



Contents

Acknowledgments	ii
Abstract	v
Contents	xvii
I Introduction and literature review	1
1 Introduction, contents and aims of the thesis	3
1.1 Introduction	3
1.2 Characteristics of 'omic' data	5
2 Common strategies for the analysis of metabolomic data	9
2.1 Classical bivariate tests	9
2.2 Linear modelling of omic data	12
2.3 Corrections for multiple comparisons	13
2.4 Principal Component analysis	16

3	Modern techniques for the analysis of metabolomic data	19
3.1	Projection based methods	19
3.2	Penalization methods	22
3.3	Other methods	29
4	Challenges for analyzing metabolomics data. Strategies and aims of the thesis	31
4.1	Challenges for analyzing metabolomic data.	31
4.2	Strategies and aims of the thesis.	32
II	Materials and methods	35
5	Multiway data, methods for its analysis	37
5.1	From 2D matrices to 3D arrays	37
5.2	Exploration and description of N-way arrays.	38
5.3	Regression methods for N -way arrays, N -PLS.	41
5.4	Software for analyzing three-way data	43
6	Variable selection techniques	45
6.1	VIP scores	45
6.2	Selectivity Ratio	48
6.3	Variable selection through L1 penalization	50
III	Results	55
7	Sparse N -PLS, a method for variable selection in multiway data sets	57
7.1	Sparse N -PLS, integration of L1 penalization in the N -PLS algorithm	57
7.2	Hyperparameters of the sparse N -PLS algorithm.	58

8 sNPLS package, a comprehensive software for N-PLS and sparse N-PLS analysis	63
8.1 Implementation of the sNPLS algorithm in \mathbf{R}	63
8.2 The sNPLS package	70
9 Validation of the sparse N -PLS method and sNPLS package	85
9.1 Random synthetic data sets	85
9.2 Data driven synthetic data sets	88
9.3 Real data sets	90
9.4 Comparison with other methods	96
IV Conclusions and future work	107
10 Conclusions	109
10.1 Developed topics and contributions	109
10.2 Future work and research lines	110
Bibliography	115