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Analyzing volatile compound measurements using traditional Multivariate techniques and Bayesian networks

A thesis presented in partial fulfillment of the requirements for the degree of

Master of Arts in Statistics

at Massey University, Albany, New Zealand

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2009
The purpose of this project is to compare two statistical approaches, traditional multivariate analysis and Bayesian networks, for representing the relationship between volatile compounds in kiwifruit. Compound measurements were for individual vines which were progeny of an intercross. It was expected that groupings in the data (or compounds) would give some indication of the generic nature of the biochemical pathways. Data for this project was provided by the Flavour Biotech team at Plant and Food Research. This data contained many non-detected observations which were treated as zero and to deal with them, we looked for appropriate value of \( c \) for data transformation in \( \log(x+c) \). The data is ‘large \( p \) small \( n \)’ paradigm – and has much in common with data, although it is not as extreme as microarray. Principal component analysis was done to select a subset of compounds that retained most of the multivariate structure for further analysis. The reduced set of data was analyzed by Cluster analysis and Bayesian network techniques. A heat map produced by Cluster analysis and a graphical representation of Bayesian networks were presented to scientists for their comments. According to them, the two graphs complemented each other; both graphs were useful in their own unique way. Along with clusters of compounds, clusters of genotypes were represented by the heat map which showed by how much a particular compound is present in each genotype while the relation among different compounds was seen from the Bayesian networks.
Acknowledgments

I would like to sincerely thank my supervisor, Dr Beatrix Jones for her constant guidance and support right from the beginning through the end of this project. Her encouragement enabled me to widen my understanding of the subject.

I would like to extend my thanks towards Ross Atkinson and Robert Winz from the Flavour Biotech team at Plant and Food Research for allowing me to use their data and providing their comments on the results. I would also like to thank Foundation for Research, Science and Technology (contract C06X0403) for funding this project and Marsden Fast Start Grant to Beatrix Jones (MAU0501) for partial support in completion of this work.

I would like to specially thank my husband Jugal, whose enduring love and support enabled me to complete my thesis.

Finally, I would like to thank my sister, Neha for her help with proof reading.
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