Evaluating Temporal Dynamics using Gaussian Processes in Longitudinal Metabolomics Data

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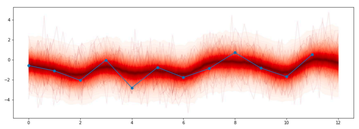
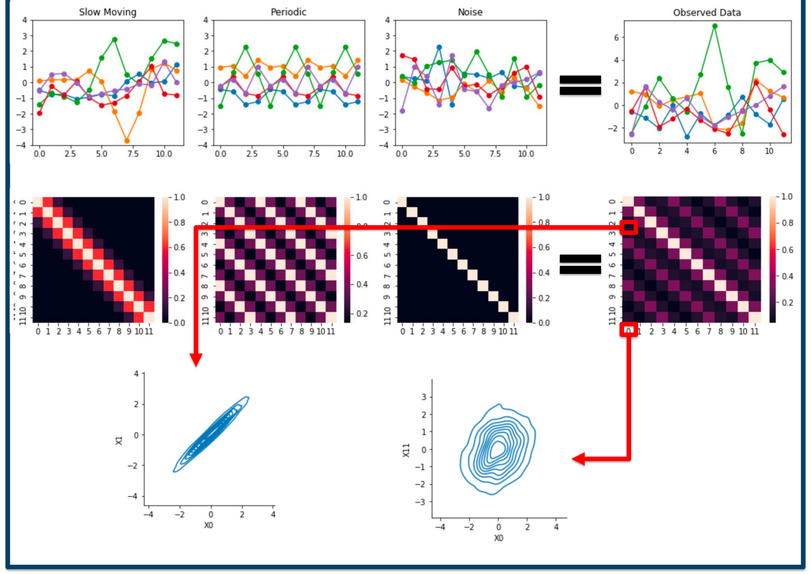
1 Introduction

We are interested in uncovering plausible **functional representations** of temporal dynamics given observed longitudinal omics data. These representations can then be investigated for biologically meaningful **component characteristics** as well as **contributions**. Potential applications include omics normalization and predictive modeling.

2 Gaussian Processes

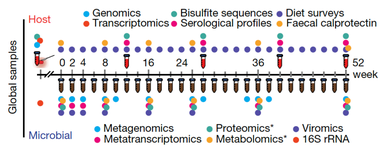
$$y \sim MVN(g(\mu), \Sigma)$$
$$g(\mu) = 0, \Sigma = K(x, x')$$

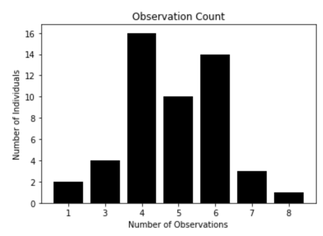


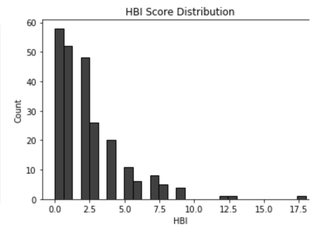


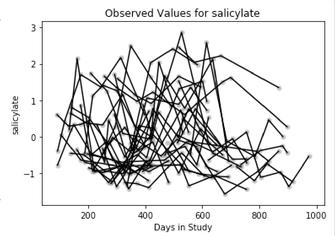
3 iHMP Data Subset Overview

241 samples
50 individuals
100 metabolites



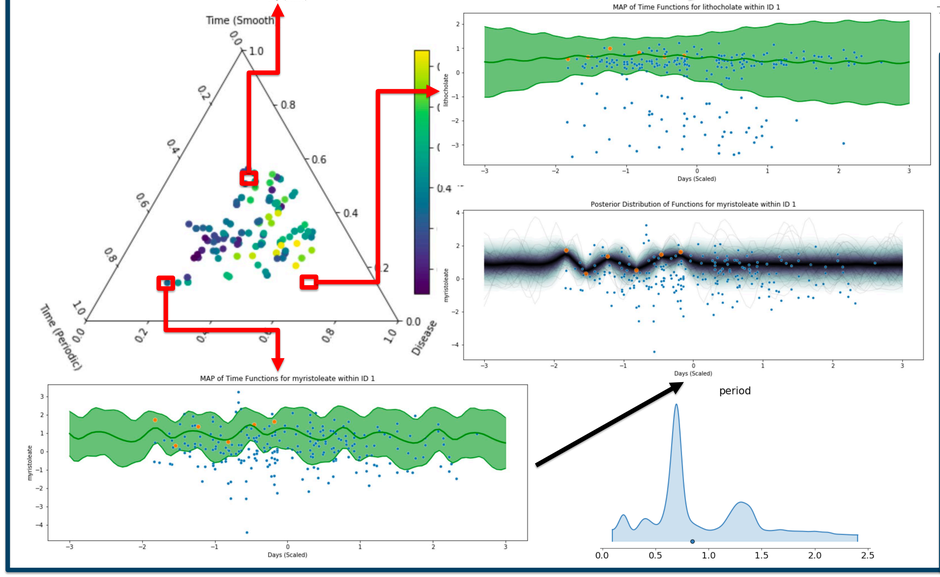


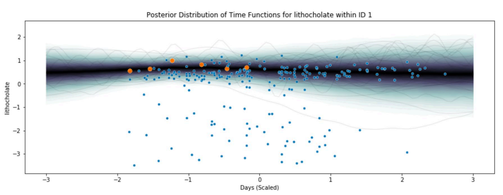


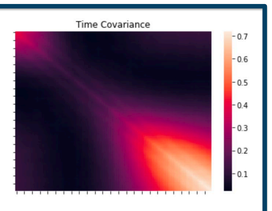


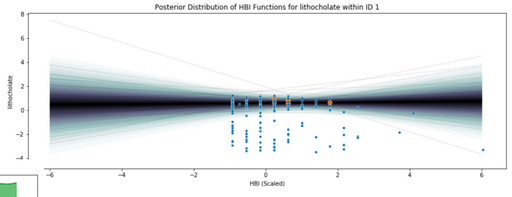
4 Metabolite Gaussian Processes

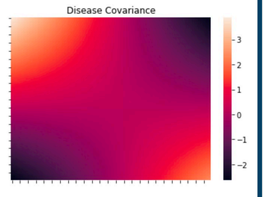
$$K(x, x') = B\left[x_i, x_i'^T\right] \begin{pmatrix} \sigma_s^2 EQ(x_t, x_t') \\ +\sigma_p^2 Per(x_t, x_t') \\ +\sigma_d^2 Poly(x_d, x_d') \end{pmatrix} + \sigma_n^2$$











5 Conclusions

- Nontrivial covariance relationships detected
- Posterior sampling is important but difficult

Next Steps

- Kernel learning
- Clustering
- Multi-omics
- Temporal interrelationship structures
- Approximate inference

6 Software

This work will be incorporated into *Waveome*, a software library that analyzes longitudinal omics data. More information including documentation, manuals, and tutorials will be available at waveome as resources are updated.

Data Source

Inflammatory Bowel Disease Multi'omics Database

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