

Predictioneer

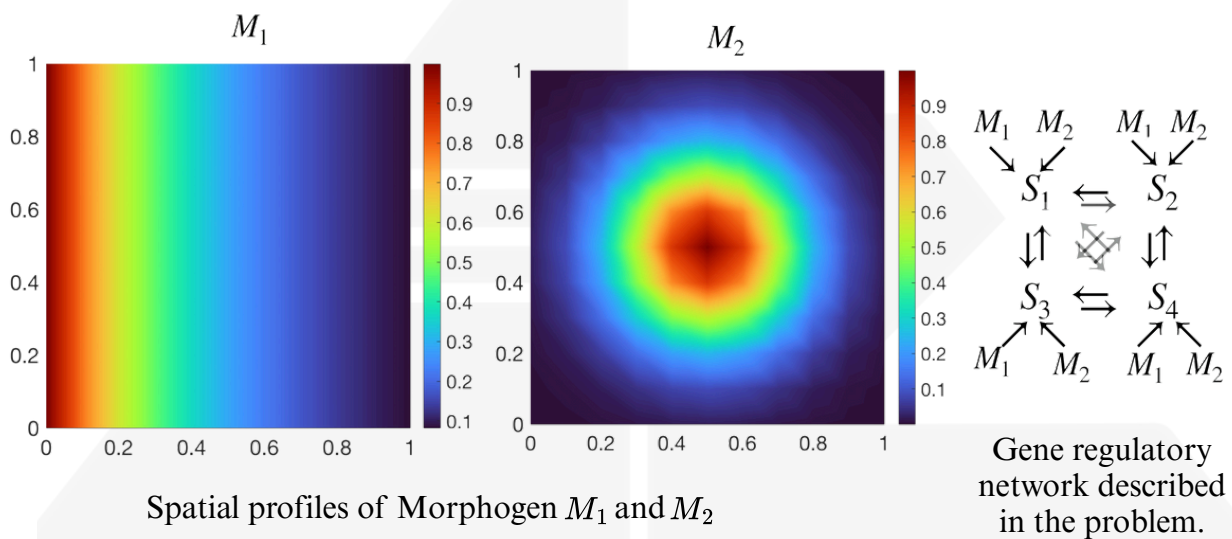
Problem Statement Inferring a Gene Regulatory Network from Spatial Expression Dynamics

Background :

Consider a two-dimensional tissue exposed to two spatially varying morphogens :

$$M_1(x, y) = e^{-2.5x}, \quad M_2(x, y) = \exp\left(-\frac{(x - 0.5)^2 + (y - 0.5)^2}{2(0.18)^2}\right)$$

These morphogens regulate a four-gene network. These morphogens regulate the genes (promotes or inhibits). The genes also regulate each other. Rather than modeling absolute concentrations, we study *deviations from a baseline expression level*. Let $S_i(x, y, t)$ be this deviation. There is an auto regulation in the system that wants to keep the gene expression to the baseline level (i.e. $S_i(x, y, t)$ to zero). By construction, deviations may take positive or negative values: positive means “above baseline”, negative means “below baseline”. At the same time morphogens and the other genes control each other.



Experimental Design :

The tissue is first held under both morphogens (M_1, M_2) until it reaches a spatial steady state $\mathbf{S}(x, y, t = 0) = \mathbf{0}$.

Two perturbation experiments are then performed:

1. **Experiment A (provided dataset):** The system is initialized at steady state, and morphogen M_2 is instantly removed. Time-dependent gene expression deviations $S_i(x, y, t)$ are recorded over a grid of (x, y) and exported in the provided CSV file **GRN_experiment_M2_removal.csv**.
2. **Experiment B (held out):** The system is again initialized at the same steady state, but now morphogen M_1 is removed. Your goal is to use your inferred model to predict the spatial-temporal dynamics under this perturbation.

Both experiments include multiple time points and full spatial sampling, but only Experiment A is available to you

Your task and submission details :

1. **Model reconstruction from time series** Using only the dataset from Experiment A and the analytic forms of $M_1(x, y)$ and $M_2(x, y)$:
 - (a) Estimate the gene regulatory network (i.e. return a 4×4 matrix with entries +1, -1, or 0). +1 means promote, -1 means inhibit, 0 means no interaction. Diagonal elements of the matrix are irrelevant in this context. (**Note** : The element ij refers to the interaction/influence of gene j on gene i .)
 - (b) Estimate the morphogen coupling matrix B . This will be a 4×2 matrix. with entries +1, -1, or 0.

(text file for both matrix is required)

You may use finite difference approximations of dS/dt and linear regression techniques.

2. **Prediction Task (Experiment B)** Using your fitted model parameters (A, B, α) , simulate the dynamics resulting from the removal of M_1 :

$$M_1(x, y, t) = 0 \quad M_2(x, y, t) = M_2(x, y)$$

Export your prediction as a CSV file for comparison with the held-out dataset. Please use the same data points in same order as Experiment A.

3. Please attach a report (<5 pages) that describes your findings and insights from this exercise

Evaluation Criteria:

The points weightage of the problem statement are as follows:

Part I (40 %) 20-20 % weightage will be given to the correct identification of gene regulatory matrix and morphogen coupling matrix.

Part II (30 %)

The accuracy of the results will be assessed using Root Mean Square(RMS) values between the predicted and actual gene expression values.

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (Predicted_i - Actual_i)^2}{N}}$$

Part III (30 %)

This part will be graded on the overall presentation and the problem-solving approach. In this section, creativity will be put to the test.

Participation Procedure:

- A group of **2 to 4** members are allowed per team. Each team should have at least one chemical engineering student.
- No participant can register in more than **one team**. In such an instance, both teams will be subjected to **disqualification**.

Certification Prizes:

- The top **5 teams** will be awarded cash prizes worth **25K INR total** and the **top 10 teams** will receive a **certificate of merit**.
- The rest of the teams making a valid final submission and qualifying all the eligibility criteria will receive a **certificate of appreciation**.

NOTE: The final decision-making authority lies with team AZeotropy. Participants also consent to the free use of their submissions by the team AZeotropy. Proper attribution shall be given to the authors in case their submissions are published on the symposium

In case of any queries , participants can contact:

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