

EXPLAINABLE METRIC LEARNING FOR SMALL-SIZED MEDICAL DATASETS

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by

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Department of Electrical Engineering

Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy
to the



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Dedicated to

My Children : Kabir & Veer

Certificate

This is to certify that the thesis entitled “**Explainable Metric Learning for small-sized Medical Datasets**” being submitted by **Ms. Shipra Madan** to the Department of Electrical Engineering, Indian Institute of Technology-Delhi, for the award of the degree of **Doctor of Philosophy** is the record of the bonafide research work carried out by her under our supervision. In our opinion, the thesis has reached the standards fulfilling the requirements of the regulations relating to the degree.

The results contained in this thesis have not been submitted either in part or in full to any other university or institute for the award of any degree or diploma.

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A handwritten signature in cursive script that reads "Shipra Madan". The signature is written in dark ink and is positioned above the printed name.

Shipra Madan

Abstract

In recent years, Deep Learning has garnered significant attention within the research community, owing to its remarkable performance across a spectrum of tasks. Consequently, deep learning models have found successful applications in diverse domains, including but not limited to speech recognition, autonomous vehicle navigation, medical image analysis, disease diagnosis, as well as broader tasks like segmentation and classification. Despite the widespread adoption of deep learning, there remains ample room for improvement, particularly in scenarios where data availability is limited. Additionally, deep learning models are often regarded as enigmatic "black-box" systems, making it challenging to elucidate the rationale behind the labels they assign. This thesis centers on addressing two critical areas: first, the effective handling of small datasets through the utilization of the deep metric learning paradigm, and second, the development of methods for explaining the decisions made by neural networks trained with limited data. These endeavors are specifically tailored to the domain of medical imaging.

To begin, I present the notion of metric learning, an approach centered on the use of a distance metric to discern the similarity or dissimilarity between images. This technique leverages a limited number of images from each category to facilitate classification. In this context, I employ Siamese networks and Triplet nets, both stemming from the metric learning paradigm, to construct classification models tailored for small-sized medical datasets. Some of the medical problems which are tackled in various experimental studies in this work are bone-age assessment in 0-3 years of age, COVID-19 detection, pneumonia classification and lung cancer prediction.

Subsequently, the thesis shifts its focus towards crafting interpretable frameworks, de-

veloped through the metric learning approach, and trained on compact medical datasets. These frameworks not only yield meaningful insights but also come accompanied by comprehensive explanations that elucidate the underlying mathematical models. To commence this exploration, I provide a concise introduction to Explainable Artificial Intelligence (XAI) techniques, delving into their extensive categories applicable in the realm of deep learning for the analysis of medical images. Following that, I outline the methodology employed to explain the models that have been trained on the aforementioned medical datasets with limited data, employing various explanation methods, including post-hoc, model-specific, model-agnostic, local, and counterfactual techniques.

In the later part of the thesis, a systematic comparison of Explainable Artificial Intelligence (XAI) methods with their suitability of application to different dataset scenarios is discussed. To evaluate both the quantitative and qualitative effectiveness of each interpretation method introduced in this study, we have devised two comprehensive validation metrics.

In summary, these frameworks pave the way to not only create new classification frameworks which work for small-scale medical datasets but also provide logical explanations to the decisions made by models trained using small datasets.

सार

नवीनतम वर्षों में, विभिन्न कार्यों में अपने उल्लेखनीय प्रदर्शन के कारण, डीप लर्निंग ने अनुसंधान समुदाय के भीतर महत्वपूर्ण ध्यान आकर्षित किया है। नतीजतन, डीप लर्निंग मॉडल को विभिन्न डोमेन में सफल अनुप्रयोग मिले हैं, जिनमें भाषण पहचान, स्वायत्त वाहन नेविगेशन, चिकित्सा छवि विश्लेषण, रोग निदान, साथ ही विभाजन और वर्गीकरण जैसे व्यापक कार्य शामिल हैं। डीप लर्निंग को व्यापक रूप से अपनाने के बावजूद, सुधार की पर्याप्त गुंजाइश बनी हुई है, खासकर उन परिदृश्यों में जहां डेटा उपलब्धता सीमित है। इसके अतिरिक्त, डीप लर्निंग मॉडल को अक्सर रहस्यमय "ब्लैक-बॉक्स" सिस्टम के रूप में माना जाता है, जिससे उनके द्वारा दिए गए लेबलों के पीछे का कारण समझना कठिन हो जाता है। यह थीसिस दो महत्वपूर्ण क्षेत्रों पर ध्यान केंद्रित करती है: पहला, डीप मीट्रिक लर्निंग प्रतिमान के उपयोग के माध्यम से छोटे डेटासेट का प्रभावी संचालन, और दूसरा, सीमित डेटा के साथ प्रशिक्षित न्यूरल नेटवर्क द्वारा किए गए निर्णयों को समझाने के तरीकों का विकास। ये प्रयास विशेष रूप से मेडिकल इमेजिंग के क्षेत्र के अनुरूप हैं।

पसबसे पहले, मैं मीट्रिक सीखने की धारणा प्रस्तुत करती हूँ, जो छवियों के बीच समानता या असमानता को समझने के लिए दूरी माप का उपयोग करती है। इस तकनीक ने प्रत्येक श्रेणी से एक सीमित संख्या की छवियों का उपयोग कर क्लासिफिकेशन को सुविधाजनक बनाने में मदद की है। इस संदर्भ में, मैं मीट्रिक लर्निंग परिदृश्य से उत्पन्न दो मॉडल्स, सियामी नेटवर्क और ट्रिपलेट नेट्स का उपयोग करती हूँ। इस कार्य में विभिन्न प्रायोगिक अध्ययनों में जिन कुछ चिकित्सीय समस्याओं का समाधान किया गया है उनमें 0-3 वर्ष की आयु में हड्डी आयु का मूल्यांकन, कोविड-19 (COVID-19) पता लगाना, न्यूमोनिया वर्गीकरण और फेफड़ों के कैंसर की पूर्वानुमान शामिल हैं।

इसके बाद, थीसिस अपना ध्यान व्याख्यात्मक रूपरेखा तैयार करने की ओर केंद्रित करती है, जिसे मीट्रिक शिक्षण दृष्टिकोण के माध्यम से विकसित किया जाता है, और कॉम्पैक्ट मेडिकल डेटासेट पर प्रशिक्षित किया जाता है। ये ढाँचे न केवल सार्थक अंतर्दृष्टि प्रदान करते हैं बल्कि व्यापक स्पष्टीकरण के साथ आते हैं जो अंतर्निहित गणितीय मॉडल को स्पष्ट करते हैं। इस अन्वेषण को शुरू करने के लिए, मैं चिकित्सा छवियों के विश्लेषण के लिए डीप लर्निंग के क्षेत्र में लागू होने वाली उनकी व्यापक श्रेणियों पर प्रकाश डालते हुए व्याख्या योग्य कृत्रिम बुद्धिमत्ता (एक्सएआई) तकनीकों का एक संक्षिप्त परिचय प्रदान करती हूँ। इसके बाद, मैं उन मॉडलों को समझाने के लिए नियोजित कार्यप्रणाली की रूपरेखा तैयार करती हूँ, जिन्हें सीमित डेटा के साथ उपरोक्त मेडिकल डेटासेट पर प्रशिक्षित किया गया है, जिसमें पोस्ट-हॉक, मॉडल-विशिष्ट, मॉडल-अज्ञेयवादी, स्थानीय और प्रतितथ्यात्मक तकनीकों सहित विभिन्न स्पष्टीकरण विधियों को नियोजित किया गया है।

थीसिस के अंतम भाग में , विभिन्न डेटासेट परिदृश्यों में उनके अनुप्रयोग की उपयुक्तता के साथ व्याख्या योग्य कृत्रिम बुद्धिमत्ता (एक्सएआई) विधियों की एक व्यवस्थित तुलना पर चर्चा की गई है। इस अध्ययन में प्रस्तुत प्रत्येक व्याख्या पद्धति की मात्रात्मक और गुणात्मक प्रभावशीलता दोनों का मूल्यांकन करने के लिए, हमने दो व्यापक सत्यापन मेट्रिक्स तैयार किए हैं।

संक्षेप में, ये ढाँचे न केवल नए वर्गीकरण ढाँचे बनाने का मार्ग प्रशस्त करते हैं जो छोटे पैमाने के चिकित्सा डेटासेट के लिए काम करते हैं बल्कि छोटे डेटासेट का उपयोग करके प्रशिक्षित मॉडलों द्वारा लिए गए निर्णयों को तार्किक स्पष्टीकरण भी प्रदान करते हैं।

Contents

Certificate	i
Acknowledgements	ii
Abstract	iv
List of Figures	xi
List of Tables	xv
Abbreviations	xvii
1 Introduction	1
1.1 General Introduction	1
1.2 Background	2
1.2.1 Metric Learning	2
1.2.2 Explainable AI	3
1.2.3 Small-Dataset Medical Problems	3
1.3 Literature Review	5
1.3.1 Metric Learning	5
1.3.2 Explainable Learning	6
1.3.3 Small Dataset Medical Problems	7
1.4 Research Gaps	8
1.5 Thesis Objectives and Scope	9
1.5.1 Objectives	9
1.5.2 Scope	9
1.5.3 Metric Learning for small-scale datasets in medical domain	10

1.5.4	Explainability of metric learning based models trained for small-size dataset classification problems	10
1.6	Thesis Outline	11
1.7	Thesis Contribution	13
2	Skeletal Bone-age Assessment using a Small Dataset of Hand X-rays	14
2.1	Introduction	16
2.2	Methods	20
2.2.1	Dataset	20
2.2.2	Data Preprocessing	20
2.2.3	Architecture	21
2.2.4	Loss Function	23
2.2.5	Triplet Mining	25
2.3	Results	26
2.3.1	Evaluation	26
2.3.2	Test Accuracy and Error Analysis	26
2.3.3	Visualization	27
2.3.4	ROC Curve	28
2.3.5	Visualising Embeddings	30
2.3.6	Prediction Results	31
2.4	Discussion	34
2.4.1	Comparison with Previous Works	34
2.4.2	How to Improve the System?	34
2.4.3	Clinical Application	35
2.5	Limitations and Future Directions	35
2.6	Conclusions	37
3	Automated Detection of COVID-19 on a Small Dataset of Chest CT Images using Metric Learning	38
3.1	Introduction	40
3.2	Materials and Methods	41
3.2.1	Dataset	41
3.2.2	Experimental Setup	43

3.2.3	Architecture	44
3.3	Results	49
3.3.1	Prediction Results	51
3.3.2	Comparative Analysis	51
3.4	Discussion	53
3.4.1	The Proposed Framework Is Able to Identify COVID-19 cases Accurately	53
3.4.2	The Explainable COVID-19 Framework Performs At Par with the State-of-Art methods	54
3.4.3	Triplet Network Effectively Handles Small COVID-19 Chest X-ray dataset	54
3.4.4	Limitations and Future Directions	54
3.5	Conclusion	55
4	Pneumonia Classification using Small-Sized Lung-CT dataset and their explainability	57
4.1	Introduction	59
4.2	Background	61
4.3	Materials and Methods	62
4.3.1	Pneumonia classification using Siamese Networks and explanations using LRP (Layer-wise Relevance propagation) and SmoothGrad	64
4.3.2	Pneumonia Classification in chest X-ray images using Explainable Slot-Attention Mechanism	71
4.3.3	Pneumonia Classification in chest X-ray images using Metric Learning and back-propagation XAI method	78
4.4	Results	83
4.4.1	Pneumonia classification using Siamese Networks and explanation using LRP (Layer-wise Relevance propagation) and SmoothGrad	84
4.4.2	Pneumonia Classification in chest X-ray images using Explainable Slot-Attention Mechanism	86
4.4.3	Pneumonia Classification in chest X-ray images using Metric Learning and back-propagation XAI method	92
4.5	Discussion	96

4.5.1	Impact of different pre-trained CNN architectures and k-shot variations on model employing Siamese architecture for classifying multiple classes	97
4.5.2	Impact of varying layers in CNN models on explainable AI methods	98
4.5.3	Limitations and Future Directions	99
4.6	Conclusions	99
5	Lung Cancer Identification using Deep Neural Nets with Counterfactual Explanations	101
5.1	Introduction	103
5.2	Materials and Methods	105
5.2.1	Dataset	105
5.2.2	DNN Classifier	106
5.2.3	Counterfactuals	107
5.2.4	Counterfactual Exaggeration	109
5.3	Results	109
5.3.1	DNN Classifier	109
5.3.2	Counterfactual explanations	111
5.3.3	Counterfactual Exaggeration	114
5.4	Discussion	114
5.4.1	DNN Classifier Identified Lung Cancer Types with High Accuracy	115
5.4.2	Counterfactual Exaggeration Unveils Subtle Image Features Crucial for DNN Classifications	115
5.4.3	The Counterfactual Activations Generated were Highly Convincing and Misled the Classifiers	115
5.4.4	Limitations and Future Directions	116
5.5	Conclusion	117
6	General Discussion: Summary, Scope for Future Work and Conclusions	119
6.1	Summary of the findings	119
6.2	Discussion	122
6.2.1	Towards building ‘effective’ classifiers for small medical datasets	122
6.2.2	Towards building models trained on small datasets ‘explainable’	124
6.3	Future Scope	126

6.4 Conclusions	128
Bibliography	128
List of Publications	146
Biodata	147

List of Figures

2.1	Images showcasing hand anatomy and skeletal maturity across various age groups: (a) Representation of an immature hand displaying the areas of ossification, (b) Hand anatomy at age 0, (c) Hand anatomy at age 1, (d) Hand anatomy at age 2, and (e) Hand anatomy at age 3.	19
2.2	The preparatory processing pipeline showcases example images at different pre-processing stages. (a) Unprocessed input images (b) Segmented images (c) Black background-normalized and centered images (d) The final images with CLAHE-enhanced contrast.	21
2.3	The Triplet Net architecture processes input image samples through the embedding function to generate respective embeddings.	23
2.4	The suggested triplet loss positions the anchor in close proximity to the positive sample and more distantly from the negative sample.	24
2.5	Validation set prediction results for the RSNA dataset are shown in (a), while those for the DHA dataset are displayed in (b).	27
2.6	Carefully selected attention maps for (a) RSNA and (b) DHA datasets to illustrate the overall pattern across different classes.	29
2.7	ROC curves for bone age assessment in the test set using the triplet network for (a.) binary and (b.) multi-class configurations	30
2.8	Visualizations of the embeddings using t-SNE for both training and test data are displayed before and after training. These visualizations are shown for the binary class (0-1, 1-2 years) in (a) and for the multi-class (0-1, 1-2, 2-3 years) scenario in (b).	32
2.9	Results of bone-age estimation for the multi-class case using a few test set images.	33

3.1	Sample unprocessed CT scans of the chest for a) COVID-19 patients and b) non-COVID-19 patients.	42
3.2	Diagram illustrating the complete pipeline for the detection of COVID-19 . .	44
3.3	Illustration of the Triplet Network structure, depicting the input samples as Anchor, Positive, and Negative. The Convolutional Neural Network (CNN) generates embeddings, which are subsequently used to compute the distances.	45
3.4	The network aims to reduce the gap between the Anchor and the Positive sample while increasing the distance between the Anchor and the Negative sample.	47
3.5	Receiver operating characteristic curve analysis for the triplet network	49
3.6	The model generates embedding clusters via PCA for both training (above) and test data (below) pre- and post-training.	50
3.7	The illustration displays the output distances generated by our model for Anchor-Positive and Anchor-Negative pairs when the test image is from the COVID class. Reduced distance post-training between the test image and the Positive sample implies similarity, while an increased distance from the Negative sample suggests dissimilarity.	51
3.8	This figure illustrates the output distances of our model between Anchor-Positive and Anchor-Negative pairs when the test image belongs to the non-COVID class. A reduced distance after training between the test image and the Positive sample indicates image similarity, while an increased distance between the test image and the Negative sample indicates dissimilarity.	52
4.1	Sample chest radiographs illustrating (a) a normal lung and (b) a lung affected by pneumonia. In the pneumonic image, the red arrows indicate the presence of white infiltrates, which are a distinctive characteristic of pneumonia. . . .	60
4.2	Data distribution for various disease classes from covid-chestxray-dataset. . .	63
4.3	Figure summarizing the proposed method for detecting pneumonia in CXR images using Siamese networks.	65
4.4	High-level schematic of the Siamese Networks architecture.	65
4.5	Figure illustrating Test Image and Support Set example in a 4-Way 5-Shot learning scenario	66
4.6	CNN architecture used in the pneumonia detection model	67

4.7	A comprehensive overview of the proposed pneumonia identification methodology is presented. Both the query image and support set images undergo processing through the xSlot Attention Module. The backbone network is responsible for feature extraction, which leads to the generation of attention maps. Flattened feature vectors for both the query and support images are concatenated to enable pairwise matching, and prediction scores are then computed.	73
4.8	A comprehensive look at the proposed methodology for identifying pneumonia. The reconstructed sequential model goes through the DeepLift module, computing and visually displaying importance scores.	79
4.9	Diagram illustrating the concept of a 4-way 1-shot scenario.	81
4.10	Visual representations of the input image with four target labels are shown using (a.) LRP and (b.) SmoothGrad. The top row exhibits support set images, while the bottom row demonstrates heatmap explanations for the query image. The predicted image is highlighted with a green border.	87
4.11	Visualization of patterns for a query image and support set for COVID-19 (a.) and MERS-CoV (b.) class. Consolidated image depicts the aggregate of attention over patterns from various slots and pattern 1-5 shows the patterns learned from various regions of the image.	90
4.12	Matching matrix indicating similarity scores in percentage. First row and column indicate the consolidated attention for both query and support images of each category.	91
4.13	Figure depicting the prediction results of a few-shot classifier on a few samples with similarity scores between pairs of images.	93
4.14	Figure displaying distinct visualization techniques highlighting crucial areas on chest CT samples with pneumonia.	94
4.15	The outcomes show the prioritization of pixel masking when transitioning from the 'SARS' class to the target class 'Influenza.' Our proposed technique demonstrates improved accuracy in identifying pixels for transforming an image from one disease category to another.	95
4.16	Boxplots depicting the rise in log-odds scores between the target class and the original class following the application of the mask.	96

5.1	An overall pipeline explaining the suggested counterfactual framework for lung cancer prediction	105
5.2	Sample images from IQ-OTH/NCCD dataset distributed over 3 categories: normal, benign, and malignant	106
5.3	DNN classifier for lung cancer prediction. The DNN classifier(on top) used is a standard deep CNN and the output is a one-hot vector representing 3 lung cancer types. Training accuracy over time is depicted in a graph (bottom) for validation and test set.	110
5.4	Sample counterfactuals generated for NORMAL and MALIGNANT class . .	112
5.5	Counterfactual explanation for a misclassification event: The DNN initially misclassifies the image, categorizing a "NORMAL" image as "MALIGNANT" (a). To investigate this incorrect decision, a counterfactual image is generated (b). The counterfactual explanation is established by performing pixel-wise subtraction between the maps in (b) and (a), shedding light on why the image was mistakenly classified as "MALIGNANT" rather than "NORMAL" (c). .	113
5.6	Iterative transformation of image by the generator toward class	114

List of Tables

2.1	A comparative analysis of analogous techniques concerning dataset size and the age group under consideration.	19
2.2	Validation accuracy for predictions made within the age groups of one and two years on the DHA and RSNA datasets.	26
2.3	Analyzing Performance Differences Among Different Deep Neural Network Designs on DHA and RSNA Datasets	34
3.1	Specifications of the input dataset utilized for both training and testing purposes.	42
3.2	Comparison of our method’s performance with conventional deep learning models using a comparable volume of data.	53
4.1	Number of frontal CXR images for various pneumonia types categorized by their genus or species, sourced from the covid-chestxray-dataset.	69
4.2	Disease classifications utilized across various experiments based on their type and genus or species for the datasets used for training and testing.	70
4.3	Assessing the performance of our approach in relation to ResNet50, InceptionV3, and Reptile, employing a similar amount of data for comparison . . .	71
4.4	The number of frontal CXR images depicting various types of pneumonia, categorized by their type, genus, or species from the covid-chestxray-dataset.	77
4.5	Evaluating performance differences between 2-Way and 3-Way classification tasks across various 5-Shot, 10-Shot, and 20-Shot settings using Dataset-1. . .	84
4.6	Assessing the performance of 2-Way, 3-Way, and 4-Way classification tasks across 5-Shot, 10-Shot, and 20-Shot setups utilizing Dataset-2 for evaluation .	84
4.7	Classification Performance on covid-chestxray-dataset	88

4.8	Performance comparison of the proposed technique for pneumonia identification with conventional deep CNN networks utilizing a similar number of images.	88
4.9	A comparative assessment of performance is conducted for both 2-Way and 4-Way classification settings with 5, 10, and 20 shots using the COVID-ChestXray-Dataset and RSNA Pneumonia Dataset.	92
4.10	Analyzing the comparative performance of the sub-networks based on the Siamese architecture on both datasets.	97
4.11	Comparative performance assessment of 2-Way and 4-Way classification settings with 5, 10, and 20 Shot configurations using the COVID-ChestXray-Dataset and the RSNA Pneumonia dataset.	98
6.1	An overview of the implementation challenges of various explainable pneumonia identification methods proposed in the study.	
	✓ signifies Yes	
	× signifies No	129
6.2	Summary of interpretation performance of various explainable pneumonia identification methods proposed in the study	130

Abbreviations

AP	Antero Posterior Supine
AUC	Area Under Curve
AUROC	Area Under the receiver operator Curve
BAA	Bone Age Assessment
CAD	Computer Aided Design
CAM	Class Activation Mapping
CLAHE	Contrast-Limited Adaptive Histogram Equalization
CNN	Convolutional Neural Networks
COVID19	Corona Virus Disease
CT	Computed Tomography
CXR	Chest X-ray
DeepLIFT	Deep Learning Important FeaTures
DHA	Digital Hand Atlas Database
DICOM	Digital Imaging and Communications in Medicine
DML	Distance Metric Learning
DNN	Deep Neural Networks
FN	False Negative
FP	False Positive
FPR	False Positive Rate
GAN	Generative Adversarial Networks
GP	Greulich–Pyle
GPU	Graphics Processing Unit
GRU	Gated Recurrent Unit
Grad-CAM	Gradient-weighted Class Activation Mapping

GRU	Gated Recurrent Unit
IITD	Indian Institute of Technology-Delhi
IQ-OTH/NCCD	Iraq-Oncology Teaching Hospital/National Center for Cancer Disease
LIME	Local Interpretable Model Agnostic Explanation
LRP	Layerwise Relevance Propagation
MERS-Co	Middle East Respiratory Syndrome Coronavirus
MLP	Multi Layer Perceptron
MRI	Magnetic Resonance Imaging
PCA	Principal Component Analysis
RISE	Randomized Input Sampling for Explanation
RNN	Recurrent Neural Networks
ROC	Reciever Operating Characterstic
ROI	Regions of Interest
RSNA	Radiological Society of North America
RT-PCR	Reverse Transcription Polymerase Chain Reaction
SARS	Severe Acute Respiratory Syndrome
SGD	Stochastic Gradient Descent
TN	True Negative
TP	True Positive
TPR	True Positive Rate
tSNE	t-Distributed Stochastic Neighbour Embedding
TW	Tanner–Whitehouse
WHO	World Health Organization
XAI	Explainable Artifical Intelligence