

Development of an R Toolbox for Near-Infrared Spectroscopy Data Processing and Analysis of Plant Metabolic Phenotypes

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MSC. LIFE SCIENCE INFORMATICS

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Chapter 1

Introduction

The advancement and widespread use of high-throughput experimental technologies in the field of plant biology have introduced significant challenges in managing and analysing the vast datasets effectively. Addressing these challenges require innovative methods that maximize the data utility while minimizing computational inefficiencies and resource consumption, ensuring robust insights into complex biological systems (<https://www.frontiersin.org/research-topics/6856/machine-learning-in-plant-science/articles>).

1.1 Related Work

The related work include, the followings

Chapter 2

Background

The background of this study include

2.1 Near Infrared Spectroscopy (NIRS)

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2.1.1 Introduction

2.2 Metabolomics

2.2.1 Introduction

2.2.2 Mass Spectrometry

2.3 Machine Learning

2.3.1 Introduction

2.3.2 Partial Least Square Regression (PLS)

2.3.3 Random Forest (RF)

2.3.4 Convolutional Neural Network (CNN)

Chapter 3

Methods and Implementation

3.1 MSNovelist

3.1.1 Basic Idea of the Software

3.1.2 Deep Learning Architecture

3.1.3 Preparation of Data

3.2 Data

3.2.1 Data Records

3.2.2 File Formats

3.3 Evaluation of the Training

3.4 Implementations in the TensorFlow Framework

3.4.1 Preprocessing of Data

3.4.2 Training

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3.4.4 Termination Criterion

3.4.5 Training on the Pubchem Dataset

3.5 Implementations in the PyTorch Framework

3.5.1 Reimplementation of the LSTM Architecture

3.5.2 Training with DeepSMILES and SELFIES

3.5.3 Transformer Implementation

3.6 Software

3.7 Hardware

Chapter 4

Results and Discussion

4.1 Data charecterestics

histogram, spectra

4.2 Baseline Machine Learning Models Pablo

PLS, RF, CNN

4.2.1 Variable importance

4.3 Variations in Baseline systems

4.3.1 modifying the Test and Training split

4.3.2 input data length

4.4 Sues

4.4.1 QBMG Tokenization