proceedings

Abstract

Analysis and Prediction of Postprandial Metabolic Response to Multiple Dietary Challenges Using Dynamic Mode Decomposition †

Viktor Skantze [1,2,*], Mats Jirstrand [2], Carl Brunius [1], Ann-Sofie Sandberg [1], Rikard Landberg [1] and Mikael Wallman [2]

[1] Department of Life Sciences, Division of Food and Nutrition Science, Chalmers University of Technology, 412 96 Gothenburg, Sweden; carl.brunius@chalmers.se (C.B.); ann-sofie.sandberg@chalmers.se (A.-S.S.); rikard.landberg@chalmers.se (R.L.)
[2] Department of Systems and Data Analysis, Fraunhofer-Chalmers Research Centre for Industrial Mathematics, 412 88 Gothenburg, Sweden; mats.jirstrand@fcc.chalmers.se (M.J.); mikael.wallman@fcc.chalmers.se (M.W.)
* Correspondence: vikska@chalmers.se
† Presented at the 14th European Nutrition Conference FENS 2023, Belgrade, Serbia, 14–17 November 2023.

Abstract: Background: In the field of precision nutrition, predicting high-dimensional metabolic response to diet and identifying groups of differential responders are two highly desirable steps towards developing tailored dietary strategies. However, proper data analysis tools are currently lacking, especially for complex settings such as crossover studies. Current methods of analysis often rely on matrix or tensor decompositions, which are well suited for identifying differential responders but lacking in predictive power, or on dynamical systems modelling, which may be used for prediction but typically requires detailed mechanistic knowledge of the system under study. Objectives: To remedy these shortcomings, we aimed to explore dynamic mode decomposition (DMD), which is a recent, data driven method for deriving low-rank linear dynamical systems from high dimensional data. Methods: To allow integration of complex data from several dietary inputs to the metabolic system, we combine parametric DMD (pDMD) with DMD with control (DMDc). The resulting method allows (i) to predict the postprandial metabolic response of a new diet given only the metabolic baseline and dietary input, and (ii) to identify inter-individual differences in metabolic regulation, useful in determining metabotypes, i.e., metabolic phenotypes in dynamic data. To our knowledge, this is the first time DMD has been applied to metabolomics data. Results: pDMDc enabled a data-driven construction of low-dimensional dynamical models, able to capture the underlying dynamics of the metabolome after three dietary challenges. We demonstrate the utility and accuracy of the model in a crossover study setting on both measured and simulated data. Using simulated data, metabolic response to a new diet was accurately predicted having trained on four diets, with an average cosine similarity score of 0.6 (SD = 0.27). In measured data, we identified previously published metabolic groups with 100% overlap. Discussion: Accurate predictions via pDMDc require data from several dietary exposures with large variation, which can be costly to collect to confirm the efficacy of the method. A possible remedy is to share data among individuals using the mixed-effects framework. Employing pDMDc paves the way towards using control theory to approach PN by estimating the optimal input given a target metabolite trajectory.

Keywords: precision nutrition; dynamic mode decomposition; differential responders; metabotypes

Citation: Skantze, V.; Jirstrand, M.; Brunius, C.; Sandberg, A.-S.; Landberg, R.; Wallman, M. Analysis and Prediction of Postprandial Metabolic Response to Multiple Dietary Challenges Using Dynamic Mode Decomposition. *Proceedings* **2023**, *91*, 38. https://doi.org/10.3390/proceedings2023091038

Academic Editors: Sladjana Sobajic and Philip Calder

Published: 15 November 2023

Author Contributions: V.S.: Writing—original draft, review & editing, conceptualization, methodology, project administration, formal analysis; M.W.: Writing—review & editing, conceptualization, methodology, formal analysis; C.B.: Writing—review & editing, methodology; A.-S.S.: Data curation; M.J.: Writing—review & editing, methodology; R.L.: Writing—review & editing. All authors have read and agreed to the published version of the manuscript.

Funding: This work has been supported by the Swedish Foundation for Strategic Research (SSF, FID17-0020) and the Swedish Research Council for Sustainable Development (FORMAS, 2016-00314), and has been developed as part of the FORMAS project "Diet × gut microbiome-based metabotypes to determine cardio-metabolic risk and tailor intervention strategies for improved health" (2017-02003) funded by the European Joint Programming Initiative "A Healthy Diet for a Healthy Life" (www.healthydietforhealthylife.eu) (R.L., C.B.). All funders are gratefully acknowledged.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The measured data analyzed in this study can be provided upon reasonable request. The simulated data along with a MATLAB implementation of pDMDc is available at https://github.com/FraunhoferChalmersCentre/pDMDc.

Conflicts of Interest: The authors declare no conflict of interest.