Applications of numerical linear algebra for the study of complex networks and systems

Laplacian of a non-negative matrix.
Z matrices and Metzler matrices.
Positive and compartmental systems.

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Roma Tor Vergata, November 22-23-24 2022

Summary

- Laplacian matrix and Laplacian flow. Example: opinions dinamic.
- Equilibrium of the Laplacian flow and rank of the Laplacian.
- Convergent and semi convergent matrices in continuous time. Rate of convergence.
- Necessary and sufficient condition for consensus of the Laplacian flow.
- Z matrices and Metzler matrices. Positive systems. Application to opinions dynamic.
- Compartmental systems. Example: biokinetic models.

Laplacian matrix

A matrix L is defined Laplacian if:

- $Le = 0$, namely the sum of the entries of each row is equal to zero;
- the entries outside the main diagonal are less or equal than zero.

The definition implies that the diagonal entries of a Laplacian are greater or equal than zero and that the matrix is singular.

If A is non negative, the matrix $L_A = \mathrm{diag}(Ae) - A$ is a Laplacian defined Laplacian of A. Notice that, given a Laplacian L, if D is a diagonal matrix such that $A = D - L \geq 0$ then

$$L_A = \mathrm{diag}(De - Le) - D + L = \mathrm{diag}(De) - D + L = L.$$

Hence, given a Laplacian L there are infinite matrices A such that $L = L_A$.

Some spectral properties of the Laplacian

Let us denote with $\mu(A)$ the spectral abscissa of a matrix A namely the maximum of the real parts of its eigenvalues.

Theorem

If L is a Laplacian $\mu(L) \geq 0$ and $\mu(L) = 0$ if and only if $L = 0$. Moreover $\mu(-L) = 0$.

Proof Gershgorin theorem implies that all the eigenvalues of L different from 0 have positive real part, hence $\mu(L) \geq 0$ and $\mu(-L) = 0$. If $\mu(L) = 0$ then all the eigenvalues are equal to zero, then the trace of L is zero, hence the diagonal is made up of zero entries, hence $L = 0$.

Opinions dynamic: Abelson continuous model

In continuous models of opinions dynamic all the nodes, or actors, of a social network have a variable $x_i(t)$ representing their opinions as functions of time, usually abbreviated to x_i. The Abelson model takes the form

$$\dot{x}_i = \sum_{j=1}^{n} A_{i,j}(x_j - x_i),$$

where $A_{i,j} \geq 0$ represents a rate at which actor j attempts to persuade actor i.
The differences of the opinions between the actors is highlighted: if $x_j > x_i$ for $j \neq i$ then x_i has non negative derivative.

Opinions dynamic and Laplacian flow

Notice that

$$\dot{x}_i = \sum_{j=1}^{n} A_{i,j}(x_j - x_i) = \sum_{j=1}^{n} A_{i,j}x_j - \Big(\sum_{j=1}^{n} A_{i,j}\Big)x_i.$$

In matrix form this becomes

$$\dot{x} = Ax - \mathrm{diag}(Ae)x = -(\mathrm{diag}(Ae) - A)x = -L_A x.$$

- The equation $\dot{x} = -L_A x$ is known as Laplacian flow.
- We are interested in the possible convergence towards consensus of the Laplacian flow meaning that asymptotically all the opinions coincide.

Equilibrium points of the Laplacian flow and nullspace of the Laplacian matrix

- Clearly the equilibrium points of the equation $\dot{x} = -Lx$ satisfy $Lx = 0$, hence it is important to study the nullspace of L.
- Since $Le = 0$ the nullspace has dimension at least 1 so that the maximum rank is $n - 1$.

Now we discuss a theorem on the rank of the Laplacian. The case where the rank is $n - 1$ and the nullspace are just the multiples of e will be for us of particular importance.

Rank of the Laplacian

Let us observe that if $L_A = \mathrm{diag}(Ae) - A$, and $D \geq 0$ is a diagonal matrix then:

- $L_{A+D} = \mathrm{diag}((A + D)e) - (A + D) = L_A$;
- $L_{DA} = \mathrm{diag}(DAe) - DA = DL_A$.

If A is non-negative let $D = \mathrm{diag}(I + A)$. Notice that D is non singular and that $\bar{A} = D^{-1}(I + A)$ is row stochastic. Hence

$$L_{\bar{A}} = L_{D^{-1}(I+A)} = D^{-1}L_{I+A} = D^{-1}L_A$$

so that the ranks of L_A and $L_{\bar{A}}$ coincide.
In summary for the study of the rank of a Laplacian L_A it is always possible to assume that A is row stochastic.

Equilibrium points of the Laplacian flow and nullspace of the Laplacian matrix

Theorem

Let A be a row stochastic matrix and let $G = D(A)$. If there are d sinks in the condensation digraph of G then the rank of $L_A = I - A$ is $n - d$.

Before the proof of the theorem, recall the condensation digraph of G, being by construction acyclic, has a unique sink if and only if it has a globally reachable node but this is true if and only if G itself has a globally reachable node. Hence, the theorem implies that the rank of $L = I - A$ is $n - 1$ if and only if G has a globally reachable node. In particular the rank is $n - 1$ if G is strongly connected (A irreducible) but the condition is not necessary: consider for example

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} \quad \Rightarrow \quad L_A = \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix}.$$

Proof

The d sinks in the condensation digraph of G correspond to d equivalence classes of the nodes of G: notice that a node of a class corresponding to a sink can only have arcs towards nodes of the same class. Hence after a suitable permutation of row and columns the matrix A becomes

$$\begin{bmatrix} A_{1,1} & & & \\ & \ddots & & \\ & & A_{d,d} & \\ A_{d+1,1} & \cdots & A_{d+1,d} & A_{d+1,d+1} \end{bmatrix}.$$

The matrices $A_{i,i}$, for $i = 1, \ldots, d$ are row stochastic and irreducible , since they are the matrices of equivalence classes of nodes, and for Perron-Frobenius theorem 1 is a simple eigenvalue of these matrices. This implies that the dimension of the nullspace of $I - A_{i,i}$ is 1.

Proof (continue)

The matrix $A_{d+1,d+1}$ cannot be row stochastic since otherwise its nodes could be partitioned in one or more equivalence classes corresponding to sinks in the condensation digraph of G. Hence $A_{d+1,d+1}$ is row substochastic and given a node with out degree equal to one there should be a path from that node to a node having out degree less than one in $A_{d+1,d+1}$. Hence $\rho(A_{d+1,d+1}) < 1$ so that $I - A_{d+1,d+1}$ has full rank.

Equilibrium points of the Laplacian flow

We deduce that if G contains a globally reachable node the only possible equilibrium points of the Laplacian flow are multiples of e.

It is interesting to observe that we used a similar permutation technique in the proof about achievement of consensus of the dynamical system $x(k) = Ax(k-1)$, in the case where the condensation digraph of $G = D(A)$ has a unique sink.

Convergence of a matrix in continuous time

As well known, the solution of the system $\dot{x}(t) = Ax(t)$ given $x(0)$ is

$$x(t) = \exp(At)x(0),$$

where

$$\exp(A) = \sum_{k=0}^{\infty} \frac{A^k}{k!}.$$

For this reason a matrix A is defined

- continuous time semi convergent if $\lim_{t\to+\infty} \exp(At)$ exists and is a specific matrix;
- continuous time convergent or Hurwitz if $\lim_{t\to+\infty} \exp(At) = 0$.

Convergence of a matrix in continuous time

By means of JCF (or more easily if A can be diagonalized) it is not difficult to prove that

$$\sigma(\exp(A)) = \{\exp(\lambda) | \lambda \in \sigma(A)\},$$

and moreover

Theorem

- A is continuous time convergent if and only if $\mu(A) < 0$;
- A continuous time semi convergent if and only if it is convergent or $\mu(A) = 0$ and 0 is a semisimple eigenvalue of A and all the other eigenvalues have negative real part.

if L is a Laplacian matrix this theorem implies that $-L$ cannot be convergent since $\mu(-L) = 0$, but can be semi-convergent in the case where 0 is semisimple since all the other eigenvalues have negative real part.

Rate of convergence

We can obtain a result on rate of convergence analogous to the one obtained for the discrete systems, in the case where 0 is a simple eigenvalue of A, the other eigenvalues have negative real part and A is diagonalizable. Then

$$At = V \begin{bmatrix} 0 & O \\ O & \Lambda t \end{bmatrix} V^{-1},$$

where Λ is a diagonal matrix of order $n-1$ containing the eigenvalues of A different from 0. Clearly

$$\exp(At) = V \begin{bmatrix} 1 & O \\ O & \exp(\Lambda t) \end{bmatrix} V^{-1}.$$

If $V = [e, *]$ and $(V^{-1})^T = [w, *]$ by proceeding as for the discrete systems we obtain

$$\| \exp(At) - ew^T \|_2 \leq \| V \|_2 \| V^{-1} \|_2 \exp(\mu_{\mathrm{ess}}(A)t),$$

where $\mu_{\mathrm{ess}}(A) = \mu(\Lambda) < 0$.

Consensus for the Laplacian flow

We now state a theorem about the convergence to consensus of the Laplacian flow $\dot{x} = -Lx$ in many respects analogous to the one regarding the discrete case.

Theorem

Let A be non-negative, let $G = D(A)$ and let L be the Laplacian of A. The following statements are equivalent:

- 0 is a simple eigenvalue of $-L$ and all other eigenvalues have negative real part;
- $\lim_{t\to+\infty} \exp(-Lt) = ew^T$ where w is the left eigenvector of L with eigenvalue 0 such that $e^T w = 1$;
- G contains a globally reachable node.

Comments

- Notice that it is not required that the subgraph of the globally reachable nodes of G is aperiodic.
- The theorem can be seen as a sort of extended Perron theorem for Laplacian matrices.
- A digraph has a globally reachable node if and only if there is a unique sink in its condensation digraph $C(G)$. Again consensus is reached if and only if in $C(G)$ there is a unique sink, but the theorem can be extended to the case where $C(G)$ has $M \geq 2$ sinks. This can be shown to be equivalent to the case where 0 is a semi simple eigenvalue of $-L$ of multiplicity M and the remaining eigenvalues have negative real parts.

Proof (sketch)

We would like to use the theorem about the discrete case. With this aim let $\epsilon > 0$ and small as needed so that $B_{\epsilon,L} = I - \epsilon L$ is row stochastic. The proof of the theorem can be obtained by proving the following three double implications

- 0 is a simple eigenvalue of $-L$ and all other eigenvalues have negative real part if and only if 1 is a simple eigenvalue of $B_{\epsilon,L}$ and all other eigenvalues modulus less than one (suggestion: remember that ϵ can be chosen sufficiently small);
- $\lim_{t\to+\infty} \exp(-Lt) = ew^T$ if and only if $\lim_{k\to+\infty} B_{\epsilon,L}^k = ew^T$ (suggestion: $\sigma(B_{\epsilon,L}) = 1 - \epsilon\sigma(L)$).
- $G = D(A)$ contains a globally reachable node if and only if $D(B_{\epsilon,L})$ contains a globally reachable node and the set of globally reachable nodes is aperiodic (suggestion: besides the weights, the arcs of the two graphs differ possibly for the presence of the loops that guarantee aperiodicity).

Positive entries of w

Clearly $w^T L = 0^T$ if and only if $w^T B_{\epsilon,L} = w^T$. Notice that $D(B_{\epsilon,L}) = D(A)$ apart possibly for the loops that do not influence the globally reachable nodes. Hence the condensation digraphs of $D(A)$ and $D(B_{\epsilon,L})$ coincide and have an unique sink associated with the same equivalence class of nodes. By virtue of what we proved in the theorem about achievement of consensus of systems $x(k) = Ax(k-1)$ the components of w associated to the nodes of this class are positive while the remaining are equal to zero (of course if A is irreducible then $w > 0$).

Example: opinions dynamic

Let us consider again the application to opinions dynamic. The theorem tells us that if one of the actors is globally reachable, hence it can influence, even if indirectly, all the other actors, then consensus is reached. Moreover the effective value of the consensus is a convex combination of the initial opinions only of the actors corresponding to globally reachable nodes.

Z matrices and Metzler, or quasipositive, matrices

- A matrix whose entries outside the main diagonal are less or equal than zero is known as Z matrix. Hence a Laplacian is a Z matrix.
- The opposite of a Z matrix is known as a Metzler o quasipositive matrix.

One of the reasons of the importance of Metzler matrices is their connection with positive systems.

Metzler matrices and positive systems

A system $\dot{x} = Ax + b$ is defined to be positive if $x(0) \geq 0$ implies $x(t) \geq 0$ for $t \geq 0$.

Theorem

The system $\dot{x} = Ax + b$ is positive if and only A is Metzler and $b \geq 0$.

Proof First of all let us assume that $\dot{x} = Ax + b$ is positive. If $x(0) = 0$ then $\dot{x}(0) = b$ and this implies $b \geq 0$. If $n > 1$ let $i \neq j$ and $A_{i,j} < 0$. Then it is easy to select an initial vector having $x_i(0) = 0$ and $x_j(0) > 0$ so that $\dot{x}_i(0) = A_{i,j}x_j(0) + b_i < 0$, so that the system cannot be positive.
Now let us assume that A is Metzler and $b \geq 0$, if for some t, $x(t) \geq 0$ and $x_i(t) = 0$ then $\dot{x}_i(t) \geq 0$ and this guarantees that the system is positive.

Example Clearly Laplacian flows, $\dot{x} = -L_A x$, and in particular Abelson model of opinions dynamic, are positive systems.

Opinions dynamic with stubborn agents

Let us modify Abelson model in such a way that some of actors, say the first m, are directly influenced by biases of external individuals that do not change their own opinion. Then for $i = 1, \ldots, m$ the model, known in this form as Taylor model, becomes

$$\dot{x}_i = \sum_{j=1}^{n} A_{i,j}(x_j - x_i) + (u_i - x_i),$$

where $u_i \geq 0$ is known as prejudice of the agent i. In matrix form we obtain the system

$$\dot{x} = -(L_A + W)x + u, \qquad W = \sum_{i=1}^{m} e_i e_i^T$$

easily recognized as positive, since $-(L + W)$ is quasipositive and $u \geq 0$.

Opinion dynamics with stubborn agents

The equilibria of the system can be obtained by solving the linear system of equations

$$(L_A + W)x = u.$$

- If A is irreducible then $L_A + W$ is non-singular. Actually if $L_A + W$ is singular and if $\gamma > 0$ is sufficiently large then $\rho(-(L + W) + \gamma I) \geq \gamma$ but this is impossible since $\rho(-(L_A + W) + \gamma I) < \max(-(L_A + W) + \gamma I)e \leq \gamma$.
- If $(L_A + W)w(k) = e_k$ then $\sum_{k=1}^{m} w(k) = e$ and $x = \sum_{k=1}^{m} u_k w(k)$.

If we prove that $w(k) \geq 0$ then we would obtain that the equilibrium, for each actor, is a convex combination of the prejudices.

Perron and Perron-Frobenius for Metzler matrices

The attribute "quasipositive" for Metzler matrices is justified by the observation that the fundamental theorems about non-negative matrices can be applied to them with some "cosmetics". Actually if A is quasipositive there exists $\alpha \geq 0$ such that $\alpha I + A \geq 0$. Notice that

$$\sigma(\alpha I + A) = \alpha + \sigma(A),$$

while the eigenvectors of the two matrices are the same. Hence if A is quasipositive

- it has a real eigenvalue λ such that $\lambda > \Re(\nu)$ for all $\nu \in \sigma(A)$, $\nu \neq \lambda$, and the left and right eigenvectors associated to λ can be selected non negative;
- if in addition A is irreducible it has a real simple eigenvalue λ such that $\lambda > \Re(\nu)$ for all $\nu \in \sigma(A)$, $\nu \neq \lambda$ and the left and right eigenvectors associated to λ can be selected positive.

A theorem on inverses of Metzler matrices

Theorem

A Metzler matrix A is such that all its eigenvalues have negative real part if and only if A is non-singular and $-A^{-1} \geq 0$. If in addition A is irreducible then $-A^{-1} > 0$.

Before the proof let us observe that since $-A^{-1} = (-A)^{-1}$ the theorem could be formulated focusing on Z matrices. A Z matrix having all the eigenvalues with positive real part is known as non singular M matrix. Hence the theorem could be restated by saying that a non-singular M matrix has non-negative inverse which becomes positive if the matrix is irreducible.

Proof

Let us assume that all the eigenvalues of A have negative real part. This clearly implies that A is nonsingular. Now, let us exploit quasipositivity as follows: let $\epsilon > 0$ and let $A_\epsilon = I + \epsilon A$. Of course if ϵ is sufficiently small then $A_\epsilon \geq 0$. In addition let $a + \imath b$, where $a < 0$ an eigenvalue of A. The corresponding eigenvalue of A_ϵ is $1 + \epsilon a + \imath\epsilon b$ and notice that

$$|1 + \epsilon a + \imath\epsilon b|^2 < 1 \Leftrightarrow \epsilon(a^2 + b^2) < -2a,$$

and since $a < 0$, if ϵ is sufficiently small $\rho(A_\epsilon) < 1$. Hence

$$(-\epsilon A)^{-1} = (I - A_\epsilon)^{-1} = \sum_{k=0}^{\infty} A_\epsilon^k \geq 0.$$

Hence $-A^{-1} \geq 0$. If in addition A is irreducible and ϵ is sufficiently small then A_ϵ is primitive having positive diagonal entries so that it has a positive power.

Proof

Let us assume that A is non-singular and that $-A^{-1} \geq 0$. Since A is quasipositive it has a real eigenvalue λ such that $\lambda > \Re(\nu)$ for every $\nu \in \sigma(A)$, $\nu \neq \lambda$ with associated eigenvector $v \geq 0$, $v \neq 0$.

$$Av = \lambda v \Rightarrow \lambda(-A^{-1} v) = -v \Rightarrow \lambda < 0.$$

Opinion dynamics with stubborn agents

Let us consider again the system $\dot{x} = -(L + W)x + u$. The matrix $-(L + W)$ is Metzler and if L is irreducible it is nonsingular and has eigenvalues with negative real part. Hence the system has the unique equilibrium $(L + W)^{-1}u = -(-(L + W))^{-1}u$. The matrix $(L + W)^{-1}$ is positive so that each element of the equilibrium is a convex combination of the entries of u. Since the eigenvalues of $-(L + W)$ have negative real parts the system converges towards the equilibrium.

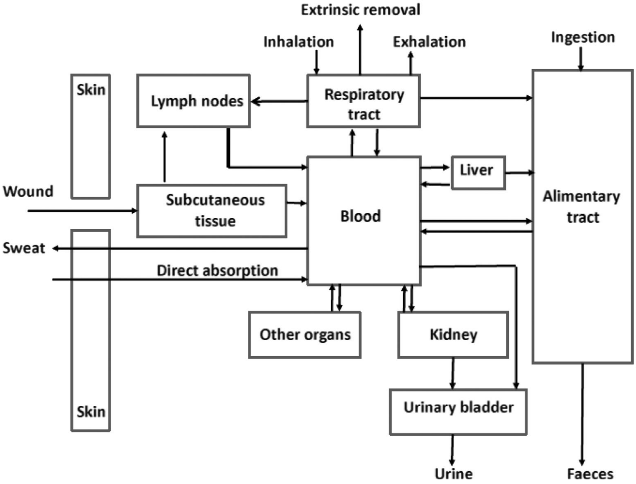
Metzler matrices and compartmental systems

Metzler matrices are important in the study of compartmental systems, that are characterized by conservation laws (e.g. mass, fluid, energy) and by the flow of material between units known as compartments, that store the material. It is natural to represent these systems by means of a digraph. The nodes represent the compartments and the arcs the flow of the material between two compartments.

Example: biokinetic models

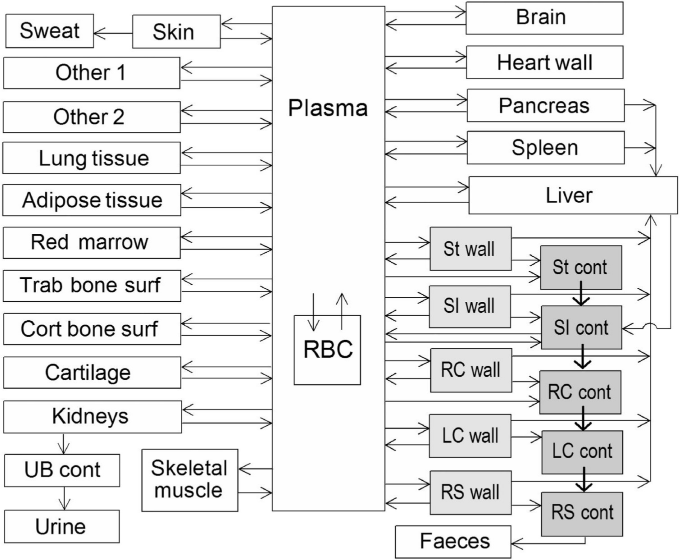
Biokinetic models are an example of compartmental models used to describe the time-dependent distribution and excretion of radioactive material that enters the human body via inhalation, ingestion or through wounds.
A typical biokinetic model is composed of a respiratory tract model, an alimentary tract model and a systemic model (for material absorbed into blood and distributed systemically to organs/tissues).
Here we show first a figure that highlights entrance and exit points in the body of radionuclides and is largely independent from the specific radioactive element. The second figure describes a systemic model specific for caesium.

Example: main routes of intake, transfer, and excretion of radionuclides in the body



Source: International Commission on Radiological Protection.

Example: systemic biokinetic model for caesium



Source: International Commission on Radiological Protection.

Example: biokinetic models

- The compartments represent whole organs or specific tissues and a biokinetic model for a single radionuclide may contain up to 70-80 compartments.
- The flows between compartments are linear in the quantity contained in the compartment. Flows are specified by transfer rates (fraction per day), to account for the absorption into blood from the entry point (e.g. the oral cavity, for ingestion), the distribution via blood to systemic organs/tissues and finally the excretion via urine and faeces.
- The physical decay of a radionuclide could be included in the model (at the price of incrementing the number of compartments).

Equations of a compartmental system

Let us denote with $q_i(t)$ the quantity of material stored in compartment i at time t. We model the variation of q_i by means of the equation

$$\dot{q}_i(t) = \sum_{j \neq i} \left(F_{j \to i} - F_{i \to j} \right) - F_{i \to O} + u_i,$$

where

- $F_{i \to j} \geq 0$ represents the mass flow from compartment i to compartment j, it is assumed that $F_{i \to j} = 0$ if $q_i = 0$;
- $F_{i \to O} \geq 0$ represents the mass flow from compartment i to the environment, it is assumed that $F_{i \to O} = 0$ if $q_i = 0$;
- $u_i \geq 0$ represents the mass flow from environment to compartment i.

Equations of a compartmental system

Notice that:

- if $q_i(t) = 0$ then $\dot{q}_i(t) = \sum_{j \neq i} F_{j \to i} + u_i \geq 0$ so that q_i does not become negative;
- $\sum_i \dot{q}_i(t) = -\sum_i F_{i \to O} + \sum_i u_i$ implying that, without inflows and outflows, the total mass is constant.

Equations of a linear compartmental system

Now, let us assume that the flows depend linearly from the stored quantities so that $F_{i\to j} = c_{i,j}q_i$, $c_{i,j} \geq 0$, and $F_{i\to O} = w_i q_i$, $w_i \geq 0$. The equations of the system become

$$\dot{q}_i = \sum_{j\neq i}\Big(c_{j,i}q_j - c_{i,j}q_i\Big) - w_i q_i + u_i.$$

Setting $C = (c_{i,j})$, $w = (w_i)$, $u = (u_i)$ we can represent the equations in compact form

$$\dot{q} = (C^T - \mathrm{diag}(Ce))q - \mathrm{diag}(w)q + u = Mq + u,$$

where $M = C^T - \mathrm{diag}(Ce + w)$ is known as compartmental matrix.

Properties of compartmental matrices

Notice that M:

- is a Metzler matrix whose diagonal entries are less or equal than zero (the i-th diagonal entry is zero only if the i-th compartment is a sink);
- $-M^T = -C + \mathrm{diag}(Ce) + \mathrm{diag}(w)$ is the sum of a Laplacian and of a non-negative diagonal matrix, so that it is diagonally dominant by rows;
- it is normally very sparse since the number of edges is generally a very small multiple of the number of compartments.

Since M is Metzler and $u \geq 0$ the system $\dot{q} = Mq + u$ is positive.

A basic property of a linear compartmental system

A compartment i is defined:

- outflow connected if $F_{i \to O} > 0$ or there exists a directed path from i to a compartment j such that $F_{j \to O} > 0$;
- inflow connected if $u_i > 0$ or there exists a directed path from a compartment j with $u_j > 0$ to i.

It is possible to prove what follows.

Theorem

If the system is outflow connected then M is continuous time convergent and every solution tends to the unique equilibrium $q^* = -M^{-1}u \geq 0$. Moreover $q^*_i > 0$ if the compartment i is inflow connected.

Conclusions

- If $A \geq 0$ then the rank of the Laplacian L_A is strictly related to the connection properties of $D(A)$.
- The Laplacian flow $\dot{x} = -L_A x$ converge toward consensus if and only if $D(A)$ contains a globally reachable node.
- By means of the fundamental theorems about non negative matrices it is possible to deduce useful spectral properties of Metzler matrices.
- A non singular Metzler matrix has non positive inverse (as well as a non singular M matrix has non negative inverse).
- The dynamical system $\dot{x} = Mx + b$ is positive if and only if M is Metzler and $b \geq 0$.
- Compartmental systems are an important class of positive systems.

Suggested readings

F. Bullo
Lectures on network systems
Create space, 2018.

G. Fedele, E. B., L. D'Alfonso
On the impact of agents with influenced opinions in the swarm social behaviour
Submitted, 2022.

Occupational Intakes of Radionuclides: Part 1.
ICRP Publication 130. Ann. ICRP 44(2), 2015

Occupational Intakes of Radionuclides: Part 2.
ICRP Publication 134. Ann. ICRP 45(3/4), 2016

Exercises

1. Let $A \geq 0$ and $A = A^T$. State and prove a theorem on the rank of L_A.
2. State and prove the theorem on positive systems in the case where $n = 1$.
3. Let $A \geq 0$ and let $G = D(A)$ contain a globally reachable node. Does this imply that $L_A + W$ is non singular?
4. Consider the system $\dot{q} = Mq + u$ where $M = \begin{pmatrix} -\gamma & 0 & 1 \\ \gamma & -2 & 0 \\ 0 & 1 & -1 \end{pmatrix}$ and $u = e_1$. Draw the graph of the compartmental system that it describes. Compute q^*. What happens if $\gamma \to 0$ and if $\gamma \to +\infty$?
5. Prove the theorem on compartmental systems with the stronger hypotheses that M is irreducible and $w_i > 0$ for some i.