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Using machine-learning on metabolomics data to predict complex phenotypes

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The metabolome is often seen as the ultimate cellular phenotype, resulting from all biochemical processes taking place in an organism. Using a robotized high throughput platform to prepare samples and modern mass spectrometers coupled with chromatography, it is nowadays possible to obtain both targeted and untargeted metabolomic data on hundreds of samples in a few days. Those experiments lead to thousands of metabolic features representing a precise description of the cell state at a given time. This state is a good proxy of the past, the present and the future of a given tissue, combining the result of the previous developmental stages, the current status and the bricks enabling the future development of the cells. Moreover, by applying different types of stresses to an organism, it is possible to increase the diversity of the metabolome, hence displaying broader characteristics.

By combining metabolomic and phenotypic data and using machine-learning approaches, we were able to accurately predict several complex phenotypes such as relative growth rate [1], grafting success [2], plant elevation [3] or resistance to pathogens [4] on various plant matrices. Besides, enabling prediction of those complex phenotypes, those techniques permit the discovery of biomarkers that give insights into mechanisms controlling the phenotypes.

Here we will present the different cases studied recently by our laboratory and metabolomic platform. The accuracies of the predictions and the physiological knowledge acquired thanks to those models will be detailed. Perspectives about the integration of knowledge acquired through the use of those machine-learning models into more mechanistic models will also be discussed.

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