

Annual Report Year 1

Anticipating the Chemistry of Life (ACOL)

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1 Introduction

2 Markov Random Field

2.1 WP 1

$$\mathbf{\Lambda}_c = \begin{pmatrix} -\alpha_c & \alpha_c \\ 1 - \alpha_c & \alpha_c - 1 \end{pmatrix} \quad (1)$$

We changed from μ_0 and μ_1 to a single parameter α which is the change rate to go from 0 to 1.

$$\mathbf{P}(n) = \exp(\mathbf{\Lambda}_c \nu_c b(n)). \quad (2)$$

We now have an additional parameter ν_c which is the rate parameter of the clique.

Root state probabilities are given by the stationary distribution of the Markov chain:

$$\mathbf{P}_\infty = (1 - \alpha_c, \alpha_c). \quad (3)$$

$$\mathbb{P}(L_{ms}|\mathbf{x}(m, s), R_{ms}) = \begin{cases} \epsilon & \text{if } \mathbf{x}(m, s) = 0, L_{ms} = 1, \\ 1 - \epsilon & \text{if } \mathbf{x}(m, s) = 0, L_{ms} = 0, \\ R_{ms} & \text{if } \mathbf{x}(m, s) = 1, L_{ms} = 1, \\ 1 - R_{ms} & \text{if } \mathbf{x}(m, s) = 1, L_{ms} = 0. \end{cases} \quad (4)$$

Added an error rate ϵ in case a molecule was wrongly added to LOTUS.

$$R_{ms} = (1 - e^{-\gamma_0 P_m})(1 - e^{-\gamma_1 Q_s}) \quad (5)$$

Changed equation for research effort.

2.2 WP 2

Implementation still in discussion but we are planning to move from ViMMS [1] to just using outputs of annotation tools. We might use a combination of Sirius, Metfrag, CFM-ID and maybe weight these outputs.

2.3 Fake extract

Plate 3 was performed by a bachelor student, but results are weird, so we'll pass everything again. Plate 1 is done.

3 LOTUS Expanded

In silico chemical expansion of molecules in LOTUS. Produced $3 \cdot 10^6$ molecules.

4 EMI-Monorepo

Helped Luca on the Monorepo for a couple of crates. Lost a bit the track of what he is doing.

5 Perspectives

I'd like to continue working with Luca in Rust as it is a skill that I want to master by the end of the PhD.

References

- [1] J. Wandy et al. "ViMMS 2.0: A Framework to Develop, Test and Optimise fragmentation Strategies in LC-MS Metabolomics". In: *Journal of Open Source Software* 7.71 (30, 2022). DOI: [10.21105/joss.03990](https://doi.org/10.21105/joss.03990).