# Spectra of multilayer networks - mathematical foundations, metrics, spectral properties

**Dipl.Eng. Mircho Jordanov Mirchev**

Faculty of Telecommunications, Technical University of Sofia, 8 Kl. Ohridski Blvd, 1000 Sofia +359 887 412 248, mircho@mirchev.eu

*This paper reviews a generalize approach of network models of complex systems and networks by introducing layers, thus defining multilayer networks. Having the multilayer property on the network model, it can better describe the complex system and give better results in the analysis of network science. In this paper are given the mathematical foundations and definitions of generalized multilayer networks, as well as typical classes of multilayer networks with example references. The approaches of deriving the spectra of such networks are also given. Based on the mathematical foundations and given approaches, it is possible to analyze and compare networks with different layers and from different classes.*

***Спектрални характеристики на многонивови мрежи - математическа база, метрики и спектрални свойства (Мирчо Йорданов Мирчев).*** *Настоящата разработка разглежда генерализиран модел на мрежи, като въвежда отделни слоеве в мрежовото описание на комплексните системи. Въвеждането на слоеве в мрежовите модели на комплексните системи позволява по точното им описание и анализ с инструментариума на науката за мрежи. В разработката са представени математически описания и дефиниции на слоестите мрежови модели, както и различните класове такива с примери от литературата. Показани са насоките за изчисление и анализ на спектралните характеристики на моделите. На база на посочените математически модели е възможно и сравнението на мрежови модели с различни слоеве и от различни класове.*

## Introduction

Network theory is an important tool for describing and analysing complex systems throughout the social, biological, physical, information and engineering sciences. The broad applicability of networks and their success in providing insights into the structure and function of both natural and designed systems have thus generated considerable excitement across myriad scientific disciplines. For example, networks have been used to represent interactions between proteins, friendships between people, hyperlinks between Web pages, and much more. Importantly, several features arise in a diverse variety of networks. For example, many networks constructed from empirical data exhibit heavy-tailed degree distributions, the small-world property, and/or modular structures; such structural features can have important implications for information diffusion, robustness against component failure, and many other considerations. Traditional studies of networks generally assume that nodes are connected to each other by a single type of static edge that encapsulates all connections between them. So we can initially think each network layer as a separate analysis and optimization problem. This assumption is almost always a gross oversimplification, and it can lead to misleading results and even the sheer inability to address certain problems. Most real and engineered systems usually have multiple subsystems and layers of connectivity, and the data produced by such systems are very rich.[1]–[4] To represent such systems consisting of networks with multiple types of links, or other similar features, we consider structures that have layers in addition to nodes and links. In its more general form, in a multilayer framework a node $u$ in layer $\alpha$ can be connected to any node $v$ in any layer$\beta$. In practice problems become coupled as upper layer “links” become lower layer “demands”. In technological multilayer networks (examples of which are given below) the layers are usually defined be the OSI model and upper layer “links” are implemented via lower level “paths” **[5]**. In this case also often each upper layer node is associated with one lower layer node (adaptation “links”), while the opposite is not true [6].

Examples of technological networks that can and should be considered multilayer in their analysis and optimizations are:

- IP over some L2 protocol
- IP over MPLS over some L2 protocol
- Ethernet over WDM
- Ethernet over TDM
- WAN tunnelling
- TDM over WDM
- etc.

As above examples usually follow the OSI layered model, this is not always the case. Today’s technological advances led to the concept of overlay networks, which is considered as a lower level layer network over a higher level network, e.g. L2 (Ethernet) transport over IP (VXLAN/EVPN).

In the terms of today’s social networks and our *hyper connected* [7], [8]world, multilayer network are also broadly covered. In example one person can know others (i.e. is connected) via several social networks - Facebook, LinkedIn, etc. In essence this is also considered as a multilayer network, where nodes are people, links are social connections and layers are the different means of social networks. Usually in the case of social multilayer networks there is strict one-to-one mapping of nodes between layers and such networks are a subset of multilayer networks called *multiplex networks*[3], [9], [10].

In the case of transportation networks, different means of transportation, or different airlines or operators also create multilayer networks. Such networks can be multiplex (in the air transportation, e.g.), but this is not always the case. In land and sea transportation networks, there is middle (inter-layer) network that defines the relation between nodes in the different layers [11]–[13].

Most recently, there have been increasingly intense efforts to investigate networks with multiple types of connections and so-called “network of networks[3], [4], [14]”. Such systems were examined decades ago in disciplines like sociology and engineering, but the explosive attempt to develop frameworks to study multilayer complex systems and to generalize a large body of familiar tools from network science is a recent phenomenon.

So studying the properties of multilayer networks as such, and not simply studying them layer by layer, is the key to successful understanding of the structure, dynamics and behaviour to the real life complex systems represented by networks.

## Types of multilayer networks

In this article we start by presenting the most general notion of a multilayer-network structure and by defining various constraints for that structure. We then show how this structure can be represented as an adjacency tensor and how the rank of such a tensor can be reduced (i.e. order) by constraining the space of possible multilayer networks or by ‘flattening’ the tensor. Taken to its extreme, such flattening process yields “supra-adjacency matrices” (i.e. “super-adjacency matrices”), which have the advantage over tensors of being able to represent missing nodes in a convenient way - when implementing methods of computation, especially on eigenvalues and eigenvectors, there are much more tools and mechanisms for working with matrices than with tensors[15], [16].

Multilayer networks generally inherit the properties of graphs, but also introduce new properties. The new properties are related to the additional term of layers and the relationship between them. The properties of various multilayer-network structures from the literature, represented using the general multilayer-network structure, are shown in Table 1

Some the properties that differentiate the types of multilayer networks are:

- Aligned - Is the network node aligned?
- Disjoint - Is the network layer-disjoint?
- Equivalent Size - Do all of the layers have the same number of nodes?
- Diagonal - Are the couplings diagonal?
- Layer couplings - Do the inter-layer couplings consist of layer couplings?
- Categorical - Are the inter-layer couplings categorical?
- Additionally each network has a number of possible layers “L|, and also different number of “aspects” (*d*).

Also some network structures can be represented in multiple different ways using the multilayer-network framework. For example, a network structure that consists of a sequence of graphs that share the same set of nodes can be represented using either categorical or ordinal couplings - this is usually dependant on the goal of the analysis.

*Table 1 - Various types of multilayer networks with different properties and references in the literature*

| **Name** | **Algn** | **Disj** | **Eq.size** | **Diag.** | **Lcoup.** | **Cat** | **\|L\|** | **d** | **Example refs.** |
|---|---|---|---|---|---|---|---|---|---|
| Multilayer network | | | | ✓ | ✓ | ✓ | Any | 1 | [13][1] |
| Multiplex network | ✓ | | ✓ | ✓ | ✓ | ✓ | Any or 2 | 1 | [17][18][19][20][10][21][22][23][24] |
| Multivariate network | ✓ | | ✓ | ✓ | ✓ | ✓ | Any | 1 | [25] |
| Multinetwork | ✓ | | ✓ | ✓ | ✓ | ✓ | Any | 2 | [26][27] |
| Multirelational network | ✓ | | ✓ | ✓ | ✓ | ✓ | Any | 1 | [11][28][29][30] |
| Multislice network | ✓ | | ✓ | ✓ | | | Any | 1 | [31][32][33][34] |
| Multiplex of independent networks | ✓ | | ✓ | ✓ | ✓ | ✓ | Any | 1 | [35] |
| Hypernetwork | ✓ | | ✓ | ✓ | ✓ | ✓ | Any | 1 | [36][37] |
| Overlay network | ✓ | | ✓ | ✓ | ✓ | ✓ | 2 | 1 | [38][39] |
| Composite network | ✓ | | ✓ | ✓ | ✓ | ✓ | 2 | 1 | [40] |
| Multilevel network | | ✓ | | | | | Any | 1 | [41][42] |
| Multiweighted graph | ✓ | | ✓ | ✓ | ✓ | ✓ | Any | 1 | [43] |
| Heterogeneous network | | ✓ | | | | | 2 | 1 | [44][28] |
| Multitype network | | ✓ | | | | | Any | 1 | [45][46][47] |
| Interconnected networks | | ✓ | ✓ | | | | 2 | 1 | [48][49] |
| Interdependent networks | | ✓ | ✓ | | | | 2 | 1 | [50][51][52][53][54][55][56] |
| Network of networks | | | ✓ | | | | Any | 1 | [14] |
| Coupled networks | | | | ✓ | ✓ | ✓ | Any | 1 | [57] |
| Interconnecting networks | | | | ✓ | ✓ | ✓ | 2 | 1 | [58] |
| Interacting networks | | ✓ | | | | | Any or 2 | | [59][60] |
| Heterogeneous information network | | ✓ | | | | | Any | 2 | [61] [61], [62] [63][64] |
| Meta-matrix, meta-network | | | | | | | Any | 2 | [65][66][67] |

**Mathematical representation**

The issues posed by the multiscale modelling of both natural and artificial complex systems call for a generalization of the "traditional" network theory, by developing a solid foundation and the consequent new associated tools to study multilayer and multicomponent systems in a comprehensive fashion.

A lot of work has been done during the last years to understand the structure and dynamics of these kind of systems. Related notions, such as networks of networks, multidimensional networks, multilevel networks, multiplex networks, interacting networks, interdependent networks, and many others have been introduced, and even different mathematical approaches, based on tensor representation or otherwise, have been proposed [1], [9]. The purpose of this section is to survey and discuss a general framework for multilayer networks and review some attempts to extend the notions and models from single layer to multilayer networks. As we will see, this framework includes the great majority of the different approaches addressed so far in the literature.

***General form***

A multilayer network is the pair $\mathcal{M} = (\mathcal{G}, \mathcal{C})$, where $\mathcal{G} = \{G_\alpha;\ \alpha \in \{1, \dots, M\}\}$ is a family of (directed or undirected, weighted or unweighted) graphs $G_\alpha = (N_\alpha, E_\alpha)$, called layers of $\mathcal{M}$, and

$$\mathcal{C} = \{E_{\alpha\beta} \subseteq X_\alpha \times X_\beta;\ \alpha, \beta \in \{1, \dots M\}, \alpha \neq \beta\} \quad (1)$$

is the set of interconnection between nodes in different layers $G_\alpha$ and $G_\beta$ with $\alpha \neq \beta$. The elements of $\mathcal{C}$ are called *crossed layers,* and the elements of each $E_\alpha$ are called *intralayer* connections of $\mathcal{M}$ in contrast with the elements of each $E_{\alpha\beta}$ $(\alpha \neq \beta)$ that are called *interlayer* connections.

The set of nodes of the layer $G_\alpha$ is denoted by $N_\alpha = \{n_1^\alpha, \cdots, n_{N_\alpha}^\alpha\}$ and the adjacency matrix of each layer $G_\alpha$ is denoted by $A^{[\alpha]} = (a_{ij}^\alpha) \in \mathbb{R}^{N_\alpha \times N_\alpha}$, where

$$a_{ij}^\alpha = \begin{cases} 1, & if\ (n_i^\alpha, n_j^\alpha) \in E_\alpha, \\ 0, & otherwise \end{cases} \quad (2)$$

for $1 \le i, j \le N_\alpha$ and $1 \le \alpha \le M$. The *interlayer adjacency matrix* corresponding to $E_{\alpha\beta}$ is the matrix $A^{[\alpha,\beta]} = (a_{ij}^{\alpha\beta}) \in \mathbb{R}^{N_\alpha \times N_\beta}$ given by:

$$a_{ij}^{\alpha\beta} = \begin{cases} 1, & if\ (n_i^\alpha, n_j^\beta) \in E_{\alpha\beta}, \\ 0, & otherwise. \end{cases} \quad (3)$$

The projection network of $\mathcal{M}$ is the graph $proj(\mathcal{M}) = (N_\mathcal{M}, E_\mathcal{M})$, where:

$$X_\mathcal{M} = \bigcup_{\alpha=1}^{M} X_\alpha, \quad (4)$$

$$E_\mathcal{M} = \left(\bigcup_{\alpha=1}^{M} E_\alpha\right) \bigcup \left(\bigcup_{\substack{\alpha,\beta=1 \\ \alpha\neq\beta}}^{M} E_{\alpha\beta}\right).$$

The adjacency matrix of $proj(\mathcal{M}) = (N_\mathcal{M}, E_\mathcal{M})$, is denoted as $\overline{A_\mathcal{M}}$.

***Tensor representation***

There have been some attempts in the literature for modelling multilayer networks properly by using the concept of tensors.[9] There are two main ways to think about tensors:

- tensors as multilinear maps;
- tensors as elements of a tensor product of two or more vector spaces.

The former is more applied. The latter is more abstract but more powerful. The tensor product of two real vector spaces $\mathcal{V}$ and $\mathcal{L}$, denoted by $\mathcal{V} \otimes \mathcal{L}$ (i.e., the Kronecker product), consists of finite linear combinations of $v \otimes w$, where $v \in \mathcal{V}$ and $w \in \mathcal{L}$.

The dual vector space of a real vector space $\mathcal{V}$ is the vector space of linear functions $f: \mathcal{V} \longrightarrow \mathbb{R}$, indicated by $\mathcal{V}^*$. Denoting by $Hom(\mathcal{V}^*, \mathcal{L})$ the set of linear functions from $\mathcal{V}^*$ to $\mathcal{L}$, there is a natural isomorphism between the linear spaces $\mathcal{V} \otimes \mathcal{L}$ and $Hom(\mathcal{V}^*, \mathcal{L})$. Moreover, if $\mathcal{V}$ is a finite dimensional vector space, then there exists a natural isomorphism (depending on the bases considered) between the linear spaces $\mathcal{V}$ and $\mathcal{V}^*$. In fact, if $\mathcal{V}$ is finite-dimensional, the relationship between $\mathcal{V}$ and $\mathcal{V}^*$ reflects in an abstract wat the relation between $(1 \times N)$ row-vectors and the $(N \times 1)$ column-vectors of a $(N \times N)$ matrix. However, if $\mathcal{V}$ and $\mathcal{L}$ are finite-dimensional, them the linear spaces $\mathcal{V} \otimes \mathcal{L}$ and $Hom(\mathcal{V}, \mathcal{L})$ can be identified. Thus a tensor $\sigma \in \mathcal{V} \otimes \mathcal{L}$ can be understood as a linear function $\sigma: \mathcal{V} \longrightarrow \mathcal{L}$, and therefore, once the two bases of the corresponding vector spaces are fixed, a tensor may be identified with a specific matrix.

Multilayer networks, multidimensional networks, hypergraphs, and some other objects can be represented with tensors, which represent a convenient formalism to implement different models. Specifically, tensor-decomposition methods and multiway data analysis have been used to study various types of networks. These kind of methods are based on representing multilayer networks as adjacency higher-order tensors and then applying generalizations of methods such as Singular Value Decomposition (SVD), and the combination of CANDECOMP (canonical decomposition) and PARAFAC (parallel factors) leading to CANDECOMP/PARAFAC (CP). These methods are used to extract communities, to rank nodes and to perform data mining [1], [68].

### *Supra-adjacency representation*

The adjacency-matrix representation for monoplex (single-layer) networks is powerful because of the numerous tools, methods and theoretical results that have been developed for matrices can be exploited. To get access to these tools for investigations of multilayer networks, such networks can be represented using supra-adjacency matrices. An additional advantage of supra-adjacency matrices over adjacency tensors is that they provide a natural way to represent multilayer networks that are not node-aligned without having to append empty nodes. However, this boon comes with a cost: flattening a multilayer network to obtain a supra-adjacency matrix loses some of the information about the aspects. Partitioning a network's edge set into intra- layer edges, inter-layer edges and coupling edges makes it possible to retain some of this information.

If the multilayer network is a multiplex network (i.e. there each node participates in all layers), it can be represented as network $\mathcal{M}$ made of $M$ layers $\{G_\alpha; 1 \leq \alpha \leq M\}, G_\alpha = (N_\alpha, E_\alpha)$ , with $N_1 = \cdots = N_M = \{n_1, \dots, n_N\} = N$ and described as a tensor product:

$$\mathcal{M} = \langle N \rangle \otimes \langle \{\ell_1, \dots, \ell_M\} \rangle, \quad (5)$$

where $\ell_i$ represents the layer $G_i$.

Then according to [xx], a multilayer network $\mathcal{M}$ of $N$ nodes and with layers $\{\ell_1, \dots, \ell_M\}$ can be identified with a linear transformation $\sigma: \mathcal{V} \otimes \mathcal{L} \longrightarrow \mathcal{L} \otimes \mathcal{V}$ and therefore $\mathcal{M}$ is completely determined by the matrix associated with $\sigma$ on the basis

$$n_i \otimes \ell_\alpha; 1 \leq i \leq N, 1 \leq \alpha \leq M \quad (6)$$

Also if A and B are two different matrices assigned to the same tensor, there exists a permutation matrix $P$ such that $B = P \cdot A \cdot P^{-1}$, and thus both matrices have the same spectral properties.

So for any tensor of a multilayer network we can get an adjacency matrix, called *supra-adjacency matrix* of $\mathcal{M}$, which can be written in the usual form

$$\mathcal{A} = \begin{pmatrix} A_1 & \cdots & I_N \\ \vdots & \ddots & \vdots \\ I_N & \cdots & A_M \end{pmatrix} \quad (7)$$

Note that, unlike the case of multiplex networks, the blocks in the supra-adjacency matrix of a general multilayer networks are not necessarily square matrices.

Now a supra-Laplacian matrix can be derived from a supra-adjacency matrix in a manner that is analogous to the way that one derives a Laplacian matrix from the adjacency matrix of a monoplex graph. For example, the combinatorial supra-Laplacian matrix is $\mathcal{L}_\mathcal{M} = D_\mathcal{M} - \mathcal{A}_\mathcal{M}$, where $D_\mathcal{M}$ is the diagonal supra-matrix that has node-layer strengths (i.e. weighted degrees) along the diagonal and $\mathcal{A}_\mathcal{M}$ denotes the supra-adjacency matrix that corresponds to the graph $G_\mathcal{M}$. Hence, each diagonal entry of the supra-Laplacian $\mathcal{L}_\mathcal{M}$ consists of the sum of the corresponding row in the supra-adjacency matrix $\mathcal{A}_\mathcal{M}$ , and each non-diagonal element of $\mathcal{L}_\mathcal{M}$ consists of the corresponding element of $\mathcal{A}_\mathcal{M}$ multiplied by $-1$. The eigenvalues and eigenvectors of this supra-Laplacian are important indicators of several structural features of the corresponding network, and they also give crucial insights into dynamical processes that evolve on top of it [69], [70]. The second smallest eigenvalue and the eigenvector associated to it, which are sometimes called (respectively) the "algebraic connectivity" and "Fiedler vector" of the corresponding network, are very important diagnostics for the structure of a network [71], [72].

## Spectra of multilayer networks

### *Supra-Laplacian matrix*

Generally, the Laplacian matrix of a graph with adjacency matrix A, or simply the Laplacian, is given by:

$$L = D - A \quad (8)$$

where $D = diag(k_1, k_2 \cdots)$ is the degree (or identity) matrix.

Thus, it is natural to define the *supra-Laplacian* matrix of a Multiplex network as the Laplacian of its supra-graph:

$$\mathcal{L} = \mathcal{D} - \mathcal{A} \quad (9)$$

where $\mathcal{D} = diag(K_1, K_2, \dots)$ is the degree matrix. Besides the Laplacian for each layer graph $G_\alpha$ can be defined as

$$L^\alpha = D^\alpha - A^\alpha \quad (10)$$

and the Laplacian of the coupling graph:

$$\boldsymbol{\mathcal{L}_C = \Delta - \mathcal{C}} \quad (11)$$

where $\boldsymbol{\Delta = diag(c_1, c_2, \dots, c_N)}$ is the coupling-degree matrix.

By definition:

$$\boldsymbol{\mathcal{L}} = \underbrace{\bigoplus}_{\alpha} \boldsymbol{\mathcal{L}^\alpha + \mathcal{L}_C} \quad (12)$$

Eq. (12) takes a very simple form in the case of a node-aligned multiples, i.e.:

$$\boldsymbol{\mathcal{L}} = \underbrace{\bigoplus}_{\alpha} . (\boldsymbol{L^\alpha + cI_N}) - \boldsymbol{K_m \otimes I_n} \quad (13)$$

where $\boldsymbol{K_m}$ is the adjacency matrix of a complete graph of *m* nodes, $\boldsymbol{I_n}$ is the $k \times k$ identity matrix and $\boldsymbol{c_i = c}, \forall \boldsymbol{i} \in \boldsymbol{N}$ is the coupling degree of a node-layer pair.

### *Individual layer spectra*

In [68] using perturbation theory, is showed that the largest eigenvalue of the multiplex network is equal to the one of the adjacency matrix of the dominant layer of the system at a first order approximation. Similarly, in [73] is studied thee eigenvalues of the Laplacian in the context of multilayer networks. They show that the eigenvalues of the quotient (a coarsening of the original network) are interlaced with the eigenvalues of its parent network. This fact has deep consequences as, for example, the relaxation time on a multiplex network is at most the one of the aggregated network, which in turn can result in faster diffusion processes on multiplex networks than in their aggregated counterparts.

### *Combined spectrum*

The eigenvalues and eigenvectors of this supra-Laplacian are important indicators of several structural features of the corresponding network, and they also give crucial insights into dynamical processes that evolve on top of it [15], [74]. The second smallest eigenvalue and the eigenvector associated to it, which are called (respectively) the “algebraic connectivity” and “Fiedler vector” of the corresponding network, are very important diagnostics for the structure of a network.

For example, the algebraic connectivity of a multilayer network with categorical couplings16has two distinct regimes [3], [15], [48]when examined as a function of the relative strengths of the inter-layer edges and the intra-layer edges. Additionally, there is a discontinuous (i.e. first-order) phase transition — a so-called “structural transition” — between the two regimes. In one regime, the algebraic connectivity is independent of the intra-layer adjacency structure, so it is determined by the inter-layer edges. In the other, the algebraic connectivity of the multilayer network is bounded above by a constant multiplied by the algebraic connectivity of the unweighted superposition of the layers. Combinatorial supra-Laplacian matrices have also been used to study a diffusion process on multiplex networks [1].

### *Eigenvalues and eigenvectors of tensors*

The Z-eigenvalue problem for tensors involves finding nontrivial solutions of in homogeneous polynomial systems in several variables. The Z-spectrum of A, denoted $\mathcal{Z}(A)$ is defined to be the set of all Z-eigenvalues of $\mathcal{A}$. It is proven in [75], that for a symmetric tensor $\mathcal{A}$, the set of $E$-eigenvalues of $\mathcal{A}$ is nonempty and finite. We therefore define the Z-spectral radius of a symmetric tensor A, denoted $\varrho(\mathcal{A})$, to be $\varrho(\mathcal{A}) := max\{|\lambda| \mid \lambda \in \mathcal{Z}(\mathcal{A})\}$.

### Conclusion and future works

Based on the mathematical representation of multilayer networks, much better multilayer models can be created and analysed. Moreover complex systems can be modelled in different aspects and also can be related to each other based not only on typical graph properties, but also based on the spectral properties. The generalized model of multilayer networks using tensors is good in the modelling complex systems, but on the other hand spectrum is very difficult to compute. The supra-Laplacian matrix is a good way of reduction the tensor to a matrix and for it to be done spectral analysis.

Future works in this field include better eigenvalue and eigenvector decomposition of tensors, so the information for the systems that is lost in flattening the tensors to supra-Laplacian and supra-adjacency matrices is preserved, while keeping the computation to bearable degrees.

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