A Slightly Different Approach to Network Environ Analysis

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Outline

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Model Network Structure

- A network with n compartments:

$$x_1,\, x_2,\, \ldots.,\, x_n$$

- Linear interactions among compartments:

$$x_j \longrightarrow x_i, \qquad 1 \leq i\,,\, j \leq n$$

- Inputs to and outputs from individual compartments:

$$x_i \longrightarrow \circledcirc, \qquad \circledcirc \longrightarrow x_j, \qquad 1 \leq i,\, j \leq n$$

Contents of NEA

- Pathway analysis
  - Number of possible pathways among compartments.
- Storage Analysis
  - Mapping of input values to storage values at steady state.
- Flow Analysis
  - Mapping of input values to sum of flows from/to each compartment.
- Utility Analysis
  - Analysis of $+/-$ relationships among compartments.

Mass-Action Type Interactions

- Partial turnover coefficient of $x_j \longrightarrow x_i$ is denoted as c_{ij} (∼community matrix).
- Then the actual flow intensity of $x_j \longrightarrow x_i$ is $c_{ij}x_j$.
- Output flow intensity of $x_j \longrightarrow \circledcirc$ is $c_{0j}x_j = y_j$.
- Input flow intensity of $\circledcirc \longrightarrow x_j$ is just $z_j = c_{j0}$.
- Turnover rate is defined for each compartment x_k as follows:

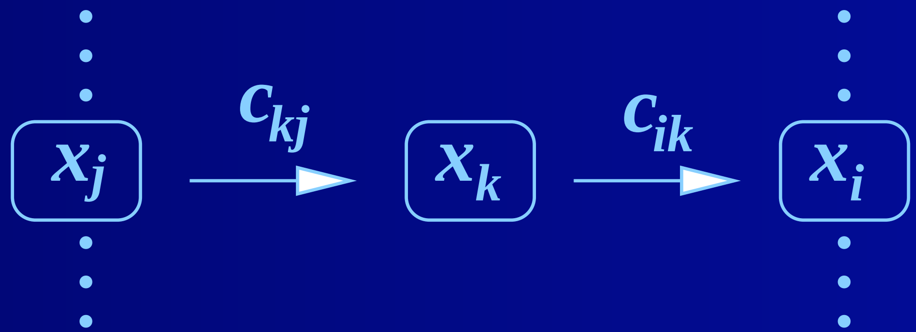
$$\tau_k = \sum_{i=0,\, i \neq k}^{n} c_{ik}, \quad k = 1, \ldots, n$$

Rate of Change of Storage Values

The rate of change of compartment x_k can be formulated as:

$$\frac{dx_k}{dt} = \underbrace{\sum_{j=0,\, j\neq k}^{n} x_j\, c_{kj}}_{\text{inflow}} - \underbrace{x_k \sum_{i=0,\, i\neq k}^{n} c_{ik}}_{\text{outflow}}, \qquad 1 \leq k \leq n$$

where $x_0 = 1.$



Construction of ODE

The rate of change of compartment x_k can be formulated as:

$$\frac{dx_k}{dt} = -\underbrace{x_k \sum_{i=0,\, i\neq k}^{n} c_{ik}}_{\text{outflow}} + \underbrace{\sum_{j=0,\, j\neq k}^{n} x_j\, c_{kj}}_{\text{inflow}}, \qquad 1 \leq k \leq n$$

where $x_0 = 1$. Then

$$\frac{dx_k}{dt} = -x_k \tau_k + \sum_{j=0,\, j\neq k}^{n} x_j\, c_{kj}, \qquad 1 \leq k \leq n$$

Using vector notation, we get

$$\frac{dx_k}{dt} = [c_{k1}\ c_{k2}\ \cdots - \tau_k \cdots c_{kn}]\, [x_1\ x_2 \cdots x_n]^T + c_{k0}$$

ODE System

Let

$$x = [x_1 \; x_2 \cdots x_n]^T, \qquad z = [z_1 \; z_2 \cdots z_n]^T$$

Then

$$\dot{x} = C\,x + z$$

where

$$C = \begin{bmatrix} -\tau_1 & c_{12} & \cdots & c_{1n} \\ c_{21} & -\tau_2 & \cdots & c_{1\,(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ c_{n1} & c_{(n-1)\,1} & \cdots & -\tau_n \end{bmatrix}$$

Storage Analysis

Storage Analysis immediately follows from this ODE system:

$$\dot{x} = C\,x + z$$

Assuming the system is at steady state $(\dot{x}^* = 0)$, we get

$$\begin{aligned} -C\,x^* &= z \\ x^* &= \left(-C^{-1}\right) z \\ x^* &= S\,z \end{aligned}$$

The mapping represented by the matrix S

$$S : z \longrightarrow x^*$$

maps *inputs* into *steady-sate storage values*.

Flow Analysis

To accommodate flow analysis we define the flow matrix F as follows:

$$F := \begin{cases} f_{ij} &= \quad c_{ij}x_j^* \\ f_{ii} &= \quad -\tau_i x_i^* = -T_i \end{cases}$$

where x^* is the state of the system at steady-state, i.e.,

$$C\,x^* + z = 0$$

The equality below follows from the definitions of F and C.

$$F\,1 = C\,x^*$$

Throughflow Analysis

We define the matrix B as follows:

$$B := \begin{cases} b_{ij} &= c_{ij}/\tau_j = f_{ij}/T_j \\ b_{ii} &= -1 \end{cases}$$

Then by definition

$$F\,1 = B\,T$$

Note that at steady state we have

$$F\,1 = C\,x^* = -z$$

Throughflow Analysis

Combining

$$F\,1 = B\,T$$

with

$$F\,1 = C\,x^* = -z$$

we get

$$\begin{aligned} -z &= B\,T \\ \underbrace{\left(-B^{-1}\right)}_{=N}\,z &= T \end{aligned}$$

The mapping represented by the matrix

$$N\;:\;z \rightarrow T$$

maps inputs to throughflows.

Non-Steady-State Throughflow Analysis

Is it possible to derive a map from inputs to throughflows

$$\bar{N} : z \longrightarrow T$$

in the non-steady-state case?

Since throughflows (T) and storages (x) will be varying in time, such a map would probably be a *differential map*.

$$\begin{aligned} \dot{x} &= C\,x + z \\ &= B\,T \,\mathbf{.}\, x + z \end{aligned}$$

where "**.**" denotes componentwise vector multiplication. Rearranging terms, we get

$$\underbrace{\left(\frac{d}{dt} - B\,T\right)}_{=\bar{N}} \mathbf{.}\, x = z$$

Utility Analysis

Utility Analysis is based on the matrix

$$U = (I - D)^{-1} \quad \text{where} \quad D = B - B'$$

The matrix B' is defined similarly to B as follows:

$$B' := \begin{cases} b'_{ij} & = & c_{ji}/\tau_j = f_{ji}/T_j \\ b'_{ii} & = & -1 \end{cases}$$

Or similarly:

$$D := \begin{cases} d_{ij} & = & (c_{ij} - c_{ji})/\tau_i = (f_{ij} - f_{ji})/T_i \\ d_{ii} & = & 0 \end{cases}$$