BAYESIAN METABOLITE FINGERPRINTING

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Sometimes in metabolomic studies we wish to classify a plant, a tissue or a tumor using its metabolic spectrum. Such studies usually have low replicates and many metabolites which should be ordered respect to their importance. In this paper a convenient model is suggested for plant data derived by mass-spectrometry gas-chromatography technology. Metabolite selection is implemented using a spike and slab distribution, and Markov chain Monte Carlo is used to sample from the posterior. The main advantage of our approach compared with methods such as principal components analysis and hierarchical clustering is that it provides a quantitative measure of importance of each metabolite. The suggested approach is applied to a real data set.