24th International Workshop on Algorithms in Bioinformatics

WABI 2024, September 2–4, 2024, Royal Holloway, London, United Kingdom

Solon P. Pissis Wing-Kin Sung



Editors

Solon P. Pissis (1)

CWI, Amsterdam, The Netherlands Vrije Universiteit, Amsterdam, The Netherlands solon.pissis@cwi.nl

Wing-Kin Sung

The Chinese University of Hong Kong, China Hong Kong Genome Institute, Hong Kong Science Park, China kwksung@cuhk.edu.hk

ACM Classification 2012

Applied computing \to Bioinformatics; Applied computing \to Computational biology; Theory of computation \to Design and analysis of algorithms; Mathematics of computing \to Discrete mathematics; Mathematics of computing \to Information theory

ISBN 978-3-95977-340-9

Published online and open access by

Schloss Dagstuhl – Leibniz-Zentrum für Informatik GmbH, Dagstuhl Publishing, Saarbrücken/Wadern, Germany. Online available at https://www.dagstuhl.de/dagpub/978-3-95977-340-9.

Publication date

August, 2024

Bibliographic information published by the Deutsche Nationalbibliothek

The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available in the Internet at https://portal.dnb.de.

License

This work is licensed under a Creative Commons Attribution 4.0 International license (CC-BY 4.0): https://creativecommons.org/licenses/by/4.0/legalcode.



In brief, this license authorizes each and everybody to share (to copy, distribute and transmit) the work under the following conditions, without impairing or restricting the authors' moral rights:

Attribution: The work must be attributed to its authors.

The copyright is retained by the corresponding authors.

Digital Object Identifier: 10.4230/LIPIcs.WABI.2024.0

ISBN 978-3-95977-340-9

ISSN 1868-8969

https://www.dagstuhl.de/lipics

LIPIcs - Leibniz International Proceedings in Informatics

LIPIcs is a series of high-quality conference proceedings across all fields in informatics. LIPIcs volumes are published according to the principle of Open Access, i.e., they are available online and free of charge.

Editorial Board

- Luca Aceto (Reykjavik University, IS and Gran Sasso Science Institute, IT)
- Christel Baier (TU Dresden, DE)
- Roberto Di Cosmo (Inria and Université Paris Cité, FR)
- Faith Ellen (University of Toronto, CA)
- Javier Esparza (TU München, DE)
- Daniel Kráľ (Masaryk University, Brno, CZ)
- Meena Mahajan (Chair, Institute of Mathematical Sciences, Chennai, IN)
- Anca Muscholl (University of Bordeaux, FR)
- Chih-Hao Luke Ong (Nanyang Technological University, SG)
- Phillip Rogaway (University of California, Davis, US)
- Eva Rotenberg (Technical University of Denmark, Lyngby, DK)
- Raimund Seidel (Universität des Saarlandes, Saarbrücken, DE and Schloss Dagstuhl Leibniz-Zentrum für Informatik, Wadern, DE)
- Pierre Senellart (ENS, Université PSL, Paris, FR)

ISSN 1868-8969

https://www.dagstuhl.de/lipics

Contents

Preface Solon P. Pissis and Wing-Kin Sung				
WABI 2024 Committees	0:ix			
Invited Talk				
Bioinformatics of Pathogens Tomáš Vinař	1:1-1:2			
Regular Papers				
On the Complexity of the Median and Closest Permutation Problems Luís Cunha, Ignasi Sau, and Uéverton Souza	2:1-2:23			
An Efficient Algorithm for the Reconciliation of a Gene Network and Species Tree Yao-ban Chan	3:1-3:17			
MEM-Based Pangenome Indexing for k-mer Queries Stephen Hwang, Nathaniel K. Brown, Omar Y. Ahmed, Katharine M. Jenike, Sam Kovaka, Michael C. Schatz, and Ben Langmead	4:1-4:17			
Memoization on Shared Subtrees Accelerates Computations on Genealogical Forests Lukas Hübner and Alexandros Stamatakis	5:1-5:22			
Cosine Similarity Estimation Using FracMinHash: Theoretical Analysis, Safety Conditions, and Implementation Mahmudur Rahman Hera and David Koslicki	6:1-6:16			
Sapling: Inferring and Summarizing Tumor Phylogenies from Bulk Data Using Backbone Trees Yuanyuan Qi and Mohammed El-Kebir	7:1-7:19			
Applying the Safe-And-Complete Framework to Practical Genome Assembly Sebastian Schmidt, Santeri Toivonen, Paul Medvedev, and	8:1-8:16			
Alexandru I. Tomescu Orientability of Undirected Phylogenetic Networks to a Desired Class: Practical Algorithms and Application to Tree-Child Orientation Tsuyoshi Urata, Manato Yokoyama, and Momoko Hayamizu	9:1-9:17			
b-move: Faster Bidirectional Character Extensions in a Run-Length Compressed Index Lore Depuydt, Luca Renders, Simon Van de Vyver, Lennart Veys, Travis Gagie, and Jan Fostier	10:1–10:18			
The mod-minimizer: A Simple and Efficient Sampling Algorithm for Long k-mers Ragnar Groot Koerkamp and Giulio Ermanno Pibiri	11:1–11:23			
24th International Workshop on Algorithms in Bioinformatics (WABI 2024). Editors: Solon P. Pissis and Wing-Kin Sung				

Leibniz International Proceedings in Informatics

Lipics Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

0:vi Contents

Reconstructing Rearrangement Phylogenies of Natural Genomes Leonard Bohnenkämper, Jens Stoye, and Daniel Dörr	12:1-12:16
PLA-index: A k-mer Index Exploiting Rank Curve Linearity Md. Hasin Abrar and Paul Medvedev	13:1-13:18
A Unifying Taxonomy of Pattern Matching in Degenerate Strings and Founder Graphs Rocco Ascone, Giulia Bernardini, Alessio Conte, Massimo Equi, Esteban Gabory, Roberto Grossi, and Nadia Pisanti	14:1-14:21
Swiftly Identifying Strongly Unique k-Mers Jens Zentgraf and Sven Rahmann	15:1–15:15
Finding Maximum Common Contractions Between Phylogenetic Networks Bertrand Marchand, Nadia Tahiri, Olivier Tremblay-Savard, and Manuel Lafond	16:1-16:24
A*PA2: Up to $19 \times$ Faster Exact Global Alignment Ragnar Groot Koerkamp	17:1–17:25
RNA Triplet Repeats: Improved Algorithms for Structure Prediction and Interactions Kimon Boehmer, Sarah J. Berkemer, Sebastian Will, and Yann Ponty	18:1–18:23
RNA Inverse Folding Can Be Solved in Linear Time for Structures Without Isolated Stacks or Base Pairs Théo Boury, Laurent Bulteau, and Yann Ponty	19:1–19:23
The Path-Label Reconciliation (PLR) Dissimilarity Measure for Gene Trees Alitzel López Sánchez, José Antonio Ramírez-Rafael, Alejandro Flores-Lamas, Maribel Hernández-Rosales, and Manuel Lafond	20:1-20:21
McDag: Indexing Maximal Common Subsequences in Practice Giovanni Buzzega, Alessio Conte, Roberto Grossi, and Giulia Punzi	21:1-21:18
Anchorage Accurately Assembles Anchor-Flanked Synthetic Long Reads Xiaofei Carl Zang, Xiang Li, Kyle Metcalfe, Tuval Ben-Yehezkel, Ryan Kelley, and Mingfu Shao	22:1-22:17
AlfaPang: Alignment Free Algorithm for Pangenome Graph Construction Adam Cicherski, Anna Lisiecka, and Norbert Dojer	23:1-23:18

Preface

This proceedings volume contains papers and abstracts presented at the 24th Workshop on Algorithms in Bioinformatics (WABI 2024), which was held in Egham, United Kingdom, from September 2nd to 4th, 2024.

The Workshop on Algorithms in Bioinformatics is an annual conference established in 2001 to cover all aspects of algorithmic work in bioinformatics, computational biology, and systems biology. The conference serves as a forum for presenting new insights about discrete algorithms and machine-learning methods that address important problems in biology, particularly those based on molecular data and phenomena. These algorithms are founded on sound models, exhibit computational efficiency, and have been implemented and tested in simulations and on real datasets. The focus of the meeting is on recent research results, including significant work-in-progress, as well as identifying and exploring directions for future research. Over the 24 instances of WABI, computational biology has significantly grown in importance. Some of these methods have been applied in different biological and clinical domains like vaccine development.

WABI 2024 was co-located with ALGO 2024. A total of 46 manuscripts were submitted to WABI 2024, of which 22 were selected for presentation at the conference and included in this proceedings volume as full papers. The 22 papers chosen for the conference underwent a rigorous peer review process, involving at least four independent reviewers per submitted paper. Following this, discussions took place among the WABI 2024 Program Committee members. The reviews were conducted by both Program Committee members and additional reviewers selected based on their expertise relevant to specific papers. The selected papers encompass a wide range of topics, including phylogenetic trees and networks, cancer phylogenetics, sequence alignment and assembly, gene and genomic-level evolution, genome rearrangement, sequence and genome analysis, RNA structure, pattern matching, data compression, and more. The conference program also featured an invited talk. The EasyChair system was utilized for handling submissions and reviews.

Extended versions of selected papers have been invited for publication in a thematic series in the journal "Algorithms for Molecular Biology" (AMB), published by BioMed Central.

We extend our gratitude to all the authors of the submitted papers, whose contributions made this conference possible. Special thanks are due to all the members of the WABI 2024 Program Committee and their sub-reviewers for their diligent efforts in reviewing the manuscripts and engaging in comprehensive discussions. These discussions informed the decision-making process and resulted in constructive review reports for the authors. We are grateful to the WABI Steering Committee for their availability, assistance, and guidance. Our thanks go to all the conference participants, session chairs, and speakers who contributed to a highly successful scientific program. In particular, we express our gratitude to the conference's keynote speaker, Tomáš Vinař (Comenius University in Bratislava, Slovakia), for his presentation titled "Bioinformatics of Pathogens". Furthermore, we would like to express our special appreciation to the ALGO 2024 Organizing Committee for their dedicated efforts and generosity in organizing the event.

Previous WABI proceedings appeared in LNCS/LNBI volumes as follows: 2149 (WABI 2001, Aarhus), 2452 (WABI 2002, Rome), 2812 (WABI 2003, Budapest), 3240 (WABI 2004, Bergen), 3692 (WABI 2005, Mallorca), 4175 (WABI 2006, Zurich), 4645 (WABI 2007, Philadelphia), 5251 (WABI 2008, Karlsruhe), 5724 (WABI 2009, Philadelphia), 6293 (WABI 2010, Liverpool), 6833 (WABI 2011, Saarbrücken), 7534 (WABI 2012, Ljubljana), 8126

0:viii Preface

(WABI 2013, Sophia Antipolis), 8701 (WABI 2014, Wroclaw), 9289 (WABI 2015, Atlanta), and 9838 (WABI 2016, Aarhus). Beginning in 2017, they appeared in LIPIcs volumes: 88 (WABI 2017, Boston), 113 (WABI 2018, Helsinki), 143 (WABI 2019, Boston), 172 (WABI 2020, held virtually in Pisa), 201 (WABI 2021, held virtually in Chicago), 242 (WABI 2022, Potsdam) and 273 (WABI 2023, Houston).

Solon P. Pissis and Wing-Kin Sung

WABI 2024 Committees

Steering Committee

Vincent Moulton University of East Anglia, UK

Nadia Pisanti University of Pisa, Italy

Jens Stoye Bielefeld University, Germany

Mona Singh Princeton University, USA

PC Chairs

Solon P. Pissis

CWI, The Netherlands; Vrije Universiteit, The Netherlands

Wing-Kin Sung

Chinese University of Hong Kong, Hong Kong

Program Committee

Tatsuya Akutsu Kyoto University, Japan

Jarno Alanko University of Helsinki, Finland

Lorraine Ayad Brunel University London, UK

Jasmijn Baaijens TU Delft, The Netherlands

Giulia Bernardini Università di Trieste, Italy

Broňa Brejová

Comenius University in Bratislava, Slovakia

Panagiotis Charalampopoulos Birkbeck, University of London, UK

Rayan Chikhi CNRS, France

Lenore Cowen

Tufts University, USA

Manuel Cáceres

Aalto University, Finland

24th International Workshop on Algorithms in Bioinformatics (WABI 2024). Editors: Solon P. Pissis and Wing-Kin Sung
Leibniz International Proceedings in Informatics

Leibniz International Proceedings in Informatics

LIPICS Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

0:x WABI 2024 Committees

Daniel Doerr

Heinrich Heine University Düsseldorf, Germany

Mohammed El-Kebir

University of Illinois at Urbana-Champaign, USA

Jonas Ellert

ENS - PSL, France

Anna Gambin

Institute of Informatics, Warsaw University, Poland

Shilpa Garg

Technical University of Denmark, Denmark

Bjarni Halldorsson

deCODE genetics and Reykjavik University, Iceland

Wing-Kai Hon

National Tsing Hua University, Taiwan

Carl Kingsford

Carnegie Mellon University, USA

Gregory Kucherov

CNRS/LIGM, France

Dominik Köppl

University of Yamanashi, Japan

Manuel Lafond

Université de Sherbrooke

Francesca Nadalin

EMBL, UK

Yuri Pirola

DISCo, Univ. degli Studi di Milano-Bicocca, Italy

Nicola Prezza

Ca' Foscari University, Italy

Mingfu Shao

The Pennsylvania State University, USA

Sharma V. Thankachan

North Carolina State University, USA

Prudence Wong

University of Liverpool, UK

Simone Zaccaria

UCL Cancer Institute, UK

Meirav Zehavi

Ben-Gurion University, Israel

Jie Zheng

ShanghaiTech University, China

WABI 2024 Committees 0:xi

Subreviewers

Eloi Araujo Bojana Kodric Kristoffer Sahlin Rocco Ascone Aleksandr Koshkarov Yoshifumi Sakai Andrej Baláž Oded Lachish Jannik Schestag Elena Biagi Benjamin Langmead Francisco Sena Maria Bochenek Rahul Shah Téo Lemane Christina Boucher Jiayi Li Yihang Shen Davide Cenzato Xiang Li Qian Shi Cedric Chauve Josipa Lipovac Jouni Sirén Ke Chen Alitzel López Sánchez Yuyao Song Neo Christopher Chung Ting Lu Michał Startek Davide Cozzi Guillaume Marçais Nadia Tahiri Gianluca Della Vedova Bertrand Marchand Siyu Tao

Gianluca Della Vedova Bertrand Marchand Siyu Tao
Riccardo Dondi Camille Marchet Haotian Teng
Shiyi Du Pierre Marijon Yue Teng
Shane Elder Robert Mercas Carlo Tosoni
Estében Cohomic Manal Mahamad

Estéban Gabory Manal Mohamed Jasper van Bemmelen

Arnab Ganguly Rahul Nihalani Leo van Iersel

Krzysztof Gogolewski Hannes P. Eggertsson Anna Vathrakokoili Pournara

Khodor Hannoush Gunnar Pálsson Hilde Verbeek

Peter Heringer Karol Pokorski Riccardo Vicedomini

Guillaume Holley Simon Puglisi Tomas Vinar
Aaron Hong Daniel Puttini Mathias Weller
Ferdoos Hossein Nezhad Yuanyuan Qi Qingyu Yang
Jesper Jansson Jakub Radoszewski Jiale Yu

Jesper JanssonJakub RadoszewskiJiale YuMark JonesNicola RizzoXin YuanRebecca Katharina PfeilDuncan RobertsonTasfia ZahinSung-Hwan KimYingfan RuiXiaofei Zang