is a poor metric in class imbalanced sub-populations since a classifier with low classification error (%) may not achieve high F-measure and performs substantially worse in class imbalanced datasets (Luque et al., 2019).

4.4 Ablation Analyses

Ablation analyses demonstrated the importance of different components in the Fair-Net's architecture. We trained multi-task neural network architectures that resembled variants of Fair-Net Branched by removing (1) the primary output Y and (2) the secondary output Y' from each of the sub-population heads in Fair-Net's architecture to evaluate whether the classification and calibration performances are affected. For the ablation analyses, we focused on the adult census dataset (Kohavi, 1996) since it contains sub-populations with a diverse range of samples and imbalance ratios.

4.4.1 With and without Primary Output *Y* for Each Sub-population

We trained a modified architecture without the primary output Y from every sub-population network head. Thus, the Fair-Net architecture was reduced to a branched neural network architecture, where each branch was trained on a different sub-population using a balanced cross-entropy loss. The balanced cross-entropy loss upweighted minority class samples to be equally prevalent as samples from the majority class for each sub-population. Empirical results (Figure 4) showed that this modified architecture incurred a drop in classification performance across minority sub-populations such B, BM and BF. Moreover, we observed that this architecture had poor calibration performance (Figure 4) when compared to a standard Fair-Net architecture with a primary output Y for each sub-population. Post-processing this modified architecture's outputs using parametric and non-parametric calibration techniques may improve the calibration performance. The standard Fair-Net Branched architecture continued to achieve the best overall classification and calibration performances across all the sub-populations of interest.



Figure 4: Ablation analyses demonstrating different components of Fair-Net are essential to improve classification and calibration performances for the adult census income dataset (Kohavi, 1996).

4.4.2 With and without Secondary Output *Y'* for Each Sub-population

We trained a modified architecture after eliminating the secondary output Y' from each of the subpopulation branches. This essentially reduced the Fair-Net architecture to a branched neural network architecture, where a separate network head was trained for each sub-population using non-weighted crossentropy loss. Hence, samples from both the majority (negatives) and the minority (positives) classes were weighted equally. The multi-task architecture without the secondary output Y' for each sub-population produced well calibrated probabilities. However, it achieved the lowest classification performance across all the under-represented sub-populations. In the standard Fair-Net architecture, the secondary output Y'was trained using a balanced cross-entropy loss so that samples from the minority class were upweighted to be equally prevalent as samples from the majority class belonging to the same sub-population thereby improving classification performance. We hypothesized that this modified architecture without the secondary output Y' would be comparatively weaker than the standard Fair-Net architecture in classification performance.

Empirically, we observed that there were drops in classification performance of this modified architecture across B, BM and BF sub-populations in terms of F-measure and ROC-AUC (Figure 4). As evident from the distribution of these sub-populations in the dataset, B, BM and BF had very few samples with a high class imbalance ratio when compared to other sub-populations. Hence, we concluded that the secondary output Y' is necessary to improve the classification performance across minority sub-populations with high class imbalance ratios. Both the variants of Fair-Net Branched continued to achieve the best classification and calibration performances across all the sub-populations of interest.

4.4.3 With and without Histogram Loss (L_H)

We introduced two variants of Fair-Nets that used the histogram loss (Datta et al., 2021b). Our case studies across COMPAS data, credit card default dataset and adult census dataset showed that the variants of Fair-Nets trained using histogram loss often outperformed the corresponding variants of Fair-Nets without the histogram loss by achieving lower ECE scores. This suggests that optimizing on the histogram loss may result in improved calibration performance. There may be other formulations for the histogram loss and fully exploring options is left for future studies.

4.5 Study Limitations & Future Directions

The proposed modeling framework requires that all sub-populations are identifiable from the outset. We explicitly identify each sub-populations in training the model, summing over the losses for each subpopulation. Hence, our modeling framework needs access to the features that were used to identify these sub-populations of interest. In our study, the secondary output Y' equally weighs the minority and the majority samples for each sub-population. However, upweighting the minority samples using a higher weight may yield better results in class imbalanced scenarios. In general, neural network architectures may often exhibit poor predictive performance and generalization due to unavailability in training data for under-represented sub-populations (Cui et al., 2015). As a result, variants of Fair-Net may exhibit degraded performance in the absence of enough training data. In our case studies, we weighted each subpopulation of interest equally by setting λ_{e} as 1 for all $g \in G$. However, upweighting under-represented or minority sub-populations may result in improved predictive performance in these subpopulations and exploring options is left for future work. Exploiting multi-task architectures may prove to be an effective way to improve predictive performance across these sub-populations, as evident in our study.

SCIENCE AND

5 CONCLUSION

In this work, we have introduced Fair-Net, a class of neural network architectures that simultaneously improved classification and calibration performances across diverse sub-populations of interest in class imbalanced datasets. Empirically, we showed that the variants of Fair-Net outperformed commonly used neural network architectures by achieving higher Fmeasure, ROC-AUC and low ECE across different sub-populations of interest in three real world datasets: UCI Credit card default dataset, UCI Adult census dataset and Propublica COMPAS datasets. Due to its simplicity, Fair-Nets can readily be incorporated in complex network architectures as the final layer to improve predictive performance across subpopulations of interest.

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REFERENCES

- Barnette, D. A., Schleiff, M. A., Datta, A., Flynn, N., Swamidass, S. J., and Miller, G. P. (2020). Meloxicam methyl group determines enzyme specificity for thiazole bioactivation compared to sudoxicam. *Toxicol. Lett.*
- Buolamwini, J. and Gebru, T. (2018). Gender shades: Intersectional accuracy disparities in commercial gender classification. In Friedler, S. A. and Wilson, C., editors, Proceedings of the 1st Conference on Fairness, Accountability and Transparency, volume 81 of Proceedings of Machine Learning Research, pages 77– 91, New York, NY, USA. PMLR.
- Chawla, N. V., Bowyer, K. W., Hall, L. O., and Kegelmeyer, W. P. (2002). Smote: Synthetic minority oversampling technique. J. Artif. Int. Res., 16(1):321–357.
- Cui, X., Goel, V., and Kingsbury, B. (2015). Data augmentation for deep neural network acoustic modeling. *IEEE/ACM Transactions on Audio, Speech, and Language Processing*, 23(9):1469–1477.
- Dal Pozzolo, A., Caelen, O., and Bontempi, G. (2015). When is undersampling effective in unbalanced classification tasks? In Appice, A., Rodrigues, P. P., Santos Costa, V., Soares, C., Gama, J., and Jorge, A., editors, *Machine Learning and Knowledge Discovery in Databases*, pages 200–215, Cham. Springer International Publishing.
- Datta, A., Flynn, N. R., Barnette, D. A., Woeltje, K. F., Miller, G. P., and Swamidass, S. J. (2021a). Machine learning liver-injuring drug interactions with non-steroidal anti-inflammatory drugs (nsaids) from a retrospective electronic health record (ehr) cohort. *PLOS Computational Biology*, 17(7):1–24.
- Datta, A., Flynn, N. R., and Swamidass, S. J. (2021b). Cal-net: Jointly learning classification and calibration on imbalanced binary classification tasks. In 2021 International Joint Conference on Neural Networks (IJCNN), pages 1–8.
- Datta, A., Matlock, M. K., Dang, N. L., Moulin, T., Woeltje, K. F., Yanik, E. L., and Swamidass, S. J. (2020). "black box" to "conversational" machine learning: Ondansetron reduces risk of hospital-acquired venous thromboembolism. *IEEE Journal of Biomedical and Health Informatics*, pages 1–1.
- Davis, J. and Goadrich, M. (2006). The relationship between precision-recall and roc curves. In Proceedings of the 23rd International Conference on Machine Learning, ICML '06, page 233–240, New York, NY, USA. Association for Computing Machinery.
- DeGroot, M. H. and Fienberg, S. E. (1983). The comparison and evaluation of forecasters. *Journal of the Royal Statistical Society. Series D (The Statistician)*, 32(1/2):12–22.
- Domingos, P. (1999). Metacost: A general method for making classifiers cost-sensitive. In *Proceedings of the Fifth ACM SIGKDD International Conference on*

Knowledge Discovery and Data Mining, KDD '99, page 155–164, New York, NY, USA. Association for Computing Machinery.

- Dua, D. and Graff, C. (2020). UCI machine learning repository.
- Elkan, C. (2001). The foundations of cost-sensitive learning. In In Proceedings of the Seventeenth International Joint Conference on Artificial Intelligence, pages 973–978.
- Esteva, A., Kuprel, B., Novoa, R. A., Ko, J., Swetter, S. M., Blau, H. M., and Thrun, S. (2017). Dermatologistlevel classification of skin cancer with deep neural networks. *Nature*, 542(7639):115–118.
- Hardt, M., Price, E., and Srebro, N. (2016). Equality of opportunity in supervised learning. In *Proceedings of the* 30th International Conference on Neural Information Processing Systems, NIPS'16, page 3323–3331, Red Hook, NY, USA. Curran Associates Inc.
- Holte, R. C., Acker, L. E., and Porter, B. W. (1989). Concept learning and the problem of small disjuncts. In *Proceedings of the 11th International Joint Conference on Artificial Intelligence - Volume 1*, IJCAI'89, page 813–818, San Francisco, CA, USA. Morgan Kaufmann Publishers Inc.
- Huang, L., Zhao, J., Zhu, B., Chen, H., and Broucke, S. V. (2020). An experimental investigation of calibration techniques for imbalanced data. *IEEE Access*, 8:127343–127352.
- Johnson, J. M. and Khoshgoftaar, T. M. (2019). Survey on deep learning with class imbalance. *Journal of Big Data*, 6(1):27.
- Kearns, M., Neel, S., Roth, A., and Wu, Z. (2019). An empirical study of rich subgroup fairness for machine learning. Proceedings of the Conference on Fairness, Accountability, and Transparency.
- Kim, M. P., Ghorbani, A., and Zou, J. Y. (2019). Multiaccuracy: Black-box post-processing for fairness in classification. In Conitzer, V., Hadfield, G. K., and Vallor, S., editors, *Proceedings of the 2019 AAAI/ACM Conference on AI, Ethics, and Society, AIES 2019, Honolulu, HI, USA, January 27-28, 2019*, pages 247–254. ACM.
- Kirchner, J. L. S. M. L. and Angwin, J. (2017). Compas dataset.
- Kohavi, R. (1996). Scaling up the accuracy of naive-bayes classifiers: a decision-tree hybrid. Proceedings of the Second International Conference on Knowledge Discovery and Data Mining.
- Küppers, F., Kronenberger, J., Shantia, A., and Haselhoff, A. (2020). Multivariate confidence calibration for object detection. In *The IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) Workshops.*
- Kubat, M. and Matwin, S. (1997). Addressing the curse of imbalanced training sets: One-sided selection. In *ICML*.
- LeCun, Y., Kavukcuoglu, K., and Farabet, C. (2010). Convolutional networks and applications in vision. In 2010 IEEE International Symposium on Circuits and Systems (ISCAS), pages 253–256.
- Ling, C. X. and Li, C. (1998). Data mining for direct marketing: Problems and solutions. In Proceedings of the Fourth International Conference on Knowledge

Discovery and Data Mining, KDD'98, page 73–79. AAAI Press.

- Luque, A., Carrasco, A., Martín, A., and de las Heras, A. (2019). The impact of class imbalance in classification performance metrics based on the binary confusion matrix. *Pattern Recognition*, 91:216–231.
- Matlock, M. K., Datta, A., Dang, N. L., Jiang, K., and Swamidass, S. J. (2019). Deep learning long-range information in undirected graphs with wave networks. In 2019 International Joint Conference on Neural Networks (IJCNN), pages 1–8.
- Merler, M., Ratha, N., Feris, R. S., and Smith, J. R. (2019). Diversity in faces. *arXiv preprint arXiv:1901.10436*.
- Mikolov, T., Sutskever, I., Chen, K., Corrado, G. S., and Dean, J. (2013). Distributed representations of words and phrases and their compositionality. In Burges, C. J. C., Bottou, L., Welling, M., Ghahramani, Z., and Weinberger, K. Q., editors, *Advances in Neural Information Processing Systems 26*, pages 3111–3119. Curran Associates, Inc.
- Pakdaman Naeini, M., Cooper, G., and Hauskrecht, M. (2015). Obtaining well calibrated probabilities using bayesian binning. *Proceedings of the ... AAAI Conference on Artificial Intelligence. AAAI Conference on Artificial Intelligence*, 2015:2901–2907.
- Platt, J. C. (1999). Probabilistic outputs for support vector machines and comparisons to regularized likelihood methods. In ADVANCES IN LARGE MARGIN CLAS-SIFIERS, pages 61–74. MIT Press.
- Tang, Y., Zhang, Y., Chawla, N. V., and Krasser, S. (2009). Svms modeling for highly imbalanced classification. *IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics)*, 39(1):281–288.
- Ting, K. M. (1998). Inducing cost-sensitive trees via instance weighting. In Żytkow, J. M. and Quafafou, M., editors, *Principles of Data Mining and Knowledge Discovery*, pages 139–147, Berlin, Heidelberg. Springer Berlin Heidelberg.
- Turiel, J. D. and Aste, T. (2020). Peer-to-peer loan acceptance and default prediction with artificial intelligence. *Royal Society Open Science*, 7(6):191649.
- Verma, S. and Rubin, J. (2018). Fairness definitions explained. In 2018 IEEE/ACM International Workshop on Software Fairness (FairWare), pages 1–7.
- Yeh, I.-C. and hui Lien, C. (2009). The comparisons of data mining techniques for the predictive accuracy of probability of default of credit card clients. *Expert Systems with Applications*, 36(2, Part 1):2473–2480.
- Zadrozny, B. and Elkan, C. (2001). Obtaining calibrated probability estimates from decision trees and naive bayesian classifiers. In *Proceedings of the Eighteenth International Conference on Machine Learning*, ICML '01, page 609–616, San Francisco, CA, USA. Morgan Kaufmann Publishers Inc.
- Zadrozny, B. and Elkan, C. (2002). Transforming classifier scores into accurate multiclass probability estimates. In Proceedings of the Eighth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD '02, page 694–699, New York, NY, USA. Association for Computing Machinery.
- Završnik, A. (2021). Algorithmic justice: Algorithms and big data in criminal justice settings. *European Journal* of Criminology, 18(5):623–642.