香港浸會大學 HONG KONG BAPTIST UNIVERSITY

DEPARTMENT OF COMPUTER SCIENCE 計算機科學系

DEPARTMENT OF COMPUTER SCIENCE

SEMINAR

2024 SERIES

Advancing Unified Deep Learning for Comprehensive Mass Spectrometry Analysis

DATE & TIME

14 OCT 2024 (MON) 10:00 – 11:00 AM

VENUE

WLB 210, The Wing Lung Bank Building for Business Studies, Shaw Campus

PROF XUEFENG CUI

School of Computer Science and Technology
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ABSTRACT

Tandem Mass Spectrometry (MS/MS) is widely utilized in proteomics for the identification and quantification of proteins, in metabolomics for the profiling of small molecules, and in lipidomics for the characterization of lipid species. MS/MS is also essential in drug discovery, biomarker identification, environmental analysis, and forensic science. Despite its broad applicability and effectiveness, current research encounters two main challenges. First, the increasing volume of peptide MS/MS spectra data demands the development of novel computational methods for swift database searches. We present MS2VEC, an innovative fingerprint embedding model designed for extensive peptide MS/MS spectra library retrieval. This model identifies the relationships between distant peaks and integrates position-sensitive fingerprint features. To achieve this, dilated convolutions are used to capture distant associations, and a position-sensitive multi-head attention pooling mechanism is applied to extract fingerprint features. Due to the scarcity of small molecule MS/MS spectral data, conventional techniques that depend on database comparisons are inadequate for newly identified molecules that are not yet included in the database. To overcome this challenge, we present MS2SMILES, an innovative method that treats hydrogen atoms as implicitly bonded to heavy atoms. This approach is tailored to precisely predict hydrogen atoms in chemical structures, which are not explicitly shown in SMILES.

SPEAKER'S BIOGRAPHY

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