RL-Driven Kinetic Modeling

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Context and Motivation

Kinetic models are essential for understanding how **cells** behave dynamically:

- How they respond to stress, grow, or adapt to changes?
- What happens when genes or enzymes are altered (e.g., in synthetic biology or disease)?

Applications include robustness analysis of metabolic phenotypes or bioreactor simulations (Figure 1).

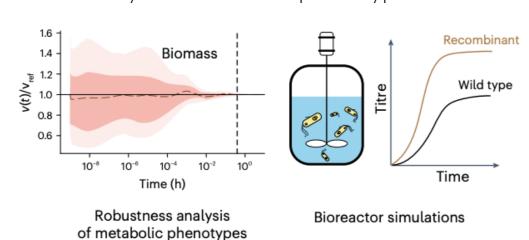


Figure 1. Showcase of usecases of kinematic models. Figure from [3].

However, these models require **thousands** of kinetic parameters, and most of them are **unknown**, **hard** to measure, or **inconsistent** across studies.

Previous Work

Traditional methods:

- use outdated parameters, rely on brute-force optimization, and assume simplified networks,
- struggle with scalability, data uncertainty, and handling multi-scale constraints.

Although attempts have been made to address these issues, they often require:

- extensive computational time [4],
- ground truth training data derived from traditional kinetic modeling approaches [1, 5, 2].

Finally, newly proposed framework **RENAISSANCE** [3] addresses both of these issues, however, it still has the following limitations:

- unstable convergence towards finding the optimal kinetic parameters,
- requires per environment re-training.

Overview of the RENAISSANCE framework is shown in Figure 2.

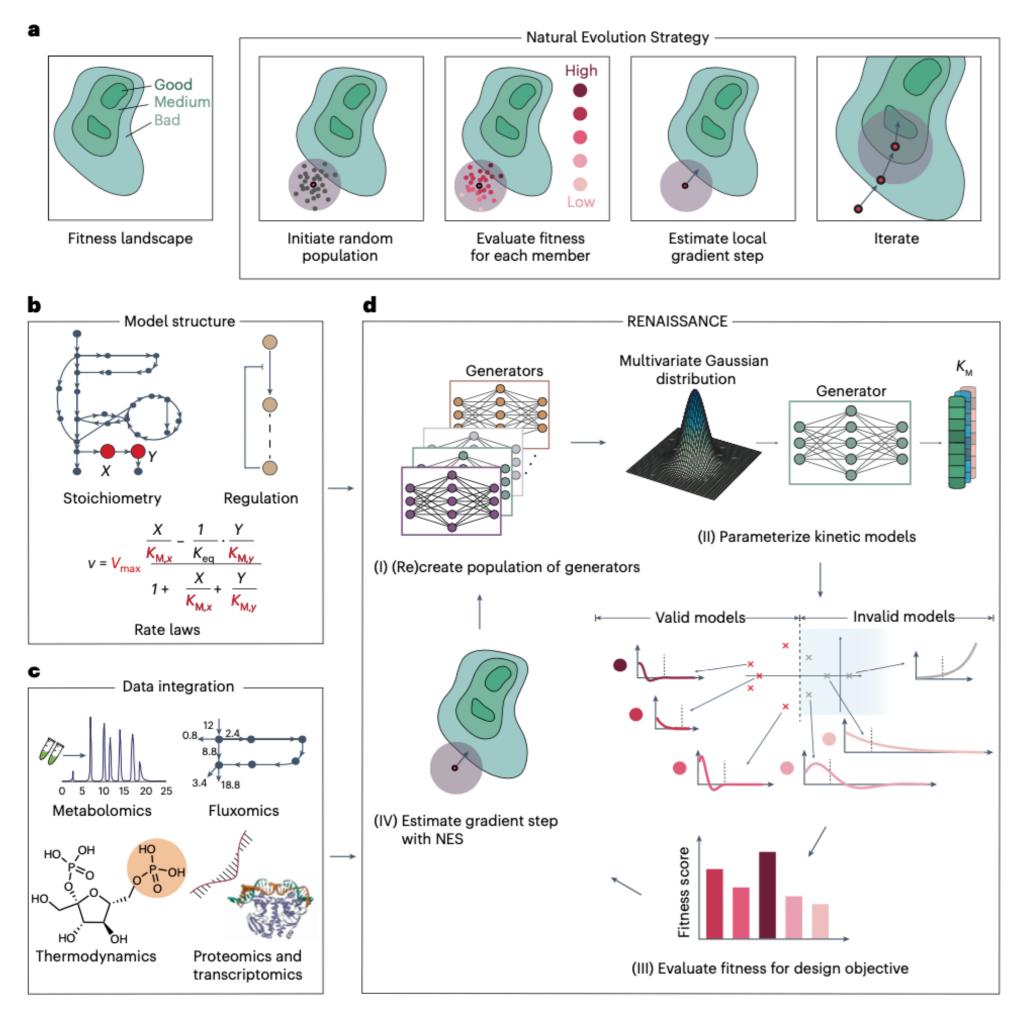


Figure 2. Overview of the RENAISSANCE framework. Figure from [3].

Key Contributions

Our contributions can be summarized as follows:

- we propose RL based alternative to the evolutionary algorithm used in RENAISSANCE,
- we provide a comparative study of the proposed RL approach vs. the traditional evolutionary algorithm,

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