Network Environ Analysis

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Model Network Structure

- A network with n compartments:

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

- Interactions among compartments:

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

- Inputs to and outputs from individual compartments:

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

Here " $\circledcirc$ " represents the environment.

From Model to ODE

To form a mathematical description of such an ecosystem model, we define the following parameters:

$$\begin{aligned} f_{ij} &: \text{ flow rate of nutrients from compartment } j \text{ to compartment } i \\ z_i &: \text{ rate of environmental input to compartment } i \\ y_i &: \text{ rate of environmental output from compartment } i \\ x_i &: \text{ storage value of compartment } i \end{aligned}$$

Based on these parameters, we define the corresponding flow matrix F, input vector z, output vector y, and the storage vector x as follows:

$$F = \begin{bmatrix} f_{11} & \cdots & f_{1n} \\ \vdots & \ddots & \vdots \\ f_{n1} & \cdots & f_{nn} \end{bmatrix} \quad z = \begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} \quad y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}.$$

For an evolving ecosystem, all parameters defined above may be varying in time, hence each will be a function of time. We can construct a differential equation for the change of storage value of compartment k ($\dot{x}_k = \frac{dx_k}{dt}$) as follows:

$$\dot{x}_k = \underbrace{\sum_{j=1}^{n} f_{kj} + z_k}_{\text{input to } x_k} \underbrace{- \sum_{j=1}^{n} f_{jk} - y_k}_{\text{output from } x_k} \,. \tag{1}$$

In general, the following differential equation holds for each compartment

$$\dot{x}_k = T_k^{in} - T_k^{out}$$

where T^{in} and T^{out} are functions of time, and

$$\begin{aligned} T_k^{in} &= \sum_{i=1}^{n} f_{ki} + z_k \\ T_k^{out} &= \sum_{i=1}^{n} f_{ik} + y_k \end{aligned} \tag{2}$$

Throughfow Analysis

At steady state, we have

$$T_k^{in} = T_k^{out} = T_k$$

Replacing T^{in} by its definition (2), we get

$$\sum_{i=1}^{n} f_{ki} + z_k = T_k \tag{3}$$

We define G, the flow matrix normalized with respect to throughlows (T), as follows:

$$g_{ik} = \frac{f_{ik}}{T_k} \tag{4}$$

Combining equation (3) with definition (4), we get

$$z_k = T_k - \sum_{i=1}^{n} g_{ki} T_i$$

Using matrix notation, the equation above can be expressed as follows:

$$z = (I - G)\, T$$

where G has zeros on its diagonals. Assuming $I - G$ is invertible, we define the *throughflow matrix* N as follows:

$$N\, z = T, \quad N = (I - G)^{-1}$$

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

Storage analysis assumes donor-controlled flows, where

$$f_{ij} = c_{ij} x_j$$

Partial turnover coefficient of $x_j \to x_i$ is denoted as c_{ij} ($\sim$community matrix).

- Then the actual flow rate of $x_j \to x_i$ is $c_{ij} x_j$.
- Outflow rate of $x_j \to \circledcirc$ is $c_{0j} x_j = y_j$.
- Inflow rate of $\circledcirc \to x_j$ is just $z_j = c_{j0}$.
- Turnover rate is defined for each compartment x_k as follows:

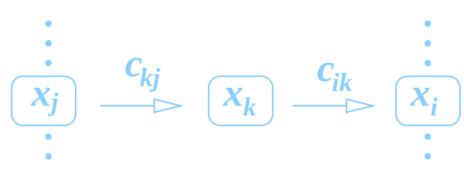
$$\tau_k = \sum_{i=0,\, i\neq k}^{n} c_{ik}, \quad k = 1, \ldots, n$$

Construction of the ODE system:

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 $x_0 = 1$.



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

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

Using vector notation, we get

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

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

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

The mapping represented by the matrix S

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

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

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:

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