Bioinformatics Algorithms Active Learning Approach

Bioinformatics Algorithms Active Learning Approach Bioinformatics Algorithms An Active Learning Approach Bioinformatics algorithms are the computational tools that drive our understanding of biological data They enable us to analyze vast datasets predict protein structures identify diseasecausing mutations and design new drugs However these algorithms often require massive amounts of labeled data which can be expensive and timeconsuming to obtain Active learning offers a potential solution by intelligently selecting the most informative data points for manual annotation minimizing the need for extensive labeling while maximizing model performance Bioinformatics algorithms active learning machine learning data annotation data efficiency prediction classification protein structure disease prediction drug discovery This article delves into the use of active learning within the realm of bioinformatics algorithms It explores the fundamental principles of active learning outlining its benefits over traditional passive learning approaches The discussion highlights how active learning strategies can be effectively implemented in various bioinformatics tasks including protein structure prediction disease diagnosis and drug design Furthermore the article investigates the potential of active learning to accelerate the development of novel bioinformatics algorithms ultimately leading to improved efficiency and accuracy in understanding and manipulating biological systems Active Learning in Bioinformatics A Paradigm Shift The field of bioinformatics is characterized by the constant generation of massive amounts of data ranging from DNA sequences and protein structures to gene expression profiles and clinical records This deluge of information necessitates sophisticated algorithms capable of extracting meaningful insights and making accurate predictions However the development and training of these algorithms rely heavily on labeled datasets which are often expensive and timeconsuming to generate Traditional passive learning methods require large amounts of manually labeled data creating a bottleneck in the development and application of bioinformatics tools In contrast 2 active learning offers a more intelligent approach by strategically selecting the most informative data points for manual annotation This results in significantly reduced labeling effort while achieving similar or even superior model performance compared to passive learning How Active Learning Works Active learning operates on the premise that not all data points are equally valuable for training a model By identifying and focusing on the most informative examples it minimizes the need for extensive labeling while maximizing model performance The process typically involves 1 Initial Training A model is trained on a small

initially labeled dataset 2 Data Selection The model identifies unlabeled data points that are most likely to improve its performance if labeled This selection is often based on the models uncertainty or disagreement with other models 3 Manual Annotation The selected data points are manually labeled by human experts 4 Model Retraining The model is retrained with the newly labeled data further enhancing its accuracy and efficiency This iterative process continues until the model achieves a desired level of performance or a budget constraint is reached Benefits of Active Learning in Bioinformatics Active learning offers several key benefits in the context of bioinformatics Data Efficiency Active learning significantly reduces the need for manual data annotation making it more efficient and costeffective than traditional passive learning methods This is especially crucial in bioinformatics where large labeled datasets are often scarce and expensive to obtain Improved Model Performance By focusing on the most informative data points active learning can achieve higher accuracy and generalization performance compared to passive learning especially when dealing with limited labeled data Faster Development Active learning can accelerate the development of new bioinformatics algorithms by reducing the time and resources required for data annotation This allows researchers to quickly iterate and refine their models leading to faster breakthroughs in understanding and manipulating biological systems Applications of Active Learning in Bioinformatics 3 Active learning has shown promise in various bioinformatics applications including Protein Structure Prediction Active learning can help reduce the computational cost of predicting protein structures by focusing on the most informative regions of the protein This can lead to more accurate and efficient prediction models Disease Diagnosis Active learning can improve the accuracy of disease diagnosis by selecting the most relevant clinical data points for annotation This can lead to earlier and more accurate identification of diseases Drug Discovery Active learning can accelerate the process of drug discovery by identifying promising candidate molecules and prioritizing them for further testing This can lead to faster development of new and effective treatments for diseases The Future of Active Learning in Bioinformatics The integration of active learning with bioinformatics algorithms has the potential to revolutionize how we analyze and interpret biological data As data generation continues to escalate active learning will play an increasingly vital role in extracting meaningful insights from complex biological systems Conclusion Active learning represents a significant advancement in the field of bioinformatics offering a path towards more efficient and accurate data analysis By intelligently selecting the most informative data points for annotation active learning allows researchers to build high performance models without relying on massive labeled datasets This paradigm shift has the potential to accelerate the development of novel bioinformatics algorithms leading to groundbreaking discoveries in areas such as protein structure prediction disease diagnosis and drug discovery As the field of bioinformatics continues to evolve active learning is poised to play an increasingly crucial role in unlocking the secrets of biological systems FAQs 1 How is active learning different from

traditional passive learning Active Learning The model actively selects data points for annotation based on its uncertainty or disagreement This approach is more efficient and often results in better performance than passively labeling all data points Passive Learning The model is trained on a fixed prelabeled dataset This approach requires large amounts of data and may not be as efficient as active learning 2 What are the challenges of using active learning in bioinformatics Data Complexity Biological data can be highly complex and require domain expertise for 4 accurate annotation Model Selection Choosing the right model for the specific task is crucial for effective data selection Human Expertise Active learning relies on human experts to label selected data points which can be timeconsuming and expensive 3 What are some popular active learning algorithms used in bioinformatics Uncertainty Sampling The model selects data points it is most uncertain about QuerybyCommittee A committee of multiple models is used and the model selects data points where the models disagree most Expected Model Change The model selects data points that are expected to cause the biggest change in the models parameters if labeled 4 How does active learning compare to other data efficiency techniques in bioinformatics Active Learning Selects specific data points for annotation based on model uncertainty Transfer Learning Leverages knowledge from previously trained models on similar datasets Data Augmentation Creates artificial data points to increase the size of the training dataset Feature Engineering Extracts relevant features from existing data to enhance model performance 5 What are some potential future directions for active learning in bioinformatics Integration with Big Data Developing active learning techniques that can handle massive datasets Automated Annotation Exploring methods to automate the annotation process reducing the reliance on human experts MultiModal Learning Using active learning to integrate data from multiple sources such as genomics proteomics and clinical data

Active LearningAnalysis Of Algorithms An Active Learning ApproachBioinformatics AlgorithmsAlgorithms for Query-Efficient Active LearningAlgorithms for Active LearningBioinformatics AlgorithmsAnalysis of AlgorithmsAdaptive and Natural Computing AlgorithmsOnline Choice of Active Learning AlgorithmsAdvances in Information RetrievalBrain Function Assessment in LearningArtificial Neural Networks – ICANN 2009Management of DataOnline Learning Algorithms for Sequence Prediction, Importance Weighted Classification, and Active LearningProceedings of the Fourth SIAM International Conference on Data MiningLearning with Online ConstraintsInformation Theoretic Active Learning in Unsupervised and Supervised ProblemsActive Relevance Feedback AlgorithmsActive Learning Algorithms for Multilayer Feedforward Neural NetworksActive Learning Challenge Burr Settles Mc Connell Phillip Compeau Songbai Yan Daniel Joseph Hsu Phillip Compeau Jeffrey J. McConnell Bernadete Ribeiro Kobi Luz Giambattista Amati Claude Frasson Cesare Alippi Nikolaos Karampatziakis Michael W. Berry Claire Elizabeth Monteleoni Jamshid Sourati Zuobing Xu Adebola Adebisi Adejumo Isabelle Guyon

Active Learning Analysis Of Algorithms An Active Learning Approach Bioinformatics Algorithms Algorithms for Query-Efficient Active Learning Algorithms for Active Learning Bioinformatics Algorithms Analysis of Algorithms Adaptive and Natural Computing Algorithms Online Choice of Active Learning Algorithms Advances in Information Retrieval Brain Function Assessment in Learning Artificial Neural Networks – ICANN 2009 Management of Data Online Learning Algorithms for Sequence Prediction, Importance Weighted Classification, and Active Learning Proceedings of the Fourth SIAM International Conference on Data Mining Learning with Online Constraints Information Theoretic Active Learning in Unsupervised and Supervised Problems Active Relevance Feedback Algorithms Active Learning Algorithms for Multilayer Feedforward Neural Networks Active Learning Challenge *Burr Settles Mc Connell Phillip Compeau Songbai Yan Daniel Joseph Hsu Phillip Compeau Jeffrey J. McConnell Bernadete Ribeiro Kobi Luz Giambattista Amati Claude Frasson Cesare Alippi Nikolaos Karampatziakis Michael W. Berry Claire Elizabeth Monteleoni Jamshid Sourati Zuobing Xu Adebola Adebisi Adejumo Isabelle Guyon*

the key idea behind active learning is that a machine learning algorithm can perform better with less training if it is allowed to choose the data from which it learns an active learner may pose queries usually in the form of unlabeled data instances to be labeled by an oracle e g a human annotator that already understands the nature of the problem this sort of approach is well motivated in many modern machine learning and data mining applications where unlabeled data may be abundant or easy to come by but training labels are difficult time consuming or expensive to obtain this book is a general introduction to active learning it outlines several scenarios in which queries might be formulated and details many query selection algorithms which have been organized into four broad categories or query selection frameworks we also touch on some of the theoretical foundations of active learning and conclude with an overview of the strengths and weaknesses of these approaches in practice including a summary of ongoing work to address these open challenges and opportunities table of contents automating inquiry uncertainty sampling searching through the hypothesis space minimizing expected error and variance exploiting structure in data theory practical considerations

recent decades have witnessed great success of machine learning especially for tasks where large annotated datasets are available for training models however in many applications raw data such as images are abundant but annotations such as descriptions of images are scarce annotating data requires human effort and can be expensive consequently one of the central problems in machine learning is how to train an accurate model with as few human annotations as possible active learning addresses this problem by bringing the annotator to work together with the learner in the learning process in active learning a learner can sequentially select examples and ask the annotator for labels so that it may require fewer annotations if the learning algorithm avoids querying

less informative examples this dissertation focuses on designing provable query efficient active learning algorithms the main contributions are as follows first we study noise tolerant active learning in the standard stream based setting we propose a computationally efficient algorithm for actively learning homogeneous halfspaces under bounded noise and prove it achieves nearly optimal label complexity second we theoretically investigate a novel interactive model where the annotator can not only return noisy labels but also abstain from labeling we propose an algorithm which utilizes abstention responses and analyze its statistical consistency and query complexity under different conditions of the noise and abstention rate finally we study how to utilize auxiliary datasets in active learning we consider a scenario where the learner has access to a logged observational dataset where labeled examples are observed conditioned on a selection policy we propose algorithms that effectively take advantage of both auxiliary datasets and active learning we prove that these algorithms are statistically consistent and achieve a lower label requirement than alternative methods theoretically and empirically

this dissertation develops and analyzes active learning algorithms for binary classification problems in passive non active learning a learner uses a random sample of labeled examples from a fixed distribution to select a hypothesis with low error in active learning a learner receives only a sample of unlabeled data but has the option to query the label of any of these data points the hope is that the active learner needs to query the labels of just a few carefully chosen points in order to produce a hypothesis with low error the first part of this dissertation develops algorithms based on maintaining a version space the set of hypotheses still in contention to be selected the version space is specifically designed to tolerate arbitrary label noise and model mismatch in the agnostic learning model the algorithms maintain the version space using a reduction to a special form of agnostic learning that allows for example based constraints this represents a computational improvement over previous methods the generalization behavior of one of these algorithms is rigorously analyzed using a quantity called the disagreement coefficient this algorithm is shown to have label complexity that improves over that of previous methods and matches known label complexity lower bounds in certain cases the second part of this dissertation develops algorithms based on simpler reductions to agnostic learning that more closely match the standard abstraction of supervised learning procedures the generalization behavior of these algorithms are also analyzed in the agnostic learning model and are shown to have label complexity similar to the version space methods therefore these algorithms represent qualitative improvements over version space methods as strict version space methods can be risky to deploy in practice the first of these algorithms is based on a relaxation of a version space method and the second is based on an importance weighting technique the second algorithm is also shown to automatically adapt to various noise conditions that imply a tighter label complexity analysis experiments using this algorithm are also presented to illustrate some of the

promise of the method

data structures theory of computation

the icannga series of conferences has been organised since 1993 and has a long history of promoting the principles and understanding of computational intelligence paradigms within the scientific community and is a reference for established workers in this area starting in innsbruck in austria 1993 then to ales in prance 1995 norwich in england 1997 portoroz in slovenia 1999 prague in the czech republic 2001 and finally roanne in france 2003 the icannga series has established itself for experienced workers in the field the series has also been of value to young researchers wishing both to extend their knowledge and experience and also to meet internationally renowned experts the 2005 conference the seventh in the icannga series will take place at the university of coimbra in portugal drawing on the experience of previous events and following the same general model combining technical sessions including plenary lectures by renowned scientists with tutorials

this book constitutes the refereed proceedings of the 29th annual european conference on information retrieval research ecir 2007 held in rome italy in april 2007 the papers are organized in topical sections on theory and design efficiency peer to peer networks result merging queries relevance feedback evaluation classification and clustering filtering topic identification expert finding xml ir ir and multimedia ir

this book constitutes the thoroughly refereed proceedings of the first international conference on brain function assessment in learning bfal 2017 held in patras greece in september 2017 the 16 revised full papers presented together with 2 invited talks and 6 posters were carefully selected from 28 submissions the bfal conference aims to regroup research in multidisciplinary domains such as neuroscience health computer science artificial intelligence human computer interaction education and social interaction on the theme of brain function assessment in learning

this volume is part of the two volume proceedings of the 19th international conf ence on artificial neural networks icann 2009 which was held in cyprus during september 14 17 2009 the icann conference is an annual meeting sp sored by the european neural network society enns in cooperation with the ternational neural network society inns and the japanese neural network society jnns icann 2009 was technically sponsored by the ieee computational intel gence society this series of conferences has been held annually since 1991 in various european countries and covers the field of neurocomputing learning systems and related areas artificial neural networks provide an information processing structure inspired by biological nervous systems they consist of a large number of highly interconnected processing elements with the capability of learning by example the field

of artificial neural networks has evolved significantly in the last two decades with active partici tion from diverse fields such as engineering computer science mathematics artificial intelligence system theory biology operations research and neuroscience artificial neural networks have been widely applied for pattern recognition control optimization image processing classification signal processing etc

this thesis studies three problems in online learning for all the problems the proposed solutions are simple yet non trivial adaptations of existing online machine learning algorithms for the task of sequential prediction a modified multiplicative update algorithm that produces small and accurate models is proposed this algorithm makes no assumption about the complexity of the source that produces the given sequence for the task of online learning when examples have varying importances the proposed algorithm is a version of gradient descent in continuous time finally for the task of efficient online active learning the implementation we provide makes use of many shortcuts these include replacing a batch learning algorithm with an online one as well as a creative use of the aforementioned continuous time gradient descent to compute the desirability of asking for the label of a given example as this thesis shows online machine learning algorithms can be easily adapted to many new problems

the fourth siam international conference on data mining continues the tradition of providing an open forum for the presentation and discussion of innovative algorithms as well as novel applications of data mining this is reflected in the talks by the four keynote speakers who discuss data usability issues in systems for data mining in science and engineering issues raised by new technologies that generate biological data ways to find complex structured patterns in linked data and advances in bayesian inference techniques this proceedings includes 61 research papers

cont second we analyze a supervised learning framework in which the observations are assumed to be iid and algorithms are compared by the number of prediction mistakes made in reaching a target generalization error we provide a lower bound on mistakes for perceptron a standard online learning algorithm for this framework we introduce a modification to perceptron and show that it avoids this lower bound and in fact attains the optimal mistake complexity for this setting third we motivate and analyze an online active learning framework the observations are assumed to be iid and algorithms are judged by the number of label queries to reach a target generalization error our lower bound applies to the active learning setting as well as a lower bound on labels for perceptron paired with any active learning rule we provide a new online active learning algorithm that avoids the lower bound and we upper bound its label complexity the upper bound is optimal and also bounds the algorithm s total errors labeled and unlabeled we analyze the algorithm further yielding a label complexity bound under relaxed assumptions using optical character recognition data we empirically compare the new algorithm to an online

active learning algorithm with data dependent performance guarantees as well as to the combined variants of these two algorithms

in machine learning the machine is a learning agent that aims to build a mapping function from a given set of objects to a specific domain of interest in many applications such as in supervised classification or constrained clustering where the output domain includes class and cluster labels respectively learning this function requires having access to a labeled data set assuming that the labels are noiseless this data set includes data samples for which the gold standard or true mapping has been evaluated and therefore can be a useful guide towards estimating the true function in other words the labeled data set let the machine observe a sample of reality from which the machine will learn and extend this knowledge to unobserved cases there are two remarkable points regarding this scenario 1 different choices of labeled samples lead to different estimations of the mapping and 2 observing the reality is always costly depending on how the labeled data set is constructed machine learning algorithms are categorized into two groups passive learners receive the labels passively and play no roles in building the labeled data set whereas active learners take part in choosing what part of the reality to observe the goal in active learning is to query those labels that lead to a good estimation of the gold standard mapping with the least cost this problem can be formulated as an optimization problem provided that we define scoring functions to measure how good we might learn from observing certain parts of the reality after paying certain costs thus one needs to define performance metrics and learning cost functions to do active learning in this thesis we focus on active learning for two specific learning problems classification and constrained clustering for both problems we consider solving the constrained optimization of maximizing the performance metrics when the cost of labeling observation is fixed however directly optimizing performance metrics is intractable in practice and therefore we use information theoretic functions as surrogate objectives under certain assumptions the learning cost is also shown to be proportional to the number of labels to be observed first we consider the problem of constrained binary clustering where a given set of samples are to be segmented into several groups constrained that some samples fall into the same clusters and some are put in different groups that is the constraints are assumed to be provided in form of must links and cannot links between pairs of samples we use spectral clustering with affinity propagation as an existing constrained clustering model and develop an edgewise active learning eal algorithm to query pairwise relationships between certain samples in this algorithm the goal is to decrease uncertainty of the model meaning that the surrogate objective is the model s entropy for optimizing this surrogate we start from an initial clustering of the data and compute confidence of the model regarding cluster assignment of each sample we then select the sample with lowest confidence and query its relationship with samples of highest confidence in each of the two clusters based on the available grouping next we switch to classification problem where the data samples

are to be classified into given set of classes in classification entropy has the shortcoming of querying redundant information and hence sub optimal we develop active learning methods based on two more sophisticated objectives our algorithms are for cases where a pool of unlabeled samples is available and the queries to be labeled will be selected from that pool one of our proposed algorithms is based on maximizing mutual information mi between the observed labels and the unlabeled samples and the other is based on minimizing a scalar function of fisher information matrix of the query distribution we give a rigorous theoretical analysis of using the so called fisher information ratio whose optimization as the surrogate objective can be asymptotically viewed as a bound optimization of a common performance metric

this volume in the challenges in machine learning series gathers the best contributions from the 2010 active learning challenge competition and the associated workshop on active learning and experimental design held in conjunction with aistats 2010 which gathered academic and industry researchers belonging to the various communities of artificial intelligence machine learning statistics and data mining the papers provided here include tutorial material on active learning reports on the competition and its results a set of active learning case studies and appendices providing definitive information about the competition datasets

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