

ABSTRACTS PDCLIFES

PARALLEL LEARNING OF WEIGHTED ASSOCIATION RULES IN HUMAN PHENOTYPE ONTOLOGY

Giuseppe Agapito, Mario Cannataro, Pietro H. Guzzi and Marianna Milano

The Human Phenotype Ontology (HPO) is a structured repository of concepts associated with diseases. The importance and the specificity of HPO terms are estimated employing the Information Content (IC). Thus, the analysis of annotated data is a critical challenge for bioinformatics. There exist several approaches to support ontology curators in maintaining and analysing data. From those, the use of Association Rules (AR) can improve the quality of annotations. Although, classical association rules algorithms cannot consider the source of annotation, either the producing rules with low IC. In this paper, we present an algorithm for the parallel extraction of Weighted Association Rules (WAR) from HPO terms and annotations, able to face high dimension of data and to result in good response time. Experiments performed on real and synthetic datasets show good speed-up and scalability.

IMPROVING THE RUNTIME PERFORMANCE OF NON-LINEAR MIXED-EFFECTS MODEL ESTIMATION

Tom Haber and Frank van Reeth

Non-linear mixed effects models (NLMEM) are frequently used in drug development for pharmacokinetic (PK) and pharmacokinetic- pharmacodynamic (PK-PD) analyses. Parameter estimation for these models can be time-consuming due to the need for numerical integration. Additionally, the structural model is often expressed using differential equations requiring computationally intensive time-stepping ODE solvers. Overall, this often leads to long computation times in the order of hours or even days. Combining the right mathematical tools as well as techniques from computer science, the computational cost can be significantly reduced. In this paper, several approaches are detailed for improving the performance of parameter estimation for NLMEM. Applying these, often easy, techniques can lead to an order of magnitude speedup.

APPLICATION OF WAVELET TRANSFORM IN TEETH SEGMENTATION OF BITEWING X-RAY IMAGES

Sina Salimzadeh, Sara Kandulu (Izadpanahi)

Within the recent twenty years, dental X-ray images have been widely used in forensic odontology for human identification where mass disasters happen. Therefore, a reliable approach for teeth segmentation can help forensic experts to determine the potential victims faster. In this paper, a novel method is proposed for the process of teeth segmentation and individual teeth isolation of Bitewing X-ray radiographs. This method has four steps and is based on separating teeth according to edge lines between crowns of teeth. Using this method, the evaluation of 681 teeth segmentation was measured by isolation accuracy and visual inspection. The results show that with 90.6% isolation accuracy of total 681 teeth and the average runtime of 0.22 seconds per tooth, this method performs better and much faster compared to the existing methods.

HYBRID MACHINE LEARNING AND POLYMER PHYSICS APPROACH TO INVESTIGATE 3D CHROMATIN STRUCTURE

Mattia Conte, Andrea Esposito, Luca Fiorillo, Carlo Annunziatella, Alfonso Corrado, Francesco Musella, Renato Sciarretta, Andrea M. Chiariello and Simona Bianco

Innovative experimental protocols from Molecular Biology provided in recent years quantitative data about the structure of the cell nucleus. These technologies, such as Hi-C, GAM or SPRITE, revealed that the genome has a non-random three-dimensional (3D) spatial organization, which serves functional purposes. In order to dissect the complexity of chromosome folding, models from Polymer Physics have been employed, highlighting many key aspects of large-scale chromatin organization. A deep understanding of the molecular mechanisms underlying the genome architecture is currently a crucial problem in Biology, since chromatin misfolding or structural variants can re-configure chromatin domains, thereby resulting in pathogenic phenotypes and disease. Here, we discuss a numerical Polymer-Physics-based approach (PRISMR), able to model 3D chromatin folding by using Machine Learning strategies informed with experimental data. Using as a case study the Pitx1 locus, a genomic region critically involved in hindlimb development, we show that the PRISMR algorithm reproduces in silico with high accuracy the experimental contact data, thus providing a powerful computational tool for analyzing and predicting the 3D chromatin structure.

ADAPTIVE DOMAIN DECOMPOSITION FOR EFFECTIVE DATA ASSIMILATION

Rossella Arcucci, Laetitia Mottet, César A. Quilodrán Casas, Florian Guitton , Christopher Pain, and Yi-Ke Guo

We present a parallel Data Assimilation model based on an Adaptive Domain Decomposition (ADD-DA) coupled with the open-source, finite-element, fluid dynamics model Fluidity. The model we present is defined on a partition of the domain in sub-domains without overlapping regions. This choice allows to avoid communications among the processes during the Data Assimilation phase. However, during the balance phase, the model exploits the domain decomposition implemented in Fluidity which balances the results among the processes exploiting overlapping regions. Also, the model exploits the technology provided by the mesh adaptivity to generate an optimal mesh we name supermesh. The supermesh is the one used in ADD-DA process. We prove that the ADD-DA model provides the same numerical solution of the corresponding sequential DA model. We also show that the ADD approach reduces the execution time even when the implementation is not on a parallel computing environment. Experimental results are provided for pollutant dispersion within an urban environment.



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