# Weighted pivot balances applied to metabolomics

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**Abstract**

Logratio methodology, which converts compositional data from their original Aitchison geometry to interpretable real orthonormal coordinates, is successfully used in compositional data analysis for many years (Pawlowsky-Glahn and Buccianti, 2011) and it is increasingly applied also to the field called metabolomics (Najdekr and others, 2015, Gardlo and others, 2016). Logratio methodology allows to perform a reasonable statistical processing and graphical outputs of compositional data. However, compositional data (especially in metabolomics) and their logratio coordinates can be influenced by artifacts resulting from processing (imputed) data below detection limit of measurement devices. Weighted pivot balances are new orthonormal logratio coordinates (Filzmoser and Hron, 2015) which capture the relevant relative information about an original component and also suppress the redundant information from the data in a controlled way. In weighted pivot balances the system of weights is used that accounts for different roles of parts in a compositional data set to find a more reasonable way to extract relative information about single components within orthonormal logratio coordinates. The only limitation is that the information about a part of interest within one orthonormal coordinate system is split into two coordinates, one capturing the relevant information of that part and the other containing its redundant residue (typically the last coordinate).

The practical part of the contribution is focused on real data from metabolomics comparing dry blood spots of healthy controls and patients suffered from Medium chain acyl-CoA dehydrogenase deficiency. Using weighted pivot balances specific markers of this disease can be found much easier comparing to other alternatives. Also different ways of choosing specific weights in weighted pivot balances are discussed.

## References

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