Machine Learning Protein Engineering

CERVANTES CRAWFORD

Enzyme Engineering Springer Nature
This book constitutes the refereed proceedings of the 19th International Conference on Industrial and Engineering Applications of Artificial Intelligence and Expert Systems, IEA/AIE 2006, held in Annecy, France, June 2006. The book presents 134 revised full papers together with 3 invited contributions, organized in topical sections on multi-agent systems, decision-support, genetic algorithms, data-mining and knowledge discovery, fuzzy logic, knowledge engineering, machine learning, speech recognition, systems for real life applications, and more.
Artificial Intelligence in Bioinformatics Machine Learning Based Protein Engineering for Microbial Chemical ProductionThe focus of this dissertation is on applications of machine learning-guided enzyme engineering for modulating metabolic pathways to produce chemicals. Enzyme engineering is especially useful for relieving bottlenecks in pathways, and machine learning strategies can accelerate enzyme engineering by efficiently leveraging data. We review machine learning-based protein engineering as a whole and demonstrate how we used machine learning-guided protein engineering to design acyl-CoA reductase enzymes that had increased activity for converting fatty acyl-ACPs to fatty alcohols. We also discuss machine learning strategies used to design a set of 1-Deoxy-D-Xylulose 5-Phosphate Synthase (DXS) enzymes (which are used for production of terpenoids) that had improved fitness in vivo and illustrate how machine learning was used to understand patterns in the fitness landscape. This dissertation demonstrates ways that machine learning tools can accelerate optimization of metabolic pathways by optimizing protein sequences, and the advances in this thesis can be used to help develop more efficient and sustainable routes to produce chemicals.Handbook of Machine Learning Applications for Genomics The focus of this dissertation is on applications of machine learning-guided enzyme engineering for modulating metabolic pathways to produce chemicals. Enzyme engineering is especially useful for relieving bottlenecks in pathways, and machine learning strategies can accelerate enzyme engineering by efficiently leveraging data. We review machine learning-based protein engineering as a whole and demonstrate how we used machine learning-guided protein engineering to design acyl-CoA reductase enzymes that had increased activity for converting fatty acyl-ACPs to fatty alcohols. We also discuss machine learning strategies used to design a set of 1-Deoxy-D-Xylulose 5-Phosphate Synthase (DXS) enzymes (which are used for production of terpenoids) that had improved fitness in vivo and illustrate how machine learning was used to understand patterns in the fitness landscape. This dissertation demonstrates ways that machine learning tools can accelerate optimization of metabolic pathways by optimizing protein sequences, and the advances in this thesis can be used to help develop more efficient and sustainable routes to produce chemicals.
Computational Tools for Chemical Biology John Wiley & Sons
Machine learning and artificial intelligence have propelled research across various molecular science disciplines thanks to the rapid progress in computing hardware, algorithms, and data accumulation. This book presents recent machine learning applications in the broad research field of molecular sciences. Written by an international group of renowned experts, this edited volume covers both the machine learning methodologies and state-of-the-art machine learning applications in a wide range of topics in molecular sciences, from electronic structure theory to nuclear dynamics of small molecules, to the design and synthesis of large organic and biological

molecules. This book is a valuable resource for researchers and students interested in applying machine learning in the research of molecular sciences.

Introduction to Protein Structure Prediction John Wiley & Sons

An introduction to machine learning methods and their applications to problems in bioinformatics Machine learning techniques are increasingly being used to address problems in computational biology and bioinformatics. Novel computational techniques to analyze high throughput data in the form of sequences, gene and protein expressions, pathways, and images are becoming vital for understanding diseases and future drug discovery. Machine learning techniques such as Markov models, support vector machines, neural networks, and graphical models have been successful in analyzing life science data because of their capabilities in handling randomness and uncertainty of data noise and in generalization. From an internationally recognized panel of prominent researchers in the field, Machine Learning in Bioinformatics compiles recent approaches in machine learning methods and their applications in addressing contemporary problems in bioinformatics. Coverage includes: feature selection for genomic and proteomic data mining; comparing variable selection methods in gene selection and classification of microarray data; fuzzy gene mining; sequence-based prediction of residue-level properties in proteins; probabilistic methods for long-range features in biosequences; and much more. Machine Learning in Bioinformatics is an indispensable resource for computer scientists, engineers, biologists, mathematicians, researchers, clinicians, physicians, and medical informaticists. It is also a valuable reference text for computer science, engineering, and biology courses at the upper undergraduate and graduate levels.

Enzyme Engineering and Evolution: General Methods John Wiley & Sons

Enzyme Engineering An authoritative and up-to-date discussion of enzyme engineering and its applications In Enzyme Engineering: Selective Catalysts for Applications in Biotechnology, Organic Chemistry, and Life Science, a team of distinguished researchers deliver a robust treatment of enzyme engineering and its applications in various fields such as biotechnology, life science, and synthesis. The book begins with an introduction to different protein engineering techniques, covers topics like gene mutagenesis methods for directed evolution and rational enzyme design. It includes industrial case studies of enzyme engineering with a focus on selectivity and activity. The authors also discuss new and innovative areas in the field, involving machine learning and artificial intelligence. It offers several insightful perspectives on the future of this work. Readers will also find: A thorough introduction to directed evolution and rational design as protein engineering techniques Comprehensive explorations of screening and selection techniques, gene mutagenesis methods in directed evolution, and guidelines for applying gene mutagenesis in organic chemistry, pharmaceutical applications, and biotechnology Practical discussions of protein engineering of enzyme robustness relevant to organic and pharmaceutical chemistry Treatments of artificial enzymes as promiscuous catalysts Various lessons learned from semi-rational and rational directed evolution A transdisciplinary treatise, Enzyme Engineering: Selective Catalysts for Applications in Biotechnology, Organic Chemistry, and Life Science is perfect for protein engineers, theoreticians, organic, and pharmaceutical chemists as well as transition metal researchers in catalysis and biotechnologists.

Protein Engineering Packt Publishing Ltd

Deep Learning (DL) is a method of machine learning, running over Artificial Neural Networks, that uses multiple layers to extract high-level features from large amounts of raw data. Deep Learning methods apply levels of learning to transform input data into more abstract and composite information. Handbook for Deep Learning in Biomedical Engineering: Techniques and Applications gives readers a complete overview of the essential concepts of Deep Learning and its applications in the field of Biomedical Engineering. Deep learning has been rapidly developed in recent years, in terms of both methodological constructs and practical applications. Deep Learning provides computational models of multiple processing layers to learn and represent data with higher levels of abstraction. It is able to implicitly capture intricate structures of large-scale data and is ideally suited to many of the hardware architectures that are currently available. The ever-expanding amount of data that can be gathered through biomedical and clinical information sensing devices necessitates the development of machine learning and AI techniques such as Deep Learning and Convolutional Neural Networks to process and evaluate the data. Some examples of biomedical and clinical sensing devices that use Deep Learning include: Computed Tomography (CT), Magnetic Resonance Imaging (MRI), Ultrasound, Single Photon Emission Computed Tomography (SPECT), Positron Emission Tomography (PET), Magnetic Particle Imaging, EE/MEG, Optical Microscopy and Tomography, Photoacoustic Tomography, Electron Tomography, and Atomic Force Microscopy. Handbook for Deep Learning in Biomedical Engineering: Techniques and Applications provides the most complete coverage of Deep Learning applications in biomedical engineering available, including detailed real-world applications in areas such as computational neuroscience, neuroimaging, data fusion, medical image processing, neurological disorder diagnosis for diseases such as Alzheimer's, ADHD, and ASD, tumor prediction, as well as translational multimodal imaging analysis. Presents a comprehensive handbook of the biomedical engineering applications of DL, including computational neuroscience, neuroimaging, time series data such as MRI, functional MRI, CT, EEG, MEG, and data fusion of biomedical imaging data from disparate sources, such as X-Ray/CT Helps readers understand key concepts in DL applications for biomedical engineering and health care, including manifold learning, classification, clustering, and regression in neuroimaging data analysis Provides readers with key DL development techniques such as creation of algorithms and application of DL through artificial neural networks and convolutional neural networks Includes coverage of key application areas of DL such as early diagnosis of specific diseases such as Alzheimer's, ADHD, and ASD, and tumor prediction through MRI and translational multimodality imaging and biomedical applications such as detection, diagnostic analysis, quantitative measurements, and image guidance of ultrasonography

Machine Learning with PyTorch and Scikit-Learn CRC Press

Advances in Protein Molecular and Structural Biology Methods offers a complete overview of the latest tools and methods applicable to the study of proteins at the molecular and structural level. The book begins with sections exploring tools to optimize recombinant protein expression and biophysical techniques such as fluorescence spectroscopy, NMR, mass spectrometry, cryo-electron microscopy, and X-ray crystallography. It then moves towards computational approaches, considering structural bioinformatics, molecular dynamics simulations, and deep machine learning technologies. The book also covers methods applied to intrinsically disordered proteins (IDPs)followed by chapters on protein interaction networks, protein function, and protein design and engineering. It provides researchers with an extensive toolkit of methods and techniques to draw from when conducting their own experimental work, taking them from foundational concepts to practical application. Presents a thorough overview of the latest and emerging methods and technologies for protein study Explores biophysical techniques, including nuclear magnetic resonance, X-ray crystallography, and cryo-electron microscopy Includes computational and machine learning methods Features a section dedicated to tools and techniques specific to studying intrinsically disordered proteins

Handbook of Machine Learning Applications for Genomics CRC Press

This book offers a fresh perspective on how computational tools can aid the chemical biology research community and drive new research.

Statistical Modeling and Machine Learning for Molecular Biology Elsevier

This new volume of Methods in Enzymology continues the legacy of this premier serial with quality chapters authored by leaders in the field. Provides the authority and expertise of leading contributors from an international board of authors Presents the latest release in the Methods in Enzymology series

Deep Learning in Science Royal Society of Chemistry

A one-stop reference that reviews protein design strategies to applications in industrial and medical biotechnology Protein Engineering: Tools and Applications is a comprehensive resource that offers a systematic and comprehensive review of the most recent advances in the field, and contains detailed information on the methodologies and strategies behind these approaches. The authors—noted experts on the topic—explore the distinctive advantages and disadvantages of the presented methodologies and strategies in a targeted and focused manner that allows for the adaptation and implementation of the strategies for new applications. The book contains information on the directed evolution, rational design, and semi-rational design of proteins and offers a review of the most recent applications in industrial and medical biotechnology. This important book: Covers technologies and methodologies used in protein engineering Includes the strategies behind the approaches, designed to help with the adaptation and implementation of these strategies for new applications Offers a comprehensive and thorough treatment of protein engineering from primary strategies to applications in industrial and medical biotechnology Presents cutting edge advances in the continuously evolving field of protein engineering Written for students and professionals of bioengineering, biotechnology, biochemistry, Protein Engineering: Tools and Applications offers an essential resource to the design strategies in protein engineering and reviews recent applications.

A Guide to Applied Machine Learning for Biologists CRC Press

This book of the bestselling and widely acclaimed Python Machine Learning series is a comprehensive guide to machine and deep learning using PyTorch's simple to code framework. Purchase of the print or Kindle book includes a free eBook in PDF format. Key FeaturesLearn applied machine learning with a solid foundation in theoryClear, intuitive explanations take you deep into the theory and practice of Python machine learningFully updated and expanded to cover PyTorch, transformers, XGBoost, graph neural networks, and best practicesBook Description Machine Learning with PyTorch and Scikit-Learn is a comprehensive guide to machine learning and deep learning with PyTorch. It acts as both a step-by-step tutorial and a reference you'll keep coming back to as you build your machine learning systems. Packed with clear explanations, visualizations, and examples, the book covers all the essential machine learning techniques in depth. While some books teach you only to follow instructions, with this machine learning book, we teach the principles allowing you to build models and applications for yourself. Why PyTorch? PyTorch is the Pythonic way to learn machine learning, making it easier to learn and simpler to code with. This book explains the essential parts of PyTorch and how to create models using popular libraries, such as PyTorch Lightning and PyTorch Geometric. You will also learn about generative adversarial networks (GANs) for generating new data and training intelligent agents with reinforcement learning. Finally, this new edition is expanded to cover the latest trends in deep learning, including graph neural networks and large-scale transformers used for natural language processing (NLP). This PyTorch book is your companion to machine learning with Python, whether you're a Python developer new to machine learning or want to deepen your knowledge of the latest developments. What you will learnExplore frameworks, models, and techniques for machines to 'learn' from dataUse scikit-learn for machine learning and PyTorch for deep learningTrain machine learning classifiers on images, text, and moreBuild and train neural networks, transformers, and boosting algorithmsDiscover best practices for evaluating and tuning modelsPredict continuous target outcomes using regression analysisDig deeper into textual and social media data using sentiment analysisWho this book is for If you have a good grasp of Python basics and want to start learning about machine learning and deep learning, then this is the book for you. This is an essential resource written for developers and data scientists who want to create practical machine learning and deep learning applications using scikit-learn and PyTorch. Before you get started with this book, you'll need a good understanding of calculus, as well as linear algebra.

Machine Learning John Wiley & Sons

This volume explores the latest techniques used by researchers to study directed evolution (DE) at each stage of the Design-Build-Test-Learn cycle. Chapters in this book cover topics such as designing overlap extension PCR primers for protein mutagenesis; antha-guided automation of Darwin assembly for the construction of bespoke gene libraries; rapid cloning of random mutagenesis libraries using PTO-Quickstep; and DE of glycosyltransferases by a single-cell screening method. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Cutting-edge and comprehensive, Directed Evolution: Methods and Protocols is a valuable resource for scientists and researchers who are interested in learning more about this field and incorporating these studies into new experimental workflows.

Proceedings of the 2nd International Conference on Data Engineering and Communication Technology World Scientific

A large international conference on Advances in Machine Learning and Systems Engineering was held in UC Berkeley, California, USA, October 20-22, 2009, under the auspices of the World Congress on Engineering and Computer Science (WCECS 2009). Machine Learning and Systems Engineering contains forty-six revised and extended research articles written by prominent researchers participating in the conference. Topics covered include Expert system, Intelligent decision making, Knowledge-based systems, Knowledge extraction, Data analysis tools, Computational biology, Optimization algorithms, Experiment designs, Complex system identification, Computational modeling, and industrial applications. Machine Learning and Systems Engineering offers the state of the art of tremendous advances in machine learning and systems engineering and also serves as an excellent reference text for researchers and graduate students, working on machine learning and systems engineering.

Deep Learning In Biology And Medicine Springer Nature
Molecular biologists are performing increasingly large and complicated experiments, but often have little background in data analysis. The book is devoted to teaching the statistical and computational techniques molecular biologists need to analyze their data. It explains the big-picture concepts in data analysis using a wide variety of real-world molecular biological examples such as eQTLs, ortholog identification, motif finding, inference of population structure, protein fold prediction and many more. The book takes a pragmatic approach, focusing on techniques that are based on elegant mathematics yet are the simplest to explain to scientists with little background in computers and statistics.
A Field Guide to Dynamical Recurrent Networks Academic Press
Machine Learning: A Bayesian and Optimization Perspective, 2nd edition, gives a unified perspective on machine learning by covering both pillars of supervised learning, namely regression and classification. The book starts with the basics, including mean square, least squares and maximum likelihood methods, ridge regression, Bayesian decision theory classification, logistic regression, and decision trees. It then progresses to more recent techniques, covering sparse modelling methods, learning in reproducing kernel Hilbert spaces and support vector machines, Bayesian inference with a focus on the EM algorithm and its approximate inference variational versions, Monte Carlo methods, probabilistic graphical models focusing on Bayesian networks, hidden Markov models and particle filtering. Dimensionality reduction and latent variables modelling are also considered in depth. This palette of techniques concludes with an extended chapter on neural networks and deep learning architectures. The book also covers the fundamentals of statistical parameter estimation, Wiener and Kalman filtering, convexity and convex optimization, including a chapter on stochastic approximation and the gradient descent family of algorithms, presenting related online learning techniques as well as concepts and algorithmic versions for distributed optimization. Focusing on the physical reasoning behind the mathematics, without sacrificing rigor, all the various methods and techniques are explained in depth, supported by examples and problems, giving an invaluable resource to the student and researcher for understanding and applying machine learning concepts. Most of the chapters include typical case studies and computer exercises, both in MATLAB and Python. The chapters are written to be as self-contained as possible, making the text suitable for different courses: pattern recognition, statistical/adaptive signal processing, statistical/Bayesian learning, as well as courses on sparse modeling, deep learning, and probabilistic graphical models. New to this edition: Complete re-write of the chapter on Neural Networks and Deep Learning to reflect the latest advances since the 1st edition. The chapter, starting from the basic perceptron and feed-forward neural networks concepts, now presents an in depth treatment of deep networks, including recent optimization algorithms, batch normalization, regularization techniques such as the dropout method, convolutional neural networks, recurrent neural networks, attention mechanisms, adversarial examples and training, capsule networks and generative architectures, such as restricted Boltzman machines (RBMs), variational autoencoders and generative adversarial networks (GANs). Expanded treatment of Bayesian learning to include nonparametric Bayesian methods, with a focus on the Chinese restaurant and the Indian buffet processes. Presents the physical reasoning, mathematical modeling and algorithmic implementation of each method Updates on the latest trends, including sparsity, convex analysis and optimization, online distributed algorithms, learning in RKH spaces, Bayesian inference, graphical and hidden Markov models, particle filtering, deep learning, dictionary learning and latent variables modeling Provides case studies on a variety of topics, including protein folding prediction, optical character recognition, text authorship identification, fMRI data analysis, change point detection, hyperspectral image unmixing, target localization, and more
Predicting Expression Levels of de Novo Protein Designs in Yeast Through Machine Learning Academic Press
Machine Learning (ML) is a sub field of artificial intelligence that uses soft computing and algorithms to enable computers to learn on their own and identify patterns in observed data, build models that explain the world, and predict things without having explicit pre-programmed rules and models. This book discusses various applications of ML in engineering fields and the use of ML algorithms in solving challenging engineering problems ranging from biomedical, transport, supply chain and logistics, to manufacturing and industrial. Through numerous case studies, it will assist researchers and practitioners in selecting the correct options and strategies for managing organizational tasks.
Advanced AI Techniques and Applications in Bioinformatics IOS Press
Proteins have been a central focus of engineering since the central dogma of biology was first described in 1957. The sheer number of functions they perform in the natural world is astounding. Many of the most important proteins involved in sustaining biological processes are enzymes and transcription factors. While many engineering attempts have been made with these types of proteins; new avenues have presented themselves in part due to the explosion of NGS, transcriptomics, and the bioinformatics methods designed to aid in these analyses. This thesis exemplifies the multidisciplinary approach of current protein engineering methods and the ways in which they must be tailored to the questions that are being asked. In the first study we examine not only how the burgeoning field of machine learning can be used to optimize plastic degrading enzymes, but interrogate how to best characterize the chemical changes occurring during degradation. In our second study we explore novel bioinformatics-based methods for pulling essential functional motifs out of a set of related enzymes using De Bruijn Graphs, a never before seen application of this powerful algorithm that we show outperforms other motif finding methods. I used this novel pipeline to isolate enzymes from metagenomic and protein databases with esterase activity and putative PETase activity. Lastly, I harness a creative directed evolution method (SELIS) developed by my colleague Simon d'Oelsnitz to engineer new transcription factor specificity for prokaryotic TF RolR and untangle how structural changes in the active site impact ligand binding. Together these studies advance our understanding of rational design, and bioinformatics, and directed evolution as applied to protein engineering
Directed Evolution CRC Press
The advanced AI techniques are essential for resolving various problematic aspects emerging in the field of bioinformatics. This book covers the recent approaches in artificial intelligence and machine learning methods and their applications in Genome and Gene editing, cancer drug discovery classification, and the protein folding algorithms among others. Deep learning, which is widely used in image processing, is also applicable in bioinformatics as one of the most popular artificial intelligence approaches. The wide range of applications discussed in this book are an indispensable resource for computer scientists, engineers, biologists, mathematicians, physicians, and medical informaticists. Features: Focusses on the cross-disciplinary relation between computer science and biology and the role of machine learning methods in resolving complex problems in bioinformatics Provides a comprehensive and balanced blend of topics and applications using various advanced algorithms Presents cutting-edge research methodologies in the area of AI methods when applied to bioinformatics and innovative solutions Discusses the AI/ML techniques, their use, and their potential for use in common and future bioinformatics applications Includes recent achievements in AI and bioinformatics contributed by a global team of researchers
Algorithms in Structural Molecular Biology Academic Press
This volume provides protocols for computational, statistical, and machine learning methods that are mainly applied to the study of metabolic engineering, synthetic biology, and disease applications. These techniques support the latest progress in cross-disciplinary research that integrates the different scales of biological complexity. The topics covered in this book are geared toward researchers with a background in engineering, computational analytical, and modeling experience and cover a broad range of topics in computational and machine learning approaches. Written in the highly successful Methods in Molecular Biology series format, chapters include introductions to their respective topics, lists of the necessary materials and reagents, step-by-step, readily reproducible laboratory protocols, and tips on troubleshooting and avoiding known pitfalls. Comprehensive and practical, Computational Biology and Machine Learning for Metabolic Engineering and Synthetic Biology is a valuable resource for any researcher or scientist who wants to learn more about the latest computational methods and how they are applied toward the understanding and prediction of complex biology.
Statistical Modelling and Machine Learning Principles for Bioinformatics Techniques, Tools, and Applications MIT Press
This book features research work presented at the 2nd International Conference on Data Engineering and Communication Technology (ICDECT) held on December 15–16, 2017 at Symbiosis International University, Pune, Maharashtra, India. It discusses advanced, multi-disciplinary research into smart computing, information systems and electronic systems, focusing on innovation paradigms in system knowledge, intelligence and sustainability that can be applied to provide feasible solutions to varied problems in society, the environment and industry. It also addresses the deployment of emerging computational and knowledge transfer approaches, optimizing solutions in a variety of disciplines of computer science and electronics engineering.

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