

8th Annual ACM Conference on Bioinformatics,
Computational Biology, and Health Informatics
acm-bcb.org



Association for
Computing Machinery



BOSTON, MA

August 20 - 23, 2017



* Logo design by Barbara Pixton

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Conference Program

Sunday, August 20, 2017									
Registration	08:00-18:00 at Salons 1-3 Foyer								
Venue	08:00-10:00	10:00-10:30	10:30-12:00	12:00-1:30pm	1:30-3:30	3:30-4:00	4:00-5:30	6:00-8:00	
Salons 1-2	MMM	Coffee Break Salons 1-3 Foyer	MMM	Lunch on your own	MMM	Coffee Break Salons 1-3 Foyer	MMM		
Concept	CSBW		CSBW		CSBW		CSBW	CSBW	Student event
Endeavor	CNB-MAC		CNB-MAC		CNB-MAC		CNB-MAC	CNB-MAC	
Salons 5-6	CAME		CAME		CAME		CAME	CAME	
Enterprise	Tutorial 1		Tutorial 1		Tutorial 1		Student Mentoring Workshop	Student Mentoring Workshop	
Discovery	Tutorial 2		Tutorial 3		Tutorial 3		PAR-BIO	Tutorial 4	

Sunday Workshops (See page 15 for detailed workshop programs)

- CNB-MAC** 4th International Workshop on Computational Network Biology: Modeling, Analysis, and Control
Organizers: Byung-Jun Yoon, Xiaoning Qian and Tamer Kahveci
- ParBio** 6th International Workshop on Parallel and Cloud-based Bioinformatics and Biomedicine
Organizers: Mario Cannataro and John A. Springer
- CWBW** The 2017 Computational Structural Bioinformatics Workshop
Organizers: Nurit Haspel, Kevin Molloy and Amarda Shehu
- MMM** Workshop on Microbiomics, Metagenomics, and Metabolomics
Organizers: Soha Hassoun, Curtis Huttenhower
- CAME** 6th Workshop on Computational Advances in Molecular Epidemiology
Organizers: Yury Khudyakov, Ion Mandoiu, Pavel Skums, Alex Zelikovsky

Tutorials (See page 21 for detailed tutorial programs)

- T1** Introducing the New eICU Collaborative Research Database
Organizers: Alistair E. W. Johnson, Tom J. Pollard, Roger G. Mark, and Leo A. Celi
- T2** Computational modeling of protein-RNA interactions
Organizer: Yaron Orenstein. Presenter: Austin Wang.
- T3** Robotics-inspired Algorithms for Modeling Protein Structures and Motions
Organizers: Amarda Shehu and Kevin Molloy
- T4** Stochastic Process Model and Its Applications to Analysis of Longitudinal Data
Organizers: Ilya Y. Zhbannikov and Konstantin G. Arbeev

Student Networking and Social Event: All students and postdocs are invited to this year's social events, featuring a scavenger hunt through Cambridge! As in previous years of ACM BCB, we anticipate that this will be a great networking opportunity for students. We encourage you to discuss some of your ongoing research and especially to make new contacts outside of your home institutions and labs. 6:00pm: Meet in **Concept** at the conference hotel to receive the list of within-walking-distance sights in Cambridge. You do

not need to have a team before you come to the event -- we can find teammates for you! If you prefer to arrive as a team, the ideal team size is 2-5 people.

Each team will be assigned a team number, and you can post selfies on social media with the hashtags #acmbcb2017 #scavengerhunt #teamX and/or email your selfies to either Shilpa or Jisoo (jp.jisoopark@gmail.com, shilpa.kobren@gmail.com). You'll have 60-75 minutes from the time you start to complete your quest! Prizes will be awarded to the top two winning teams!

9:00-10:00pm: After a break for dinner, a group of us will be heading 2 minutes down the street to Meadhall (4 Cambridge Center) where drinks, dessert, and other food will be available for purchase.

NOTE: You need to be 21+ with an official state/national ID to purchase any alcoholic beverages, although entrance to Meadhall and purchase of food/non-alcoholic beverages is open to all.

Monday, August 21, 2017				
Registration	08:00-18:00 at Salons 1-3 Foyer			
08:45-09:00	Opening and Welcome Remarks – General Chairs			
09:00-10:00	Session Chair: Nurit Haspel Keynote Speaker: Shawn Murphy Keynote: “Instrumenting the Health Care Enterprise for Discovery in the Course of Clinical Care” Venue: Salon 3			
10:00-10:30	Coffee Break at Salons 1-3 Foyer			
10:30-12:00	Session 1 Venue: Salon 3	Session 2 Venue: Salons 1-2	Session 3 Venue: Discovery	WABI Session 1 Venue: Concept
	Cancer Genomics and Inferring Phylogenies and Haplotypes	Text Mining and Classification	Proteins and RNA Structure, Dynamics, and Analysis I	
Session Chair	Kevin Liu	Eva Lee	Filip Jagodzinski	Jing Li
12:00-14:00	Lunch on your own			
14:00-15:30	Session 4 Venue: Salon 3	Session 5 Venue: Salons 1-2	Session 6 Venue: Discovery	WABI Session 2 Venue: Concept
	Genomic Variation and Disease	Clinical Databases and Information Systems	Big Data in Bioinformatics I	
Session Chair	Anna Ritz	Carlo Combi	Ananth Kalyanaraman	Sven Rahmann
15:30-16:00	Coffee Break at Salons 1-3 Foyer			
16:00-17:30	ACM SIGBIO General Meeting			WABI Session 3
Session Chair				Rob Patro
Venue	Salon 3			Salons 1-2
18:00-20:00	Poster Session and Reception at Salons 4-7			

Session 1: Cancer Genomics, and Inferring Phylogenies and Haplotypes	
Highlight	“Pancancer Modelling Predicts the Context-specific Impact of Somatic Mutations on Transcriptional Programs” Hatice Osmanbeyoglu, Eneida Toska, Carmen Chan, Jose Baselga and Christina Leslie
Long	“Beyond Perfect Phylogeny: Multisample Phylogeny Reconstruction via ILP” Paola Bonizzoni, Simone Ciccolella, Gianluca Della Vedova and Mauricio Soto
Long	“A Compatibility Approach to Identify Recombination Breakpoints in Sequence Alignments” Yi-Pin Lai and Thomas R. Ioerger
Short	“Phylogenetic tree based method for uncovering co-mutational site-pairs in influenza viruses” Fransiskus Xaverius Ivan, Xinrui Zhou, Akhila Deshpande, Rui Yin, Jie Zheng and Chee Keong Kwoh

Session 2: Text Mining and Classification	
Long	“Mapping Free Text into MedDRA by Natural Language Processing: a Modular Approach in Designing and Evaluating Software Extensions” Margherita Zorzi, Carlo Combi, Gabriele Pozzani and Ugo Moretti
Long	“Dependency Embeddings and AMR Embeddings for Drug-Drug Interaction Extraction from Biomedical Texts” Authors: Yanshan Wang, Sijia Liu, Majid Rastegar-Mojarad, Liwei Wang, Feichen Shen, Fei Liu and Hongfang Liu
Long	“Leveraging Sentiment Analysis for Classifying Patient Complaints” Adel Elmessiry, Zhe Zhang, Jan Karrass, Tom Catron, William Cooper and Munindar Singh
Short	“Identifying Harm Events in Clinical Care through Medical Narratives” Arman Cohan, Allan Fong, Raj Ratwani and Nazli Goharian

Session 3 Protein and RNA Structure, Dynamics, and Analysis I	
Highlight	“Fast, Clash-free RNA Conformational Morphing Using Molecular Junctions” Amelie Heliou, Dominik Budday, Rasmus Fonseca and Henry van den Bedem
Long	“GOstruct 2.0: Automated Protein Function Prediction for Annotated Proteins” Authors: Indika Kahanda and Asa Ben-Hur
Short	“Identification and Prediction of Intrinsically Disordered Regions in Proteins using n-grams” Mauricio Oberti and Iosif Vaisman
Short	Deep recurrent conditional random field network for protein secondary prediction Alexander Rosenberg Johansen, Casper Kaae S�nderby, S�ren Kaae S�nderby and Ole Winther

Session 4: Genomic Variation and Disease	
Long	“CERENKOV: Computational Elucidation of the REgulatory NonKODing Variome” Yao Yao, Zheng Liu, Satpreet Singh, Qi Wei and Stephen Ramsey
Long	“Exploring Frequented Regions in Pan-Genomic Graphs” Alan Cleary, Thiruvarangan Ramaraj, Indika Kahanda, Joann Mudge and Brendan Mumej
Long	“Bayesian Hyperparameter Optimization for Machine Learning Based eQTL Analysis” Andrew Quitadamo, James Johnson and Xinghua Shi
Short	“Coal-Miner: a Coalescent-based Method for GWA Studies of Quantitative Traits with Complex Evolutionary Origins” Hussein Hejase, Natalie Vandepol, Gregory Bonito, Patrick Edger and Kevin Liu

Session 5: Clinical Databases and Information Systems	
Long	“Learning Deep Representations from Heterogeneous Patient Data for Predictive Diagnosis” Chongyu Zhou, Jia Yao, Mehul Motani and Jingwei Chew
Long	“Winnow: Interactive Visualization of Temporal Changes in Multidimensional Clinical Data” Hsueh-Chien Cheng, Rainer von Coelln, Ann L. Gruber-Baldini, Lisa M. Shulman and Amitabh Varshney
Long	“Associating Genomics and Clinical Information by Means of Semantic Based Ranking” Francesca Cristiano, Giuseppe Tradigo and Pierangelo Veltri
Short	“Tailoring Training for Obese Individuals Through a Case-Based System” Fabiana Lorenzi, Rodrigo Goulart Da Rosa, Alessandra Peres, Gilson Pires Dorneles, Andre Peres and Francesco Ricci

Session 6: Big Data in Bioinformatics I	
Long	“SparkGA: A Spark Framework for Cost Effective, Fast and Accurate DNA Analysis at Scale” Hamid Mushtaq, Zaid Al-Ars, H. Peter Hofstee, Frank Liu, Carlos H. A. Costa and Gang Liu
Long	“Fast and Highly Scalable Bayesian MDP on a GPU Platform” He Zhou, Sunil P. Khatr, Jiang Hu, Frank Liu and Cliff Sze
Long	“Inferring Microbial Interactions from Metagenomic Time-series Using Prior Biological Knowledge” Chieh Lo and Radu Marculescu
Short	“Secure Cloud Computing for Pairwise Sequence Alignment” Sergio Salinas and Pan Li

WABI Session 1	
Long	“Seed-driven Learning of Position Weight Matrices from Large Sequence Sets” Jarkko Toivonen, Esko Ukkonen and Jussi Taipale
Long	“Fast Spaced Seed Hashing” Samuele Girotto, Matteo Comin and Cinzia Pizzi
Long	“Optimal Computation of Overabundant Words” Yannis Almirantis, Panagiotis Charalampopoulos, Jia Gao, Costas S. Iliopoulos, Manal Mohamed, Solon P. Pissis and Dimitris Polychronopoulos

WABI Session 2	
Long	"Rainbowfish: A Succinct Colored de Bruijn Graph Representation" Fatemeh Almodaresi, Prashant Pandey and Rob Patro
Long	"Disentangled Long-Read De Bruijn Graphs via Optical Maps" Bahar Alipanahi, Leena Salmela, Simon Puglisi, Martin Muggli and Christina Boucher
Long	"ThIEF: Finding Genome-wide Trajectories of Epigenetics Marks" Anton Polishko, Md Abid Hasan, Weihua Pan, Evelien Bunnik, Karine Le Roch and Stefano Lonardi

WABI Session 3	
Long	"Analysis of min-hashing for variant tolerant DNA read mapping" Jens Quedenfeld and Sven Rahmann
Long	"Byte-Aligned Pattern Matching in Compressed Genomic Sequences" Petr Prochazka and Jan Holub
Long	"Yanagi: Transcript Segment Library Construction for RNA-Seq Quantification" Mohamed Gunady, Hector Bravo, Stephen Mount and Steffen Cornwell

Tuesday, August 22, 2017				
Registration	08:00-18:00 at Salons 1-3 Foyer			
08:45-09:00	Session Chair: Amarda Shehu			
09:00-10:00	Keynote Speaker: Dagmar Ringe Keynote: "Challenges to Drug Design" Venue: Salon 3			
10:00-10:30	Coffee Break at Salons 1-3 Foyer			
10:30-12:00	Session 7 Venue: Salons 1-2	Session 8 Venue: Salon 3	Session 9 Venue: Discovery	WABI Session 4 Venue: Concept
	Advancing Algorithms and Methods I	Automated Diagnosis and Prediction I	Protein and RNA Structure, Dynamics, and Analysis I	
Session Chair	Mukul Bansal	May Wang	Henry van den Bedem	David Fernandez-Baca
12:00-13:30	Boxed Lunch Join Women in Bioinformatics (WiB) at Discovery			
13:30-14:00	Session Chair: Giuseppe Pozzi Keynote Speaker: Enoch Huang Keynote: "Demystifying Careers in the Biopharmaceutical Industry" Venue: Salon 3			
14:00-15:30	Industry Panel Venue: Salon 1-2	Session 10 Venue: Salon 3	Session 11 Venue: Discovery	WABI Session 5 Venue: Concept
		Advancing Algorithms and Methods II	Applications to Microbes and Imaging Genetics	
Session Chair	Soha Hassoun	Oliver Eulenstein	Adam Wright	Krister Swenson
15:30-16:00	Coffee Break at Salons 1-3 Foyer			
16:00-18:00	NSF-sponsored Student Research Forum Venue: Salons 1-2		Demos and Exhibits Venue: Discovery	WABI Session 6 Venue: Concept
Session Chair				Sangtae Kim
18:30-20:00	Dinner Banquet at Salons 3-4			

Session 7: Advancing Algorithms and Methods I	
Long	"Rich Chromatin Structure Prediction from Hi-C Data" Laraib Iqbal Malik and Robert Patro
Long	"Cophenetic Median Trees Under the Manhattan Distance" Alexey Markin and Oliver Eulenstein
Long	"DeepCCI: End-to-end Deep Learning for Chemical-Chemical Interaction Prediction" Sunyoung Kwon and Sungroh Yoon

Session 8: Automated Diagnosis and Prediction I	
Long	"A Multi-view Deep Learning Method for Epileptic Seizure Detection using Short-time Fourier transform" Ye Yuan, Guangxu Xun, Kebin Jia and Aidong Zhang
Long	"TUCUXI – An Intelligent System for Personalized Medicine: from Individualization of Treatments to Research Databases and Back" Alevtina Dubovitskaya, Thierry Buclin, Michael Ignaz Schumacher, Karl Aberer and Yann Thoma
Long	"Interpretable Predictions of Clinical Outcomes with An Attention-based Recurrent Neural Network" Ying Sha and May D. Wang
Short	"Confused or not Confused? Disentangling Brain Activity from EEG Data Using Bidirectional LSTM Recurrent Neural Networks" Zhaoheng Ni, Ahmet Cem Yuksel, Xiuyan Ni, Michael Mandel and Lei Xie

Session 9: Protein and RNA Structure, Dynamics, and Analysis II	
Highlight	“3D Genome Structure Modeling by Lorentzian Objective Function” Tuan Trieu and Jianlin Cheng
Highlight	“Folding Large Proteins by Ultra-Deep Learning” Jinbo Xu, Sheng Wang, Siqi Sun, Zhen Li and Renyu Zhang
Short	“Predicting the Effect of Point Mutations on Protein Structural Stability” Roshanak Farhoodi, Max Shelbourne, Rebecca Hsieh, Nurit Haspel, Brian Hutchinson, and Filip Jagodzinski

Session 10: Advancing Algorithms and Methods II	
Long	“Synthesizing Species Trees from Unrooted Gene Trees: A Parameterized Approach” Jucheol Moon and Oliver Eulenstein
Long	“Fleximer: Accurate Quantification of RNA-Seq via Variable-Length k-mers” Chelsea J.-T. Ju, Ruirui Li, Zhengliang Wu, Jyun-Yu Jiang, Zhao Yang and Wei Wang
Short	“A Sparse Latent Regression Approach for Integrative Analysis of Glycomic and Glycotranscriptomic Data” Xuefu Wang, Sujun Li, Wenjing Peng, Xue Dong, Yehia Mechref and Haixu Tang
Short	“Use of Structural Properties of Underlying Graphs in Pathway Enrichment Analysis of Genomic Data” Pourya Naderi Yeganeh and M. Taghi Mostafavi

Session 11: Applications to Microbes and Imaging Genetics	
Long	“Seq2seq Fingerprint: An Unsupervised Deep Molecular Embedding for Drug Discovery” Zheng Xu, Sheng Wang, Feiyun Zhu and Junzhou Huang
Long	“Detection of Differential Abundance Intervals in Longitudinal Metagenomic Data Using Negative Binomial Smoothing Spline ANOVA” Ahmed Metwally, Patricia Finn, Yang Dai and David Perkins.
Short	“Cell Neighbor Determination in the Metazoan Embryo System” Zi Wang, Dali Wang, Husheng Li and Zhirong Bao
Short	“Predictive and Comparative Network Analysis of the Gut Microbiota in Type 2 Diabetes” Mostafa Abbas and Yasser El-Manzalawy

WABI Session 4	
Long	“All fingers are not the same: Handling variable-length sequences in a discriminative setting using conformal multi-instance kernels” Sarvesh Nikumbh, Peter Ebert and Nico Pfeifer
Long	“Towards distance-based phylogenetic inference in average-case linear-time” Maxime Crochemore, Alexandre P Francisco, Solon P Pissis and Cátia Vaz
Long	“Forbidden Time Travel: Characterization of Time-Consistent Tree Reconciliation Maps” Nikolai Nøjgaard, Manuela Geiß, Daniel Merkle, Peter F. Stadler, Nicolas Wieseke and Marc Hellmuth

WABI Session 5	
Long	“A general framework for gene tree correction” Nadia El-Mabrouk and Aida Ouangraoua
Long	“Detecting Locus Acquisition Events in Gene Trees” Michał Ciach, Anna Muszewska and Paweł Górecki
Long	“Optimal Completion of Incomplete Gene Trees in Polynomial Time” Sarah Christensen, Erin Molloy, Pranjal Vachaspati and Tandy Warnow

WABI Session 6	
Long	“Outlier detection in BLAST hits” Nidhi Shah, Stephen Altschul and Mihai Pop
Long	“Assessing the Significance of Peptide Spectrum Match Scores” Anastasiia Abramova and Anton Korobeynikov
Long	“Improved De Novo Peptide Sequencing using LC Retention Time Information” Yves Frank, Tomas Hruz, Thomas Tschager and Valentin Venzin

Wednesday, August 23, 2017				
Registration	08:00-18:00 at Salons 1-3 Foyer			
08:45-09:00	Opening and Welcome Remarks			
09:00-10:00	Session Chair: Lenore Cowen Keynote Speaker: Tandy Warnow Keynote: "Genome-scale Estimation of the Tree of Life" Venue: Salon 3			
10:00-10:30	Coffee Break at Salons 1-3 Foyer			
10:30-12:00	Session 12	Session 13	Session 14	WABI Session 7
	Systems Biology I Venue: Salons 1-2	Knowledge Representation Applications Venue: Salons 5-7	Integrative Methods for Genomic Data Venue: Discovery	Venue: Concept
Session Chair	Jérôme Waldispühl	Pierangelo Veltri	Marco Masseroli	Christina Boucher
12:00-14:00	Lunch on your own			
14:00-15:30	Session 15	Session 16	Session 17	WABI Session 8
	Sequence Analysis and Genome Assembly Venue: Salons 1-2	Applications to Healthcare Processes Venue: Salons 5-7	Biological Modeling Venue: Discovery	Venue: Concept
Session Chair	Christina Boucher	Alistair Johnson	Naveena Yanamala	Su-In Lee
15:30-16:00	Coffee Break at Salons 1-3 Foyer			
16:00-17:30	Session 18	Session 19	Session 20	WABI Session 9
	Systems Biology II Venue: Salons 1-2	Automated Diagnosis and Prediction II Venue: Salons 5-7	Big Data in Bioinformatics II Venue: Discovery	Venue: Concept
Session Chair	Xinghua (Mindy) Shi	Dong Si	Tom Pollard	Leena Salmela
17:30-17:45	Closing Remarks at Salon 3			

7:00pm: For the students and postdocs still around after the conference, there will be a free multi-cultural Landmarks Dance Festival one subway stop (or a 25 min. walk) away at the Hatch Shell on the Charles River Esplanade (47 David G Mugar Way, Boston), featuring dancers from across the city!

*Please email Jisoo (jp.jisoo@gmail.com) or Shilpa (shilpa.kobren@gmail.com) with any concern or question.

Session 12: Systems Biology I	
Highlight	"Network-based Interpretation of Diverse High-throughput Datasets through the Omics Integrator Software Package" Amanda Kedaigle
Long	"Bayesian Collective Markov Random Fields for Subcellular Localization Prediction of Human Proteins" Lu Zhu and Martin Ester
Long	"Differential Community Detection in Paired Biological Networks" Raghvendra Mall, Ehsan Ullah, Khalid Kunji, Fulvio D'angelo, Halima Bensmail and Michele Ceccarelli
Short	"TINTIN: Exploiting Target Features for Signaling Network Similarity Computation and Ranking" Huey Eng Chua, Sourav S Bhowmick and Lisa Tucker-Kellogg

Session 13: Knowledge Representation Applications	
Long	"Determining Optimal Features for Predicting Type IV Secretion System Effector Proteins for Coxiella burnetii" Zhila Esna Ashari Esfahani, Kelly Brayton and Shira Broschat
Long	"Knowledge Rich Natural Language Queries over Structured Biological Databases" Hasan M. Jamil

Long	“Discovering Inconsistencies in PubMed abstracts through Ontology-based Information Extraction” Nisansa de Silva, Dejing Dou and Jingshan Huang
Short	“TRuML: A Translator for Rule-Based Modeling Languages” Ryan Suderman and William S. Hlavacek

Session 14: Integrative Methods for Genomic Data	
Highlight	“Analysis of Single Cells on a Pseudotime Scale along Postnatal Pancreatic Beta Cell Development” Francesca Mulas, Chun Zeng, Yinghui Sui, Tiffany Guan, Nathanael Miller, Yuliang Tan, Fenfen Liu, Wen Jin, Andrea C. Carrano, Mark O. Huising, Orian S. Shirihai, Gene Yeo and Maik Sander
Long	“HEMnet: Integration of Electronic Medical Records with Molecular Interaction Networks and Domain Knowledge for Survival Analysis” Edward W Huang, Chengxiang Zhai, Sheng Wang, Bingxue Li, Ran Zhang , Baoyan Liu , Runshun Zhang, Jie Liu,
Short	Xuezhong Zhou , Hongsheng Lin
Short	“A Novel Approach for Classifying Gene Expression Data using Topic Modeling” Soon Jye Kho, Hima Bindu Yalamanchili, Michael L Raymer and Amit P Sheth
Short	“Differential Compound Prioritization via Bi-Directional Selectivity Push with Power” Junfeng Liu and Xia Ning

Session 15: Sequence Analysis and Genome Assembly	
Long	“Understanding Sequence Conservation with Deep Learning” Yi Li, Daniel Quang and Xiaohui Xie
Long	“SeqyClean: a Pipeline for High-throughput Sequence Data Preprocessing” Ilya Zhbannikov, Samuel Hunter, James Foster and Matthew Settles
Short	“Distributed Memory Partitioning of High-Throughput Sequencing Datasets for Enabling Parallel Genomics Analyses”
Short	Nagakishore Jammula, Sriram P. Chockalingam and Srinivas Aluru
Short	“Scalable Genomic Assembly through Parallel de Bruijn Graph Construction for Multiple K-mers” Kanak Mahadik, Christopher Wright, Milind Kulkarni, Saurabh Bagchi and Somali Chaterji

Session 16: Applications to Healthcare Processes	
Highlight	“Drug Response Prediction as a Link Prediction Problem” Zachary Stanfield, Mustafa Coskun and Mehmet Koyuturk
Long	“Co-MEAL: Cost-Optimal Multi-expert Active Learning Architecture for Mobile Health Monitoring” Ramyar Saeedi, Keyvan Sasani and Assefaw Gebremedhin
Long	“Antidote Application: an Educational System for Treatment of Common Toxin Overdose” Jon Long, Yingyuan Zhang, Vladimir Brusic, Lou Chitkushev and Guanglan Zhang
Short	“Automated Off-label Drug Use Detection from User Generated Content” Mengnan Zhao and Christopher C. Yang

Session 17: Biological Modeling	
Highlight	“Model-based Transcriptome Engineering” Michael R. Brent
Long	“Circadian Rhythms in Neurospora Exhibit Biologically Relevant Driven and Damped Harmonic Oscillations” Hannah De Los Santos, Emily J. Collins, Jennifer M. Hurley and Kristin P. Bennett
Long	“Hybrid ODE/SSA Model of the Budding Yeast Cell Cycle Control Mechanism with Mutant Case Study” Mansoor Ahmadian, Shuo Wang, John Tyson and Young Cao
Short	“RBFNN-based Modelling and Analysis for the Signal Reconstruction of Peripheral Nerve Tissue” Qichun Zhang and Francisco Sepulveda

Session 18: Systems Biology II	
Long	“Reverse Engineering Gene Networks: A Comparative Study at Genome-scale” Sriram P. Chockalingam, Maneesha Aluru, Hongqing Guo, Yanhai Yin and Srinivas Aluru
Long	“Unsupervised Multi-View Feature Selection for Tumor Subtype Identification”

Long	Sultan Imangaliyev, Bart Keijser, Wlm Crelaard and Evgeni Levin “Computational Intractability Generates the Topology of Biological Networks”
Short	Ali Atiia, Corbin Hopper and Jérôme Waldispühl “A Flexible and Robust Multi-Source Learning Algorithm for Drug Repositioning” Huiyuan Chen and Jing Li

Session 19: Automated Diagnosis and Prediction II	
Long	“Tensor-Factorization-Based Phenotyping using Group Information: Case Study on the Efficacy of Statins” Jingyun Choi, Yejin Kim, Hun-Sung Kim, In Young Choi and Hwanjo Yu
Long	“Infer Cause of Death for Population Health Using Convolutional Neural Network” Hang Wu and May Wang
Short	“Automated Breast Cancer Diagnosis Using Deep Learning and Region of Interest Detection (BC-DROID)” Richard Platania, Shayan Shams, Seungwon Yang, Jian Zhang, Kisung Lee and Seung-Jong Park
Short	“A Physiological Thermal Regulation Model with Application to the Diagnosis of Diabetic Peripheral Neuropathy” Viktor Chekh, Peter Soliz, Mark Burge and Shuang Luan

Session 20: Big Data in Bioinformatics II	
Short	“An Out-of-Core GPU Based Dimensionality Reduction Algorithm for Big Mass Spectrometry Data and its Application in Bottom-up Proteomics” Muaaz Gul Awan and Fahad Saeed
Short	“Building Applications for Interactive Data Exploration in Systems Biology” Bjørn Fjukstad, Vanessa Dumeaux, Karina Standahl Olsen, Eiliv Lund, Michael Hallett and Lars Ailo Bongo
Short	“Mining Faces from Biomedical Literature using Deep Learning” Mitchell Dawson, Andrew Zisserman and Christoffer Nellåker
Short	“A Correlation Network Model Utilizing Gait Parameters for Evaluating Health Levels” Elham Rastegari and Hesham Ali

WABI Session 7	
Long	“Sparsification enables predicting kissing hairpin pseudoknot structures of long RNAs in practice” Hosna Jabbari, Ian Wark, Carlo Montemagno and Sebastian Will
Long	“Efficient and Accurate Detection of Topologically Associating Domains from Contact Maps” Abbas Roayaei Ardakany and Stefano Lonardi
Long	“An IP algorithm for RNA folding trajectories” Amir Bayegan and Peter Clote

WABI Session 8	
Long	“Vaquita: Fast and Accurate Identification of Structural Variation using Combined Evidence” Jongkyu Kim and Knut Reinert
Long	“Finding local genome rearrangements” Pijus Simonaitis and Krister Swenson
Long	“abSNP: RNA-Seq SNP Calling in Repetitive Regions via Abundance Estimation” Shunfu Mao, Kannan Ramachandran, David Tse, Soheil Mohajer and Sreeram Kannan

WABI Session 9	
Long	“Better Greedy Sequence Clustering with Fast Banded Alignment” Brian Brubach, Jay Ghurye, Aravind Srinivasan and Mihai Pop
Long	“Shrinkage Clustering: a fast and size-constrained algorithm for biomedical applications” Chenyue Hu, Hanyang Li and Amina Qutub
Long	“Gene Tree Parsimony for Incomplete Gene Trees” Md. Shamsuzzoha Bayzid and Tandy Warnow

Keynotes

Monday, August 21 | Shawn Murphy, Partners Healthcare



Title: Instrumenting the Health Care Enterprise for Discovery in the Course of Clinical Care

Abstract: Although patients may have a wealth of imaging, genomic, monitoring, and personal device data, it has yet to be fully integrated into clinical care. We identify three reasons for the lack of integration. The first is that “Big Data” is poorly managed by most Electronic Medical Record Systems (EMRS). The data is mostly available on “cloud-native” platforms that are outside the scope of most EMRS, and even checking if such data is available on a patient often must be done outside the EMRS. The second reason is that extracting features from the Big Data that are relevant to healthcare often requires complex machine learning algorithms, such as determining if a genomic variant is protein-altering. The third reason is that applications that present the big data need to be modified constantly to reflect the current state of knowledge, such as instructing when to order a new set of genomic tests. In some cases, the applications need to be updated nightly. A new architecture for the EMRS is evolving which could unite Big Data, machine learning, and clinical care through a microservice-based architecture which can host applications focused on quite specific aspects of clinical care, such as managing cancer immunotherapy. Informatics innovation, medical research, and clinical care go hand in hand as we look to infuse science-based practice into healthcare. Innovative methods will lead to in a new ecosystem of Apps interacting with healthcare providers to fulfill a promise that is still to be determined.

Biography: Dr. Murphy is the Corporate Director of Research Informatics and Computing at Partners HealthCare, is an Associate Professor of Neurology and Biomedical Informatics at Harvard Medical School, and serves as Associate Director for the Laboratory of Computer Science at the Massachusetts General Hospital. He received his BS in Chemistry from the University of Notre Dame, and his Ph.D. in Pharmacology and Physiology and MD from the University of Chicago. Dr. Murphy’s research interests include the creation of query methods for healthcare data that enable them to be directly used by scientists even when the data is extremely large. Dr. Murphy has created high impact and widely accepted open source projects that focus on the integration of highly diverse phenotypic, imaging, and genomic data such that new discoveries can be visualized and produced from secondary use of routinely collected healthcare data and be applied to new methods of providing clinical decision support in a learning healthcare system.

Tuesday August 22 | Dagmar Ringe, Brandeis University



Title: Challenges to Drug Design

Abstract: There are a number of problems to which these methods are being applied, and they include: the structural basis for efficient enzyme catalysis of proton and hydride transfer; the role of the metal ions in bridged bimetallo-enzyme active sites; direct visualization of proteins in action by time-resolved protein crystallography; the structural basis for reaction selectivity in enzymes; the evolution of new enzyme activities from old ones and the development of new pathways. The most important of these problems is the study of neurodegenerative diseases, especially Parkinson’s, Alzheimer’s and Lou Gehrig’s diseases, with a view toward determining the functions of gene products associated with such diseases, finding common pathways that underlie them, and the search for and design of specific inhibitors or activators as potential drugs to treat these diseases. A number of methods are being used, from development of genetic and in vitro screens to structure-based drug design methods.

Biography: Dr. Ringe received her B.A. degree in Chemistry from Barnard College in 1963 and

Ph.D. degree in Organic Chemistry from Boston University in 1968. She is currently the Harold and Bernice Davis Professor of Aging and Neurodegenerative Diseases at Brandeis University, and Adjunct Professor Neurology at Harvard Medical School. Her research is aimed at the study of the molecular mechanisms of enzymes and the functions of proteins, with a focus on the determination of function for proteins of unknown function and the development of methods for intervention on that function. The tools being used include X-ray crystallography, molecular biology, kinetics, organic synthesis, genetics, and computational approaches.

Wednesday August 23 | Tandy Warnow, The University of Illinois at Urbana-Champaign



Title: Genome-scale estimation of the Tree of Life

Abstract: Estimating the Tree of Life is one of the grand computational challenges in Science, and has applications to many areas of science and biomedical research. Despite intensive research over the last several decades, many problems remain inadequately solved. In this talk I will discuss species tree estimation from genome-scale datasets. I will describe the current state of the art for these problems, what is understood about these problems from a mathematical perspective, and identify some of the open problems in this area where mathematical research, drawing from graph theory, combinatorial optimization, and probability and statistics, is needed. This talk will be accessible to mathematicians, computer scientists, probabilists and statisticians, and does not require any knowledge of biology.

Biography: Tandy Warnow is the Founder Professor of Engineering at the University of Illinois at Urbana-Champaign, where she has a dual appointment between Computer Science and Bioengineering. She is also a member of the Carl R. Woese Institute for Genomic Biology and an affiliate in six other departments at UIUC (Statistics, Mathematics, Electrical and Computer Engineering, Plant Biology, Animal Biology, and Entomology). Tandy received her PhD in Mathematics at UC Berkeley under the direction of Gene Lawler, and did postdoctoral training with Simon Tavaré and Michael Waterman at the University of Southern California. She received the National Science Foundation Young Investigator Award in 1994, the David and Lucile Packard Foundation Award in Science and Engineering in 1996, an Emeline Bigelow Conland Fellowship at the Radcliffe Institute for Advanced Study in 2006, and a Guggenheim Foundation Fellowship for 2011. In 2016 she was elected as an ACM Fellow, and in 2017 she was elected as a ISCB Fellow. Her research combines mathematics, computer science, and statistics to develop improved models and algorithms for reconstructing complex and large-scale evolutionary histories in both biology and historical linguistics. Her current research focuses on phylogeny and alignment estimation for very large datasets (10,000 to 1,000,000 sequences), estimating species trees from collections of gene trees, and metagenomics.

Workshops

5th International Workshop on Parallel and Cloud-based Bioinformatics and Biomedicine (ParBio)

1:30-3:30pm, August 20, 2017

Organizers:

Mario Cannataro, University "Magna Græcia" of Catanzaro

John Springer, Purdue University

<http://staff.icar.cnr.it/cannataro/parbio2017/>

Due to the availability of high-throughput platforms (e.g. next generation sequencing, microarray and mass spectrometry) and clinical diagnostic tools (e.g. medical imaging), a recent trend in Bioinformatics and Biomedicine is the increasing production of experimental and clinical data. Considering the complex analysis pipeline of the biomedical research, the bottleneck is more and more moving toward the storage, integration, and analysis of experimental data, as well as their correlation and integration with publicly available data banks. The goal of the ParBio workshop is to bring together scientists in the fields of high performance and cloud computing, computational biology and medicine, to discuss, among the others, the organization of large scale biological and biomedical databases, the parallel/service-based implementation of bioinformatics and biomedical applications, and problems and opportunities of moving biomedical and health applications on the cloud.

Workshop program

1:30-1:50pm

GPU-PCC: A GPU based technique to compute pairwise Pearson's Correlation Coefficients for big fMRI data.

Taban Eslami, Muaaz Gul Awan and Fahad Saeed

1:50-2:10pm

Ensemble Convolution Neural Network Method for Lung Tumor Detection. Allison Rossetto and Wenjin Zhou

2:10-2:30pm

Training a Support Vector Machine for Peptide Identification with Imbalanced Data. Jeremy Lane and John Rose

2:30-2:50pm

Fuzzy Prediction of Incipient Alzheimer's Disease cases from Mild Cognitive Impaired cases. Destiny Anyaiwe, Gautam B. Singh and George D. Wilson

2:50-3:10pm

Using GenotypeAnalytics to analyze pharmacogenomic datasets. Giuseppe Agapito, Pietro Hiram Guzzi and Mario Cannataro

3:10-3:30pm

Discovery of regular domains in large DNA data sets. Francesca Bertacchini; Eleonora Bilotta; Pietro Pantano

4th International Workshop on Computational Network Biology: Modeling, Analysis, and Control (CNB-MAC)

9:00am-5:30pm, August 20, 2017

Organizers:

Byung-Jun Yoon, Texas A&M University

Xiaoning Qian, Texas A&M University

Tamer Kahveci, University of Florida

<https://cnbmac.org/>

CNB-MAC 2017 aims to provide an international scientific forum for presenting recent advances in computational network biology that involve modeling, analysis, and control of biological systems and system-oriented analysis of large-scale OMICS data. This year's workshop program includes presentation of thirteen original research papers, one highlight presentation, and one poster abstract.

Workshop program

9:00am-9:10am: Opening Remarks

9:10-9:30am: *Bayesian graphical models for computational network biology.* Yang Ni, Peter Mueller, Lin Wei, and Yuan Ji

9:30-9:50am: *Detangling PPI networks to uncover functionally meaningful clusters.* Sarah Hall-Swan, Jake Crawford, Rebecca Newman, and Lenore Cowen

9:50-10:10am: *SMILE: a novel procedure for subcellular module identification with localization expansion.* Lixin Cheng, Pengfei Liu, and Kwong-Sak Leung

10:10-10:30am: *Overlapping functional modules detection in PPI network with pair-wisely constrained nonnegative matrix tri-factorization.* Guangming Liu, Bianfang Chai, Kuo Yang, Xuezhong Zhou, and Jian Yu

10:30-11:00am Coffee Break

10:00-11:20am: *Heuristic algorithms for feature selection under Bayesian models with block-diagonal covariance structure.* Ali Foroughi Pour and Lori A. Dalton

11:20-11:40am: *Feature selection with Interactions in logistic regression models using multivariate synergies for a GWAS: application.* Easton Li Xu, Xiaoning Qian, Qilian Yu, Han Zhang, and Shuguang Cui

11:40am-12:00pm: *Simulating variance heterogeneity in quantitative genome wide association studies.* Ahmad

Al Kawam, Mustafa Alshawaqfeh, James Cai, Erchin Serpedin, and Aniruddha Datta

12:00-12:20pm: *Sparse tensor decomposition for haplotype assembly of diploids and polyploids.* Abolfazl Hashemi, Banghua Zhu, and Haris Vikalo

12:20-2:00pm Lunch

2:00-2:20pm: *Intrinsically Bayesian robust classifier for single-cell gene expression time series in gene regulatory networks.* Alireza Karbalayghareh, Ulisses Braga-Neto, and Edward Dougherty

2:20-2:40pm: *Constraints on signaling networks logic reveal functional subgraphs on multiple myeloma OMIC data.* Bertrand Miannay, Stephane Minvielle, Olivier Roux, Florence Magrangeas, and Carito Guziolowski

2:40-3:00pm: *Protein-protein interaction extraction using attention-based convolution neural networks.* Hao Zhang, Mary Yang, Xiaoyue Feng, William Yang, Weida Tong, and Renchu Guan

3:00-3:20pm: *Stability of the hybrid epithelial/mesenchymal phenotype.* Mohit Kumar Jolly, Satyendra C Tripathi, Dongya Jia, Steven M Mooney, Muge Celiktas, Samir Hanash, Kenneth Pienta, Eshel Ben-Jacob, and Herbert Levine

3:20-3:40pm Coffee Break

3:40-4:00pm: *Investigation of model stacking for drug sensitivity prediction.* Kevin Matlock, Carlos De Niz, Raziur Rahman, Souparno Ghosh, and Ranadip

4:00-4:20pm: *A Bayesian approach to determine the composition of heterogeneous cancer tissue.* Ashish Katiyar, Anwoy Mohanty, Sima Chao, Jianping Hua, Aniruddha Datta, and Michael L. Bittner

4:20-4:40pm: *A transfer learning approach for cancer drug sensitivity prediction.* Saugato Rahman Dhruba, Raziur Rahman, Souparno Ghosh, and Ranadip Pal

4:40-5:00pm: Announcement of student travel awards

5:00-5:15pm Closing remarks

The 2017 Computational Structural Bioinformatics Workshop (CSBW)

8:30am-5:30pm, August 20, 2017

Organizers:

Amarda Shehu, George Mason University

Kevin Molloy, George Mason University

Nurit Haspel, UMass Boston

<http://www.cs.odu.edu/~bioinfo/CSBW.php>

The rapid accumulation of macromolecular structures presents a unique set of challenges and opportunities in the analysis, comparison, modeling, and prediction of macromolecular structures and interactions. This workshop aims to bring together researchers with expertise in bioinformatics, computational biology, structural biology, data mining, optimization and high performance computing to discuss new results, techniques, and research problems in computational structural bioinformatics.

A total of 18 original research articles were submitted for review to CSBW 2017. Each submission received at least 3 reviews, and 12 submissions were selected for presentation at CSBW 2017 and publication in the workshop companion proceedings of ACM-BCB 2017.

Workshop program

8:30am-8:35am: Opening Remarks

8:35-9:10am: *Automated Protein Chain Isolation from 3D Cryo-EM Data and Volume Comparison Tool*. Michael Nissenon, Jing He, and Dong Si

9:10-9:35am: *Gaussian Mixture Models with Constrained Flexibility for Fitting Tomogram Tiltseries*. Kasra Manavi, Sahba Tashakkori, and Lydia Tapia

9:35-10:00am: *Geometry Analysis for Protein Secondary Structures Matching Problem*. Kamal Al Nasr, Feras Yousef, Christopher Jones, and Ruba Jebril

10:00-10:30am Coffee Break

10:30-10:55am: *A Method for Characterization of β -strand twist from a 3 dimensional Image of a protein*. Tunazzina Islam, Michael Poteat, and Jing He

10:55-11:20am: *A Graph Based Method for the Prediction of Backbone Trace from Cryo-EM Density Maps*. Peter Collins and Dong Si

11:20am-1:30pm: Poster session and lunch

1:50-2:15pm: *ProMuteHT: A High-throughput Compute Pipeline for Generating Protein Mutants in silico*. Erik Andersson and Filip Jagodzinski

2:15-2:40pm: *Statistical Analysis of Computed Energy Landscapes to Understand Dysfunction in Pathogenic Protein Variants*. Wanli Qiao, Tatiana Maximova, Erion Plaku, and Amarda Shehu

2:40-3:05pm: *Geometric Sampling Framework for Exploring Molecular Walker Energetics and Dynamics*. Bruna Jacobson, Jon David, Mitch Malone, Kasra Manavi, Susan R. Atlas and Lydia Tapia

3:05-3:30pm: *Evolving Conformation Paths to Model Protein Structural Transitions*. Emmanuel Sapin, Kenneth De Jong, and Amarda Shehu

3:30-4:00pm: Coffee Break and posters

4:00-4:25pm: *Computational Modeling of pH-dependent gp120-CD4 Interactions in Founder and Chronic HIV Strains*. Jonathan Howton and Joshua Phillips

4:25-4:50pm: *Feature-Based and String-Based Models for Predicting RNA-Protein Interaction*. Donald Adjeroh, Jun Tan, and Jie Lin

4:50-5:15pm: *Ranking Protein-Protein Binding Using Evolutionary Information*. Roshanak Farhoodi, Bahar Akbal-Delibas, and Nurit Haspel

5:15-5:30pm: Closing Remarks

6th Workshop on Computational Advances in Molecular Epidemiology (CAME)

8:00am-5:40pm, August 20, 2017

Organizers:

Yury Khudyakov, CDC

Ion Mandoiu, University of Connecticut

Pavel Skums, Georgia State University

Alex Zelikovsky, Georgia State University

<http://alan.cs.gsu.edu/came17/>

Molecular epidemiology is an integrative discipline that considers molecular biological processes in specific epidemiological settings. The CAME workshop provides a forum for presentation and discussion of the latest computational research in molecular epidemiology. It will bring together field practitioners of molecular epidemiology, population geneticists, medical researchers, bioinformaticians, statisticians and computer scientists interested in the latest developments in algorithms, mining, visualization, modeling, simulation and other methods of computational, statistical and mathematical analysis of genetic and molecular data in the epidemiological context.

Workshop program

8:00-8:20am: Zoya Dimitrova. NGS data from surveillance of high risk populations reveal transmission networks

8:20-8:40am: Viachaslau Tsyvina, Alex Zelikovsky and Pavel Skums. Fast signature-based algorithm for estimation of genetic relatedness between viral populations

08:40-09:00am: Finlay Campbell, Anne Cori, Neil Ferguson and Thibaut Jombart. Outbreaker2: a tool for reconstructing transmission trees from epidemiological and genetic data

09:00-09:20am: Alex Artyomenko, Pavel Skums and Alex Zelikovsky. Agent-based simulation of HCV Quasispecies Evolution

09:20-09:40am: David Stiven Campo Rendon. Network-based guide to efficient interruption of HCV transmission

09:40-10:00am: Mukul Bansal. Phylogenetic Inference

of Viral Transmission Networks

10:10-30am: Coffee break

10:30-10:50am: Yury Khudyakov. Molecular Surveillance of hepatitis C

10:50-11:10am: Atkinson Longmire. Automated Quality Control for a Molecular Diagnostic System

11:10-11:30am: James Lara. PHACELIA: a PHysical-ChEmical quasispecies-based Algorithm for identifying incidence of hepatitis C infection

11:30-11:50am: Pelin Burcak Icer, Alexander Artyomenko, Sumathi Ramachandran, Alex Zelikovsky, Yury Khudyakov and Pavel Skums. Multi-parameter analysis of intra-host viral populations and machine learning allows for accurate differentiation between recent and chronic HCV infections.

12:00-1:30pm: Lunch break

1:30-1:50pm: Jordan Force and Ion Mandoiu. Prediction of MHC-I epitopes from LC-MS/MS data

1:50-2:10pm: Tyler Daddio and Ion Mandoiu. Pairing T-cell receptor sequences using pooling and min-cost flows

2:10-2:30pm: Serghei Mangul, Igor Mandric, Harry Taegyun Yang, Nicolas Strauli, Dennis Montoya, Jeremy Rotman, Will Van Der Wey, Jiem R. Ronas, Benjamin Statz, Alex Zelikovsky, Roberto Spreafico, Sagiv Shifman, Noah Zaitlen, Maura Rossetti, K. Mark Ansel, Eleazar Eskin. Profiling adaptive immune repertoires across multiple human tissues by RNA sequencing

2:30-2:50pm: Artem Rogovskyy, Alex Zelikovsky, Yuriy Ionov and Ekaterina Gerasimova. Identification of antibody-binding epitopes associated with protection against Lyme disease pathogen

2:50-3:10pm: Chung Yin (Joey) Leung, Dwayne R. Roach, Devika Singh, Laurent Debarbieux and Joshua S. Weitz. Stochastic models of immunophagy synergy

3:10-3:30pm: Helen Piontkivska, Madeline Frederick, Michael Miyamoto and Marta Wayne. The role of

innate immune mechanisms in molecular evolution and pathogenesis of flaviviruses

3:30-4:00pm: Coffee break

4:00-4:20pm: Raj Sunderraman, Xiaojun Cao, and Anu Bourgeois. Extending and Enhancing the Epi-Info Suite

4:20-4:40pm: Jaume Jorba, Kun Zhao and Kelley Bullard. PoSE: Visualization of Patterns of Sequence Evolution using PAML and Matlab

4:40-5:00pm: Sheida Nabavi, Fatima Zare, Sardar Ansari and Kayvan Najarian. Bias and Noise Cancellation for Robust Copy Number Variation Detection

5:00-5:20pm: Robert Harrison. Evaluation of drug resistance with a fuzzy restricted Boltzmann machine

5:20-5:40pm: Huiyuan Chen and Jing Li. Multiple Incomplete Source Learning for Large-Scale Drug Combination Prediction

Workshop on Microbiomics, Metagenomics, and Metabolomics (MMM)

8:30am-5:45pm, August 20, 2017

Organizers:

Soha Hassoun, Tufts University

Curtis Huttenhower, Harvard School of Public Health

<https://sites.google.com/view/mmmworkshop-at-acmbcb-2017/home>

Efforts to characterize microbiota have greatly benefited from technical advances in DNA sequencing. In particular, low-cost culture-independent sequencing has made metagenomic and metatranscriptomic surveys of microbial communities practical, including bacteria, archaea, viruses, and fungi associated with the human body, other hosts, and the environment. The resulting data have stimulated the development of many new computational approaches to meta'omic sequence analysis, including metagenomic assembly, microbial identification, and gene, transcript, and pathway metabolic profiling. Further, recent advances in untargeted metabolomics have stimulated the development of many tools that enhance the functional profiling of microbial communities.

A hands-on tutorial will provide an introduction to computational metagenomics. Through invited talks, this workshop will highlight recent advances computational methods for metagenomics and metabolomics.

Workshop program

8:30-8:35am: Soha Hassoun and Curtis Huttenhower. Opening remarks.

8:35-9:15am: Curtis Huttenhower and lab members. Tutorial introduction (background)

9:15-10:00am: Curtis Huttenhower and lab members. Tutorial (taxonomic profiling).

10:00-10:30am: Coffee break

10:30-11:15am: Curtis Huttenhower and lab members. Tutorial (functional profiling).

11:15am-12:00pm: Curtis Huttenhower and lab members. Tutorial (statistics and integration).

12:00-1:30pm: Lunch

1:30-2:00pm: Soha Hassoun. Tutorial (metabolomics)

2:00-2:30m: Dan Knights. Fast exhaustive alignment for microbiome analysis

2:30-3:00pm: Yuzhen Ye. New computational tools for integrated meta-omics data analysis

3:00-3:30pm: Geork K. Gerber. Predictive and interpretable Bayesian machine learning models for understanding microbiome dynamics

3:30-4:00pm: Coffee break

4:00-4:30pm: Gail Rosen. Discovering the Hidden World: High-throughput Discovery of Microbial Community Structure and Interactions

4:30-5:00pm: Kyonbum Lee. Using Metabolomics and 16S rRNA Sequencing to Investigate the Impact of Environmental Chemical Perturbations on Gut Microbiota Community Composition and Function

5:00-5:30pm: Hesham Ali. Analysis of biologically relevant features of metagenomics data in health and disease

5:30-5:45pm: Soha Hassoun and Curtis Huttenhower. Concluding remarks.

Tutorials

T1: Introducing the New eICU Collaborative Research Database

Alistair E. W. Johnson, Tom J. Pollard and Roger G. Mark, Massachusetts Institute of Technology

Leo A. Celi, Beth Israel Deaconess Medical Center

Abstract: Patients in hospital intensive care units (ICUs) are physiologically fragile and unstable, generally have life-threatening conditions, and require close monitoring and rapid therapeutic interventions. They are connected to an array of equipment and monitors, and are carefully attended by the clinical staff. Staggering amounts of data are collected daily on each patient in an ICU: multi-channel waveform data sampled hundreds of times each second, vital sign time series updated each second or minute, alarms and alerts, lab results, imaging results, records of medication and fluid administration, staff notes and more. Petabytes of data are captured daily during care delivery in the country's ICUs; however, most of these data are not used to generate evidence or to discover new knowledge. Critically ill patients are an ideal population for clinical database investigations because the clinical value of many treatments and interventions they receive remains largely unproven, and high-quality data supporting or discouraging specific practices are relatively sparse. The technology now exists to collect, archive and organize finely detailed ICU data, making possible research resources of enormous potential. However, the highly sensitive nature of the data and the need to take necessary protective precautions has created a substantial barrier to access for the research community.

Over the past decade, the Laboratory of Computational Physiology at the Massachusetts Institute of Technology, Beth Israel Deaconess Medical Center (BIDMC) and Philips Healthcare, with support from the National Institute of Biomedical Imaging and Bioinformatics, have partnered to build and maintain the public-access Medical Information Mart for Intensive Care (MIMIC) database. It contains de-identified but comprehensive and highly detailed clinical data from more than 60,000 ICU admissions, and provides unprecedented detail about the pathophysiology and care of ICU patients.

The aim of this tutorial is to introduce a new and even larger publicly available database that we have released this year: the eICU Collaborative Research Database. It contains de-identified detailed information from over 200,000 admissions to intensive care units from many different hospitals around the United States, with representation from 10-12% of US ICU beds. The data were collected during routine clinical care, and will facilitate a number of research studies, including investigating treatment efficacy, providing interpretation of key clinical markers in certain illnesses, inventing new data visualizations to synthesize patient state, building decision support models, and more. The eICU Collaborative Research Database provides an unparalleled insight into ICU care. Access is made available to legitimate researchers who request it, provided they complete a training course in human subjects research and sign a data use agreement. We anticipate that the worldwide research community will use this unique resource to further human knowledge in the field of critical care.

T2: Computational modeling of protein-RNA interactions

Yaron Orenstein, Massachusetts Institute of Technology. Presented by Austin Wang.

Abstract: Protein-RNA interactions, mediated through both RNA sequence and structure, play vital role in all cellular processes. In recent years, technologies have been developed to measure these interactions in high-throughput manner. Researchers would like to infer accurate models from the experimental data in order to predict new interactions and better understand the underlying binding mechanism. In this tutorial, I will present the main computational challenges in incorporating RNA structure information into computational algorithms and models. I will describe in detail two state-of-the-art methods to infer structure-based models from experimental data and discuss their strengths and weakness. I will conclude with open problems in the field.

T3: Robotics-inspired Algorithms for Modeling Protein Structures and Motions

Kevin Molloy, David Morris and Amarda Shehu, George Mason University

Abstract: With biomolecular structure recognized as central to understanding mechanisms in the cell, computational chemists and biophysicists have spent significant efforts on modeling structure and dynamics. While significant advances have been made, particularly in the design of sophisticated energetic models and molecular representations, such efforts are experiencing diminishing returns. One of the culprits is the low exploration capability of Molecular Dynamics and Monte Carlo-based exploration algorithms. This impasse has attracted AI researchers that have exploited similarities between molecular chains and modular mechanical systems to offer adaptations of robot motion planning algorithms for modeling biomolecular structures and motions.

The objective of this tutorial is two-fold. First, the tutorial will introduce students and researchers that attend ACM-BCB to robotics-inspired treatments and methodologies for understanding and elucidating the role of structure and dynamics in the function of

biomolecules. Second, the presentation will be enhanced via an open-source software developed in the Shehu Computational Biology laboratory. The software allows researchers both to integrate themselves in a new research domain as well as drive further research via plug-and-play capabilities. The hands-on approach in the tutorial will be beneficial to students and senior researchers keen to make contributions in computational structural biology.

T4: Stochastic Process Model and Its Applications to Analysis of Longitudinal Data

Ilya Y. Zhbannikov and Konstantin G. Arbeev, Duke University

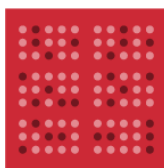
Abstract: Longitudinal studies are widely used in medicine, biology, population health and other areas related to bioinformatics. A broad spectrum of methods for joint analysis of longitudinal and time-to-event (survival) data has been proposed in the last few decades. The Stochastic process model (SPM) represents one possible framework for modeling joint evolution of repeatedly measured variables and time-to-event outcome typically observed in longitudinal studies. SPM is applicable for analyses of longitudinal data in many research areas such as demography and medicine and allows researchers to utilize the full potential of longitudinal data by evaluating dynamic mechanisms of changing physiological variables with time (age), allowing the study of differences, for example, in genotype-specific hazards. SPM allows incorporation of available knowledge about regularities of aging-related changes in the human body for addressing fundamental problems of changes in resilience and physiological norms. It permits evaluating mechanisms that indirectly affect longitudinal trajectories of physiological variables using data on mortality or onset of diseases. In this tutorial we explain the basic concepts of SPM, its current state and possible applications, corresponding software tools and show practical examples of analysis of joint analysis of longitudinal and time-to-event data with this methodology.

Posters

1. Xuefu Wang, Sujun Li, Shiyue Zhou, Yehia Mechref and Haixu Tang. A sparse latent regression approach for integrative analysis of glycomic and glycotranscriptomic data
2. Meera Garg. Study of Antidepressant Molecular Structure Leading to Safer Dosing
3. Noreen Akhtar and Ishrat Jabeen. A 2D-QSAR and Grid-Independent Molecular Descriptor (GRIND) Analysis of Quinoline-Type Inhibitors of Akt2: Exploration of the Binding Mode in the Pleckstrin Homology (PH) Domain
4. Naveena Yanamala, Marlene Orandle, Vamsi Kodali, Lindsey Bishop, Patti Zeidler-Erdely, Jenny Roberts, Vincent Castranova and Aaron Erdely. Supervised machine learning approaches predict and characterize nanomaterial exposures: MWCNT markers in lung lavage fluid.
5. Duc-Hau Le. UFO: a tool for unifying biomedical ontology-based semantic similarity calculation and visualization
6. Brandon Saiz and Padmanabhan Mahadevan. Prokaryotic Autolysin Database Construction
7. Abdul Musaweer Habib, Md. Saiful Islam, Md. Sohel, Md. Habibul Hasan Mazumder, Mohd. Omar Faruk Sikder and Shah Md. Shahik. Mining the Proteome of *Fusobacterium nucleatum* subsp. *nucleatum* ATCC 25586 for Potential Therapeutics Discovery: An In Silico Approach
8. Shah Md. Shahik. Screening of Novel Alkaloid Inhibitors for VEGF in Cancer cells: An integrated computational approach
9. Basma Abdelkarim, Vincent Maranda and Guy Drouin. The fate of retrotransposed processed genes in *Arabidopsis thaliana*
10. Basma Abdelkarim and Theodore Perkins. Super-enhancer dynamics throughout Myogenesis
11. Abdelrahman Hosny, Fatima Zare and Sheida Nabavi. VarSimLab: a Docker-based pipeline to automatically synthesize short reads with genomic aberrations
12. Neda Hassanpour, Nicholas Alden, Kyongbum Lee and Soha Hassoun. Using Enzyme Promiscuity to Advance Metabolite Annotation
13. Salvador Eugenio Caoili. Development of a Polymer-Theoretic Approach to Describing Constraints on Reactions Between Antipeptide Antibodies and Intrinsically Disordered Peptide Antigens: Implications for B-Cell Epitope Prediction
14. Huixiao Hong, Carmine Leggett and Suguna Sakkiah. Development of nicotinic acetylcholine receptor nAChR $\alpha 7$ binding activity prediction model:
15. Margaret Okomo-Adhiambo, Edward Ramos, Reagan Kelly, Yatish Jain, Roman Tatusov, Anna Montmayeur, Gregory Doho Doho, Rachel L. Marine, Terry Fei Fan Ng, Adam Retchless, Steve Oberste, Paul Rota, Xin Wang and Agha N. Khan. Automated Next Generation Sequencing Bioinformatics Pipelines for Pathogen Discovery and Surveillance
16. S M Ashiqul Islam, Ankan Choudhury, Christopher Michel Kearney and Erich J Baker. Protein classification using modified n-gram and skip-gram models
17. Xiaoli Jiao. Self-Tuning Spectral Clustering for Full-length Viral Quasispecies Reconstruction with PacBio Long Reads
18. Wen Zou, Weizhong Zhao and Roger Perkins. Best settings of model parameters in applying topic modeling on textual documents
19. Sora Kim, Han Sang Kim and Sangwoo Kim. Neopepsee: accurate genome-level prediction of neoantigens by harnessing sequence and amino acid immunogenicity information
20. Omid Ghasvand and Mary Shimoyama. Novel Unsupervised Named Entity Recognition Used in Text Annotation Tool (OntoMate) at Rat Genome Database
21. Fatima Zare, Sardar Ansari, Kayvan Najarian and Sheida Nabavi. Bias and Noise Cancellation for Robust Copy Number Variation Detection
22. Soumi Ray and Adam Wright. Applying Bayesian Changepoint Model and Hierarchical Divisive Model for Detecting Anomalies in Clinical Decision Support Alert Firing
23. Sangkyu Lee, Sarah Kerns, Barry Rosenstein, Harry Ostrer, Joseph O. Deasy and Jung Hun Oh. Preconditioned Random Forest Regression: Application to Genome-Wide Study for Radiotherapy Toxicity Prediction
24. Naveen Mangalakumar, Abed Alkhateeb, Huy Quang Pham, Luis Rueda and Alioune Ngom. Obtaining Outlier Gene Biomarkers of Breast Cancer Survivability from Time-Series Data
25. Tamsen Dunn, Gwenn Berry, Dorothea Emig-Agius, Yu Jiang, Anita Iyer, Nitin Udar and Michael Strömberg. Pisces: An Accurate and Versatile Single Sample Somatic and Germline Variant Caller
26. Michael Stromberg, Rajat Roy, Julien Lajugie, Yu Jiang, Haochen Li and Elliott Margulies. Nirvana: Clinical grade variant annotator
27. Leon Felipe Toro Navarro, Laura Inés Pinilla Mendoza and Rigoberto Ríos Estepa. *Streptomyces clavuligerus* constraint-based modeling and gene expression analysis for clavulanic acid production
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