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 AlgorithmsAnalysis of AlgorithmsBioinformatics AlgorithmsAlgorithms for Active LearningAlgorithms for Query-Efficient Active LearningHuman-in-the-Loop Machine LearningAdaptive and Natural Computing AlgorithmsActive Learning for Recommender SystemsOnline Choice of Active Learning AlgorithmsAdvances in Information RetrievalTheory of Disagreement-Based Active LearningLearning with UncertaintyActive LearningActive Learning Algorithms for Multilayer Feedforward Neural NetworksArtificial Neural Networks – ICANN 2009Learning with Online ConstraintsInteractive Machine Learning: from Theory to ScaleOnline Learning Algorithms for Sequence Prediction, Importance Weighted Classification, and Active Learning Burr Settles Mc Connell Phillip Compeau Jeffrey McConnell Phillip Compeau Daniel Joseph Hsu Songbai Yan Robert (Munro) Monarch Bernadete Ribeiro Rasoul Karimi Kobi Luz Giambattista Amati Steve Hanneke Xizhao Wang Simon Tong Adebola Adebisi Adejumo Cesare Alippi Claire Elizabeth Monteleoni Yinglun Zhu Nikolaos Karampatziakis

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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

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

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*

human in the loop machine learning lays out methods for humans and machines to work together effectively summary most machine learning systems that are deployed in the world today learn from human feedback however most machine learning courses focus almost exclusively on the algorithms not the human computer interaction part of the systems this can leave a big knowledge gap for data scientists working in real world machine learning where data scientists spend more time on data management than on building algorithms human in the loop machine learning is a practical guide to optimizing the entire machine learning process including techniques for annotation active learning transfer learning and using machine learning to optimize every step of the process purchase of the print book includes a free ebook in pdf kindle and epub formats from manning publications about the technology machine learning applications perform better with human feedback keeping the right people in the loop improves the accuracy of models reduces errors in data lowers costs and helps you ship models faster about the book human in the loop machine learning lays out methods for humans and machines to work together effectively you ll find best practices on selecting sample data for human feedback quality control for human annotations and designing annotation interfaces you ll learn to create training data for labeling object detection and semantic segmentation sequence labeling and more the book starts with the basics and progresses to advanced techniques like transfer learning and self supervision within annotation workflows what s inside identifying the right training and evaluation data finding and managing people to annotate data selecting annotation quality control strategies designing interfaces to improve accuracy and efficiency about the author robert munro monarch is a data scientist and engineer who has built machine learning data for companies such as apple amazon google and ibm he holds a phd from stanford robert holds a phd from stanford focused on human in the loop machine learning for healthcare and disaster response and is a disaster response professional in addition to being a machine learning professional a worked example throughout this text is classifying disaster related messages from real disasters that robert has helped respond to in the past table of contents part 1 first steps 1 introduction to human in the loop machine learning 2 getting started with human in the loop machine learning part 2 active learning 3 uncertainty sampling 4 diversity sampling 5 advanced active learning 6 applying active learning to different machine learning tasks part 3 annotation 7 working with the people annotating your data 8 quality control for data annotation 9 advanced data annotation and augmentation 10 annotation quality for different machine learning tasks part 4 human computer interaction for machine learning 11 interfaces for data annotation 12 human in the loop machine learning products

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

nowadays we are living in an era that is overloaded with information decision making in this environment can sometimes become a nightmare there are too many choices and we simply cannot explore them all therefore it would be really helpful to have a system to help us to find the right choice such systems which learn user preferences and provide personalized recommendations to them are called recommender systems evidently the performance of recommender systems depends on the amount of information that users provide regarding items most often in the form of ratings this problem is amplified for new users because they have not provided any rating which impacts negatively on the quality of generated recommendations this problem is called new user problem or cold start problem a simple and effective way to overcome this problem is by posing queries to new users so that they express their preferences about selected items e g by rating them nevertheless the selection of items must take into *consideration that users are not willing to answer a lot of such queries to address this problem active learning methods have been proposed to acquire the most informative ratings i e ratings from users that will help most in determining their interests the aim of this thesis is to take inspiration from the literature of active learning for machine learning and develop new methods for the new user problem in recommender systems in the recommender system context new users play the role of the oracle and provide labels ratings to the queries items in this approach we will take into consideration that although there are no data for new users but there is abundant data for existing users such additional data can help us to develop scalable and accurate active learning methods for the new user problem in recommender systems the thesis consists of two parts in the first part to be consistent with the settings of active learning in machine learning and the related works on the new user problem in recommender system it is assumed that the new user is always able to rate the queried items next this constraint is relaxed and new users are allowed not to rate the items most of the developed active learning methods exploit the characteristics matrix factorization because nevertheless recent research especially as has been demonstrated during the netflix challenge indicates that matrix factorization is a superior prediction model for recommender systems compared to other approaches*

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

describes recent advances in our understanding of the theoretical benefits of active learning and implications for the design of effective active learning algorithms it is intended for researchers and students in machine learning and statistics who are interested in gaining a deeper understanding of the developments in active learning

learning with uncertainty covers a broad range of scenarios in machine learning this book mainly focuses on 1 decision tree learning with uncertainty 2 clustering under uncertainty environment 3 active learning based on uncertainty criterion and 4 ensemble learning in a framework of uncertainty the book starts with the introduction to uncertainty including randomness roughness fuzziness and non specificity and then comprehensively discusses a number of key issues in learning with uncertainty such as uncertainty representation in learning the influence of uncertainty on the performance of learning system the heuristic design with uncertainty etc most contents of the book are our research results in recent decades the purpose of this book is to help the readers to understand the impact of uncertainty on learning processes it comes with many examples to facilitate understanding the book can be used as reference book or textbook for researcher fellows senior undergraduates and postgraduates majored in computer science and technology applied mathematics automation electrical engineering etc

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 *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*

while machine learning has made unprecedented successes in many real world scenarios most learning approaches require a huge amount of training data such a requirement imposes real challenges to the practitioners e g data annotation can be expensive and time consuming to overcome these challenges this dissertation studies interactive machine learning where learning is conducted in a closed loop manner the learner uses previously collected information to guide future decisions e g which data points to label next which in turn help make the following predictions this dissertation focuses on developing novel algorithmic principles and uncovering fundamental limits when scaling interactive machine learning into real world settings at large scales more specifically we study interactive machine learning with i noisy data and rich model classes ii large action spaces and iii model selection requirements this dissertation is thus grouped into three corresponding parts to bring the promise of interactive learning into the real world we develop novel human in the loop learning algorithms and systems that achieve both statistical efficiency and computational efficiency in the first part we study active machine learning with noisy data and rich model classes while huge successes of active learning have been observed due to technical difficulties most guarantees are developed i under low noise assumptions and ii for simple model classes we develop efficient algorithms that bypass these two fundamental barriers and thus make an essential step toward real world applications of active learning more specifically by leveraging the power of abstention we develop the first efficient general purpose active learning algorithm that achieves exponential label savings without any low noise assumptions we also develop the first deep active learning i e active learning with neural networks algorithms that achieve exponential label savings when equipped with an abstention option in the second part we study decision making with large action spaces while researchers have explored decision making when the number of alternatives e g actions is small guarantees for decision making in large continuous action spaces remained elusive leading to a significant gap between theory and practice in this part we bridge this gap by developing the first efficient general purpose contextual bandits algorithms for large action spaces in both structured and unstructured cases our algorithms make use of standard computational oracles and achieve nearly optimal guarantees and have runtime and memory independent of the size of the action space our algorithms are also highly practical they achieve the state of the art performance on an amazon dataset with nearly 3 million categories in the third part we study model selection in decision making model selection is the fundamental task in supervised learning but it faces unique challenges when deployed in decision making decisions are made online and only partial feedback is observed focusing on the regret minimization setting we establish fundamental lower bounds showing that model selection in decision making is strictly harder than model selection in standard supervised learning compared to an additional logarithmic cost suffered in supervised learning one has to pay an additional polynomial cost in decision making nevertheless we develop pareto optimal algorithms that achieve matching guarantees up to logarithmic factors focusing on the best action identification setting we develop novel algorithms and show that model selection in best action identification can be achieved without too much additional cost

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*

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