02

Model

Objective

Dataset

Issues

Alternative Idea 1

Brief other

url

Here is some text[1]

Idea:

$$\mathbf{v} = \text{MLP}(\mathbf{z_e}) \quad \text{(Reaction embeddings to flux vector)}$$

$$\text{fitness} = \mathbf{w}^\top \mathbf{v} \quad \text{(Predicted fitness from flux vector)}$$

$$\mathcal{L}_{\text{null}} = \|S\mathbf{v}\|_2^2 \quad \text{(Null-space constraint loss)}$$

$$\mathcal{L}_{\text{pFBA}} = \|\mathbf{v}\|_1 \quad \text{(Parsimonious flux balance objective)}$$

$$\mathcal{L}_{\text{fitness}} = (\mathbf{w}^\top \mathbf{v} - \text{fitness})^2 \quad \text{(Fitness constraint loss)}$$

$$\mathcal{L}_{\text{total}} = \mathcal{L}_{\text{pFBA}} + \lambda_{\text{null}}\mathcal{L}_{\text{null}} + \lambda_{\text{fitness}}\mathcal{L}_{\text{fitness}} \quad \text{(Total PINN loss)}$$

- $\mathbf{z_e}$ is the reaction embedding vector mapped via MLP to the flux vector $\mathbf{v}$.
- $\mathbf{w}$ is a binary vector indicating the biomass pseudoreaction.
- **fitness** is the experimentally measured fitness (growth ratio mutant/wildtype).
- S is the stoichiometric matrix enforcing the null-space constraint.

Brief of Other Attempts

If you think that these directions are interesting I can will expand on them. For brevity I just highlight my findings.

References

1. Corso, G., Stark, H., Jegelka, S., Jaakkola, T. & Barzilay, R. Graph neural networks. *Nat Rev Methods Primers* **4**, 1–13 (2024).