
COMPOSITIONAL METABOLIC FLUX ANALYSIS

A PREPRINT

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ABSTRACT

Metabolic Flux Analysis aims to infer the values of metabolic fluxes from measurements of isotope labelling distributions. Since these distributions are positive, sum-constrained and relatively low-dimensional, we argue that they should be analysed using specialised methods that target compositional data. We illustrate our argument using a simple pedagogical example, then show how compositional analysis leads to improved results on a typical dataset.

1 Introduction

Metabolic flux analysis is the study of

1.1 Previous work

This section briefly reviews previous work in labelling-based metabolic flux analysis. For more detailed review papers see XXXXX

1.1.1 Experimental methods

1.1.2 The forward problem

- Cumomers
- EMU

1.1.3 Software

- OpenFlux
- Freeflux
- INCA
- 13CFlux
- ...

1.1.4 Bayesian 13C MFA

1.2 Problem statement

The topic of how to statistically model isotope labelling pattern measurements has received relatively little attention in the development of metabolic flux analysis. Most presentations and software applications quantify the discrepancy between a species's measured and predicted isotope labelling distribution using a Euclidean distance, and advocate

choosing a flux configuration whose labelling pattern minimises this distance, possibly with per-species and/or per-isotope-equivalence-class weights. This is equivalent to using maximum likelihood estimation, where the likelihood is given by an independent normal distribution centered on the predicted labelling distribution, with error standard deviations determined by the weights, i.e., for each species s ,

References