Identification of cell signaling pathways based on biochemical reaction kinetics repositories

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Introduction

Cell Signaling

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Understanding the functioning of cell signaling is important in many biological areas.

Cell Signaling

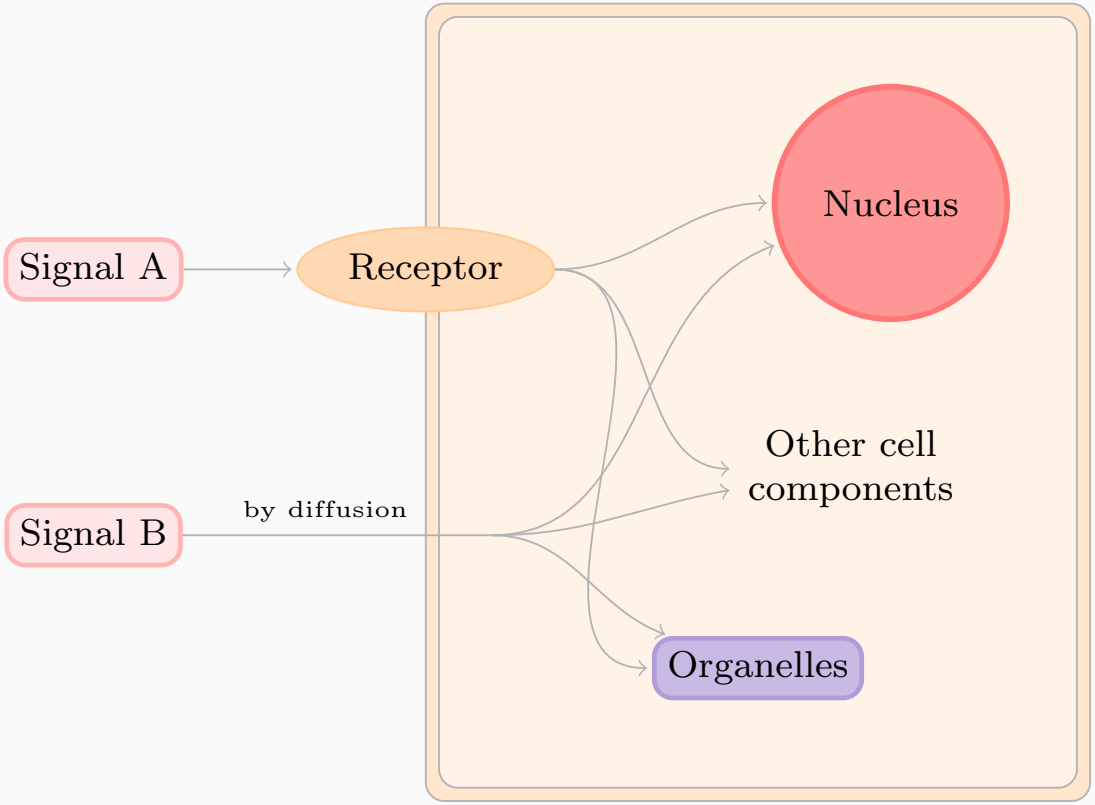

Figura 1: A general cell signaling mechanism.

Cell Signaling Pathways

A cell signaling network can be characterized by a sequence of chemical reactions that allows the presence of a signal to modify the state or behaviour of a cell.

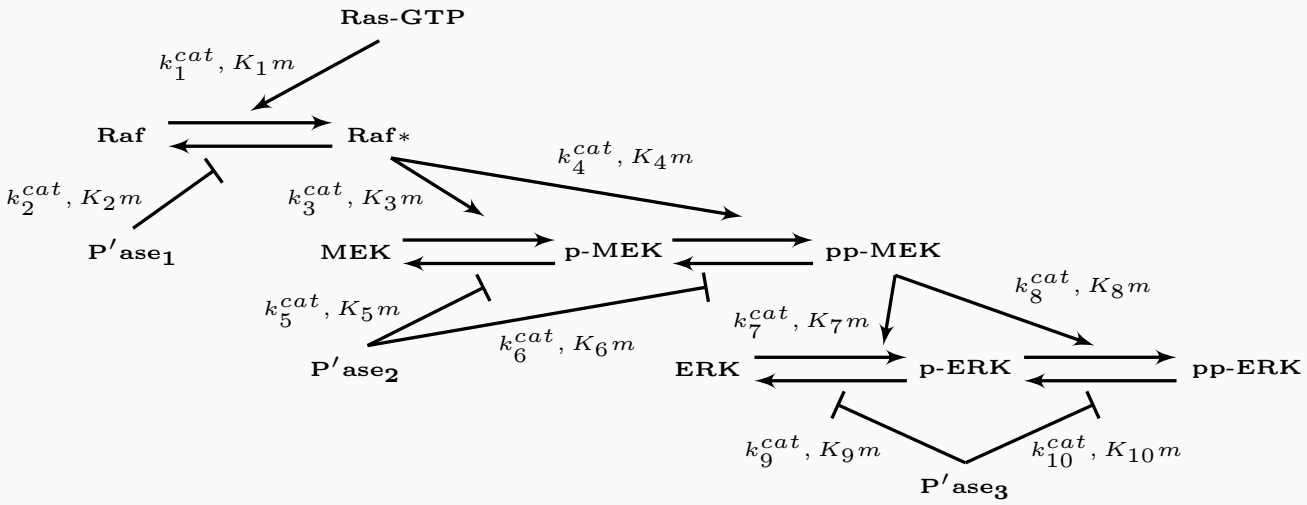

Figura 2: An example of a signaling pathway.

Mathematical Models of Signaling Networks

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Using biochemical and enzymatic kinetics, we can write equations that represent the rate of change of concentration for a chemical species.

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Repeating this procedure for all reactions of a pathway allows us to derive a system of ordinary differential equations that can model the signaling pathway.

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- a set of chemical reactions that are relevant for the biological experiment;
- information about the reaction rate constants of the model.

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Hence, it is desirable to construct a method that can systematically modify these models and choose the one that better represents the experiment.

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On her work, the problem of identification of cell signaling pathways is treated as a feature selection problem.

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The feature selection problem is a combinatorial optimization problem:

> Given a set of features S and a cost function c, find subset $X \in \mathcal{P}(S)$, with minimum cost $c(X)$.

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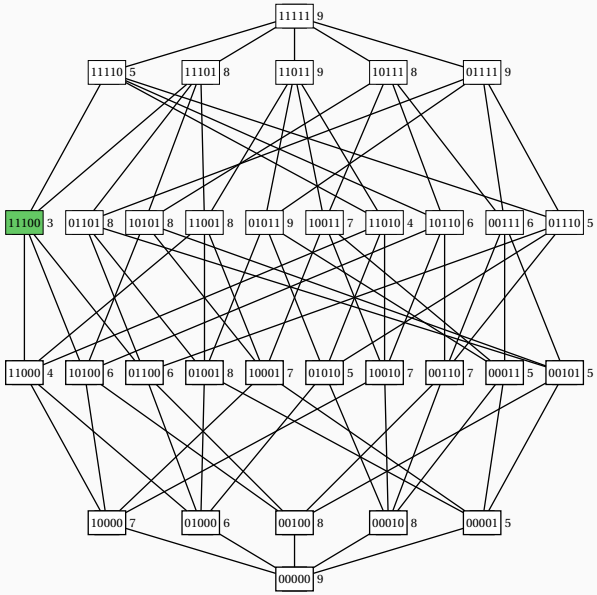

Figura 3: An example of feature selection search space with 5 features.

Feature Selection for Identification of Signaling Pathways

If we consider that the set of all possible chemical reactions is the set of features, than we can tackle the identification of signaling pathway problem as a feature selection problem.

Fundamental Concepts

Model Selection

Experiments on Model Selection

Next Steps