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

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Chapter 1

Introduction

The advancement and widespread use of heigh-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 mimnimizing 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).

The understanding of interplay between plant physiology and its hidden biochemical process is crucial for the improvement of basic plant science and addressing global challenges such as food security, crop resilience and combating climate change [1]. In recent years, advanced High-throughput analytical techniques such as Near-Infrared Spectroscopy (NIRS) and Liquid Chromatography-Mass Spectrometry (LC-MS) has instigated a paradigm shift in plant biology [2][3]. These High-throughput techniques are mostly used in areas like genomics, imaging and spectroscopy and is known for their ability to collect and analyse the data faster than traditional techniques[3]. High-throughput techniques are widely used since they enable the efficient collection of vast amount of data at various scales, from molecular to field level over significant time periods[4]. The massive amounts of data collected through this techniqes presents both opportunities and challenges to scientific communities. The vast amount of data collected require efficient processing to generate useful results in limited time frame and this is where Machine Learning (ML) becomes indispensable. ML algorithams can analyse complex, high-dimentional datasets, enabling accurate predictions of plant traits or other features based on the input data on study [4][5].

Chapter 2

Background

The background of this study include

2.1 Related Work

2.2 Near Infrared Spectroscopy (NIRS)

2.3 R Programming

2.4 Machine Learning

2.4.1 Partial Least Square Regression (PLSR)

2.4.2 Random Forest (RF)

2.4.3 Convolutional Neural Network (CNN)

2.5 Mass Spectrometry and Liquid Chromatography

Chapter 3

Implementation

3.1 Packages

Github, testing, actions

3.2 Contributions elsewhere

3.3 HPC runs

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

Chapter 5

Reference

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