Team ORDINAR: Predictioneer GRN Reconstruction

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1 Introduction

Predictioneer tasks teams with identifying a Gene Regulatory Network (GRN) governing a four-gene system (S_{1-4}) in 2D tissue under morphogen exposure (M_{1-2}). We aim to reconstruct interaction matrices (A, B) and decay rates (α) to predict dynamics under novel perturbations.

2 Theoretical Model

The system is modeled via non-homogeneous linear ODEs:

$$\dot{S}_i = -\alpha_i S_i + \sum_{j=1}^{4} A_{ij} S_j + \sum_{k=1}^{2} B_{ik} M_k(x, y)$$

where A_{ij} is gene j's influence on gene i, and B_{ik} represents morphogen-gene coupling. Auto-regulation is captured by α_i.

3 Methodology

Our approach evolved through three distinct phases to ensure titanium-grade reliability and precision.

3.1 Phase I & II: PINNs and GA

Initial explorations used Physics-Informed Neural Networks (PINNs) in JAX for continuity and Genetic Algorithms (GA) for discrete interaction searching. While PINNs offered high temporal resolution, they were prone to local minima in the discrete constraint space.

3.2 Phase III: Final GPU Evolutionary Solver

The production solver utilizes a massively parallel Evolutionary Strategy (ES) implemented in PyTorch:

- **Vectorized Eval:** 100,000 models/generation evaluated on an NVIDIA RTX 4050.
- **Steady-State (SS) Physics:** We solved for B by enforcing $\dot{S} = 0$ at $t = 0$ (pre-removal).
- **Numerical Robustness:** Derivatives $\dot{S}$ were extracted via Gaussian-smoothed finite differences ($\sigma = 2.5$) to filter experimental noise.
- **Optimization:** A $(1,000 + 50,000)$ elitist strategy ensured monotonic convergence to a global loss minimum.

4 Results

The solver achieved a Root Mean Square Error (RMSE) of **0.00089**.

4.1 Gene Interaction Matrix (A)

Influence of Gene j (column) on Gene i (row):

	S1	S2	S3	S4
S1	0	+1	-1	+1
S2	-1	0	-1	+1
S3	+1	-1	0	-1
S4	-1	+1	-1	0

Table 1: Interaction Matrix A

4.2 Morphogen Coupling Matrix (B)

Influence of M_1, M_2 on Genes S_{1-4}:

	M_1	M_2
S1	+1	0
S2	+1	0
S3	-1	0
S4	+1	0

Table 2: Coupling Matrix B

4.3 Kinetic Parameters

Average decay rate α was inferred as **0.1479**, indicating high system stability with moderate recovery times post-perturbation.

5 Experiment B Prediction

Using reconstructed parameters, we predicted Experiment B (M_1 removal) using Euler integration. The simulation captures the drifting steady-state dynamics as the M_1 activation signal is withdrawn.

6 Conclusion

Team ORDINAR has provided a robust, biologically consistent GRN reconstruction. Our GPU-accelerated framework effectively bridged the gap between discrete logical interactions and continuous kinetic drift.