universität wien
Fakultät für Informatik

MEDIZINISCHE UNIVERSITÄT WIEN

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Fakultät für Mathematik

Berufungsvorträge
"Computational Medicine"

Die Berufungsvorträge schließen folgende Punkte mit ein:

Didaktischer Vortrag (30 Minuten)
Wissenschaftlicher Vortrag (45 Minuten)
Fragen/Pause (30 Minuten)
Kommissionelles Hearing -
(Dekanatsbesprechungszimmer, 11. Stock)

Freitag, 11. Oktober 2019, HS 16

Bernhard Knapp
(International University of Catalonia, Barcelona)

09:30 Uhr: Didaktischer Vortrag

"Mapping algorithms for next generation sequencing data"

I am not an expert in next generation sequencing data. Never the less I would like to seize the opportunity to step out of my comfort zone and acquaint myself with this topic explaining the application of two very well-known computer science algorithms for the mapping of next generation sequencing data: I will explain the application of "hashing" and the "Burrows–Wheeler transformation" in simple terms and discuss the beauty of these two algorithms in the context of mapping of next generation sequencing data.
By this way I hope to show my ability to teach interdisciplinary subjects as well as my ability to learn quickly.

10:00 Uhr: Wissenschaftlicher Vortrag

"Computational prediction of T-cell receptor sequences for patient specific (cancer) antigens"

The affinity of T-cell receptors (TCRs) to peptide/MHC (pMHC) complexes (e.g. a specific cancer antigen) can be improved by introducing mutations in TCR sequences. Testing a large number of mutant TCRs experimentally is expensive and time consuming. A computational high-throughput approach could test such large numbers of TCRs in short time and at little cost. This method would be of high value in many areas of immunology such as cancer, viral infections and vaccines. However, to date no such method exists. Current computational methods are either computationally too expensive or not accurate enough. Here we propose to extend our previously developed MOSAICS protocol (Knapp et al. 2017 Bioinformatics; Sim et al. 2012 PNAS) for the prediction of TCR binding. MOSAICS implements a unique combination of hierarchical Monte Carlo, coarse-graining, stochastic chain closure, and (local) temperature annealing cycles. By this way MOSAICS will allow the prediction of association, dissociation, and binding of TCRs with peptide/MHC using structural modelling while non-essential degrees of freedom are restricted. MOSAICS is orders of magnitudes faster than conventional molecular simulation approaches and achieves high agreement with experimental data as we have shown before in multiple studies. This new MOSAICS extension together with deep learning approaches will for the first time allow computational optimisation of TCRs and antibodies on a patient specific basis. This will be of high value for precision medicine as for example in chronic viral diseases, cancer neo-antigens, orphan TCRs, and fundamental insights into autoimmune pathogenesis.