145019 Mechanistic Aware Fba Inspired Los

Here's the cleaned-up and corrected version of your text with improved grammar, spelling, and typesetting. Let me know if you'd like the markdown version too.

2025.04.08 – Possible Inclusions

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

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

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

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

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

$$\mathcal{L}_{\text{bounds}} = \sum_i \mathrm{ReLU}(-v_i) + \sum_i \mathrm{ReLU}(v_i - v_{\text{ub},i}) \quad \text{(Flux bound constraint loss)}$$

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

- $\mathbf{z_e}$ 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 of mutant to wild type)
- S is the stoichiometric matrix enforcing the null-space constraint
- $\mathbf{v}_{\text{ub}}$ is the upper bound vector for fluxes

Let me know if you want this turned into LaTeX source, markdown, or Anki format.