Deriving quantitative indices of ecosystem services from cGEMs

In the context of MPA management and the nature-based economy, the application of cGEMs on sequencing datasets holds great promise to inform quantitative indices of the status of ecosystem services. The indices can be derived from cGEMs following constraint-based approaches. Further, environmental factors and relative abundances of community members can be integrated to tailor these indices to specific environmental contexts such as those in specific MPAs, informing in this way new economic valuation models for the accounting and management of microbial natural capital . In this box, we present some examples of indices that can be readily derived from cGEMs with current methods.

Background:

The feasible flux space in cGEMs is delineated by linear constraints that represent stoichiometric, thermodynamic, and flux capacity limits of metabolic reactions. A core assumption in this modeling approach is the steady-state condition, where the net production or consumption of internal metabolites is zero. This assumption allows for the prediction of flux distributions without an explicit functional form for reaction rates, which would depend on largely inaccessible kinetic parameters.

For each community member i, the stoichiometric matrix S^i encodes the stoichiometric relationships between metabolites, represented by rows, and reactions, columns, of its metabolic network. The flux vector v^i, representing the rate of these reactions, is bound by the physiological limits of the organism, denoted by minimum (v^i_{min}) and maximum (v^i_{max}) flux values. The model also incorporates shared metabolite exchanges (E^m_x) across the community, which are crucial for understanding the inter-species metabolic dependencies and synergies. Additionally, these exchanges are modulated by the relative abundances (α_i) of each community member. The feasible flux space for the community is then defined as the set of all flux vectors that satisfy the constraints for each member and shared metabolite. We can assess this flux space by solving the following linear programming problem:

$$
\begin{aligned}
\max \quad & f(v) \\
\text{s.t.} \quad & S^i v^i = 0 \\
& v^i_{\min} \leq v^i \leq v^i_{\max} \\
& E^m_x = \sum_{i \in C} \alpha_i E^i_x \\
& v^i_{\text{bio}} > 0 \\
& \forall i \in \text{members}, \\
& \forall x \in \text{shared metabolites}.
\end{aligned}
$$

Here, $f(v)$ represents an objective function, which might vary depending on the specific application, such as community biomass production, waste degradation, or more sophisticated measures of community ecological services. In the following, we present three possible quantitative indices of ecological services that can be derived from the feasible flux space of a cGEM.

Maximum Flux Capacity (MFC):

The MFC index is designed to quantify the maximum potential of a specific metabolic function within the community. It is particularly relevant in scenarios where a certain metabolic activity is directly linked to an ecosystem service, such as carbon fixation or nitrogen cycling. The MFC is computed as the maximum summation of a particular metabolic flux across all community members:

$$\mathrm{MFC} = \max\left(\sum_{i \in C} v_k^i\right),$$

where v_k^i denotes the flux rate of key reaction k in community member i. Key reactions are selected based on the target metabolic process. For instance, carbon fixation is predominantly catalyzed by the enzyme RuBisCO within the phytoplankton, thus this would be a key reaction for carbon sequestration. This index can be used to evaluate the potential impact of environmental changes or management interventions on the metabolic output of the community. For example, the MFC of carbon fixation can be used to assess the impact of ocean acidification on the carbon sequestration potential of the community. Additionally, the MFC can be easily extended to account for multi-reaction processes, by replacing the flux v_k^i with the sum of fluxes across all reactions involved in the process.

Metabolic Flux Shift Index (MFSI):

The MFSI offers a measure of how the metabolic state of a community shifts under different environmental conditions. This index could be particularly relevant for monitoring the resilience and adaptability of microbial communities within MPAs to environmental stressors or changes, by comparing the flux state between baseline condition and a later point in time. The feasible space for MFSI includes the joint feasible spaces for both conditions. Each feasible space would be affected by the differences in environmental nutrients that are accessible to the community as well as differences in relative abundances of community members. To measure the difference between the two flux states, we can follow an approach akin to MOMA (Segrè, Vitkup, and Church 2002) and define the MFSI as the minimum of the sum of absolute flux differences across all key reactions between the two feasible flux spaces:

$$\mathrm{MFSI} = \min\left(\sum_{k \in K} |v_k - w_k|\right).$$

Here, v and w represent the flux vectors under the two conditions, respectively. By computing the minimum distance between two flux states of different environmental conditions, the MFSI provides a quantitative assessment of the divergence of the community metabolic capabilities between these two conditions. Therefore the MFSI could be instrumental in assessing the evolution of microbial ecosystem services of an MPA between time points, such as assessing the effects of a bioremediation approach by comparing with a baseline state.

Metabolic Functional Robustness Index (MFRI):

The MFRI assesses the resilience of key metabolic functions against variations in the availability of environmental nutrients by measuring how sensitive (elastic) reaction fluxes are to perturbations in nutrient uptake rates. Thus, this index quantifies the adaptive capacity of microbial communities in fluctuating environments. The elasticity of the flux of a key metabolic reaction, v_k, with respect to the perturbed exchange rate of nutrient j, $\varepsilon(k, E_j)$, is a dimensionless quantity, defined as:

$$\varepsilon_{k,\mathrm{E}_j} = \frac{\partial v_k}{\partial \mathrm{E}_j}\frac{\mathrm{E}_j}{v_k} = \frac{\partial \ln v_k}{\partial \ln \mathrm{E}_j}.$$

The MFRI for a particular reaction is then defined as the average of these elasticity values across different nutrient perturbations:

$$\mathrm{MFRI}(k) = \frac{1}{N}\sum_{j=1}^{N} \epsilon_{k,\mathrm{E}_j}.$$

This index can be pivotal in determining the critical points in a metabolic network and guiding management strategies to enhance the resilience of microbial communities. Additionally, elasticities can be readily computed within existing frameworks, such as MICOM (Diener, Gibbons, and Resendis-Antonio 2020). Finally, the MFRI can be easily extended to assess the robustness of a key community service with respect to perturbations in community structure, by replacing the nutrient exchange rates with the parameter α_i, i.e., the relative abundances of community members.

Conclusion

The indices presented above applied within the framework of cGEMs could provide a robust quantitative method to evaluate microbial ecosystem services. Further, while these indices are currently proposed to operate under the steady-state assumption, integrating cGEMs into dynamic modeling frameworks like dFBA represents a promising future direction. This approach would allow the indices to capture temporal dynamics in microbial communities, addressing the quasi-steady-state condition where different timescales of metabolic and ecological processes are considered. Such advancements in modeling will enhance the precision and applicability of these indices in managing MPAs. Beyond aligning ecological sustainability with economic valuations, they set the stage for innovative financial mechanisms that support MPAs' economic viability. Translating the ecological value of microbial services into economic terms, these indices can catalyze the creation of nature-based financial products, harmonizing conservation efforts with economic incentives.

References

Diener, Christian, Sean M. Gibbons, and Osbaldo Resendis-Antonio. 2020. “MICOM: Metagenome-Scale Modeling To Infer Metabolic Interactions in the Gut Microbiota.” *mSystems* 5 (1): 10.1128/msystems.00606-19. https://doi.org/10.1128/msystems.00606-19.

Segrè, Daniel, Dennis Vitkup, and George M. Church. 2002. “Analysis of Optimality in Natural and Perturbed Metabolic Networks.” *Proceedings of the National Academy of Sciences* 99 (23): 15112–17. https://doi.org/10.1073/pnas.232349399.