MultilayerGraphs.jl: Multilayer Network Science in Julia

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Summary

MultilayerGraphs.jl is a Julia package for the creation, manipulation and analysis of the structure, dynamics and functions of multilayer graphs.

A multilayer graph is a graph consisting of multiple standard subgraphs called *layers* which can be interconnected through bipartite graphs called *interlayers* composed of the vertex sets of two different layers and the edges between them. The vertices in each layer represent a single set of nodes, although not all nodes have to be represented in every layer.

Formally, a multilayer graph can be defined as a triple $G = (V, E, L)$, where:

- V is the set of vertices;
- E is the set of edges, pairs of nodes (u, v) representing a connection, relationship or interaction between the nodes u and v;
- L is a set of layers, which are subsets of V and E encoding the nodes and edges within each layer.

Each layer ℓ in L is a tuple (V_ℓ, E_ℓ), where V_ℓ is a subset of V that represents the vertices within that layer, and E_ℓ is a subset of E that represents the edges within that layer.

MultilayerGraphs.jl is an integral part of the JuliaGraphs ecosystem extending Graphs.jl (Fairbanks et al., 2021) so all the methods and metrics exported by Graphs.jl work for multilayer graphs, but due to the special nature of multilayer graphs the package features a peculiar implementation that maps a standard integer-labelled vertex representation to a more user-friendly framework exporting all the objects an experienced practitioner would expect such as nodes (Node), vertices (MultilayerVertex), layers (Layer), interlayers (Interlayer), etc.

MultilayerGraphs.jl features multilayer-specific methods and metrics including the global clustering coefficient, the overlay clustering coefficient, the multilayer eigenvector centrality, the multilayer modularity and the Von Neumann entropy.

Finally, MultilayerGraphs.jl has been integrated within the JuliaDynamics ecosystem so that any Multilayer(Di)Graph can be utilised as an argument to the GraphSpace constructor in Agents.jl (Datseris et al., 2022).

Statement of Need

Several theoretical frameworks have been proposed to formally subsume all instances of multilayer graphs (Aleta & Moreno, 2019; Artime et al., 2022; Bianconi, 2018; Boccaletti et al., 2014; Cozzo et al., 2018; M. D. Domenico et al., 2013; M. D. Domenico, 2022; Kivela et al., 2014; Lee et al., 2015).

Multilayer graphs have been adopted to model the structure and dynamics of a wide spectrum of high-dimensional, non-linear, multi-scale, time-dependent complex systems including physi-

39 cal, chemical, biological, neuronal, socio-technical, epidemiological, ecological and economic
40 networks (Aleta et al., 2022, 2020; Amato et al., 2017; Arruda et al., 2017; Azimi-Tafreshi,
41 2016; Baggio et al., 2016; Buldú & Porter, 2018; Cozzo et al., 2013; M. D. Domenico, 2017;
42 M. D. Domenico et al., 2016; Estrada & Gómez-Gardeñes, 2014; Gosak et al., 2018; Granell
43 et al., 2013; Lim et al., 2019; Mangioni et al., 2020; Massaro & Bagnoli, 2014; Pilosof et al.,
44 2017; Soriano-Paños et al., 2018; Timóteo et al., 2018).

45 We have chosen the Julia language for this software package because it is a modern, open-
46 source, high-level, high-performance dynamic language for technical computing (Bezanson et
47 al., 2017). At the best of our knowledge there are currently no software packages dedicated to
48 the creation, manipulation and analysis of multilayer graphs implemented in the Julia language
49 apart from MultilayerGraphs.jl itself (Moroni & Monticone, 2022).

Main Features

51 The two main data structures are `MultilayerGraph` and `MultilayerDiGraph`: collections of
52 layers connected through interlayers.

53 The **vertices** of a multilayer graph are representations of one set of distinct objects called
54 Nodes. Each layer may represent all the node set or just a subset of it. The vertices
55 of `Multilayer(Di)Graph` are implemented via the `MultilayerVertex` custom type. Each
56 `MultilayerVertex` encodes information about the node it represents, the layer it belongs to
57 and its metadata.

58 Both the **intra-layer** and **inter-layer edges** are embedded in the `MultilayerEdge` struct, whose
59 arguments are the two connected multilayer vertices, the edge weight and its metadata. It's
60 important to highlight that `Multilayer(Di)Graphs` are weighted and able to store metadata by
61 default (i.e. they have been assigned the `IsWeighted` and `IsMeta` traits from SimpleTraits.jl).

62 The **layers** are implemented via the `Layer` struct composed of an underlying graph and a
63 mapping from its integer-labelled vertices to the collection of `MultilayerVertexs` the layer
64 represents. **Interlayers** are similarly implemented via the `Interlayer` mutable struct, and they
65 are generally constructed by providing the two connected layers, the (multilayer) edge list
66 between them and a graph. This usage of underlying graphs allows for an easier debugging
67 procedure during construction and a more intuitive analysis afterwards allowing the package to
68 leverage all the features of the JuliaGraphs ecosystem so that it can be effectively considered
69 as a real proving ground of its internal consistency.

70 The `Multilayer(Di)Graph` structs are weighted and endowed with the functionality to store
71 both vertex-level and edge-level metadata by default so that at any moment the user may
72 add or remove a `Layer` or specify an `Interlayer` and since different layers and interlayers
73 could be better represented by graphs that are weighted or unweighted and with or without
74 metadata, it was crucial for us to provide the most general and adaptable structure. A
75 `Multilayer(Di)Graph` is instantiated by providing the ordered list of layers and the list of
76 interlayers to the constructor. The latter are automatically specified, so there is no need to
77 instantiate all of them.

78 Alternatively, it is possible to construct a `Multilayer(Di)Graph` making use of a graph
79 generator-like signature allowing the user to set the degree distribution or the degree sequence
80 and employs graph realisation methods such as the Havel-Hakimi algorithm for undirected
81 graphs (Hakimi, 1962) and the Kleitman-Wang algorithm for directed ones (Kleitman & Wang,
82 1973).

83 `Multilayer(Di)Graphs` structure may be represented via dedicated `WeightTensor`,
84 `MetadataTensor` and `SupraWeightMatrix` structs, all of which support indexing with
85 `MultilayerVertexs`. Once a `Multilayer(Di)Graph` has been instantiated, its layers and
86 interlayers can be accessed as their properties.

Installation and Usage

To install MultilayerGraphs.jl it is sufficient to activate the `pkg` mode by pressing `]` in the Julia
REPL and then run the following command:

```
pkg> add MultilayerGraphs
```

In the following code chunks we synthetically illustrate how to define, handle and analyse a
`MultilayerGraph` in order to showcase some of the main features outlined in the previous
section.

```julia
using Revise
using Graphs, SimpleValueGraphs
using Distributions
using MultilayerGraphs

# The objects represented by `MultilayerVertex`s are `Node`s
const n_nodes = 100
const node_list = [Node("node_$i") for i in 1:n_nodes]

#=
Each layer and Interlayer that is involved in a `Multilayer(Di)Graph` must have the same
vertex type (i.e. the type of the internal representation of vertices) and (edge) weight
We proceed by defining them:
const vertex_type = Int64
const weight_type = Float64
=#

#=
We will instantiate layers and interlayers with randomly-selected edges and vertices ado
Here, we define a layer with an underlying simple directed graph
using a graph generator-like (or "configuration model"-like) constructor which allows
for specifying both the indegree and the outdegree sequences.

Before instantiating each layer we sample its number of vertices and, optionally, of edg
=#
n_vertices = rand(1:100)                         # Number of vertices
layer_simple_directed = layer_simpledigraph(     # Layer constructor
    :layer_simpledigraph,                        # Layer name
    sample(node_list, n_vertices; replace=false), # Nodes represented in the layer
    Truncated(Normal(5, 5), 0, 20),              # Indegree sequence sample distributio
    Truncated(Normal(5, 5), 0, 20)               # Outdegree sequence sample distributi
)

#= Next, we define a layer with an underlying simple weighted directed graph.
This time we show another kind of constructor that allows the user to specify
the number of edges to be randomly distributed among the vertices.
The keyword argument `default_edge_weight` will assign a weight to such edges before the
=#
n_vertices = rand(1:n_nodes)                             # Number of vertices
n_edges = rand(n_vertices:(n_vertices * (n_vertices - 1) - 1)) # Number of edges
layer_simple_directed_weighted = layer_simpleweighteddigraph( # Layer constructor
    :layer_simpleweighteddigraph,                       # Layer name
    sample(node_list, n_vertices; replace=false),       # Nodes represented in th
    n_edges;                                            # Number of randomly dist
    default_edge_weight=(src, dst) -> rand()            # Function assigning weig
```

```julia
)

#=
## Similar constructors, more flexible at the cost of ease of use, allows for finer tuni
## NB: This constructor should be necessary only in rare circumstances, where e.g.
the equivalent simplified constructor `layer_simplevaldigraph` is not able to infer
the correct return types of the `default_vertex/edge_metadata`s, or to use underlying
graph that aren't currently supported.
=#
n_vertices = rand(1:n_nodes)                            # Number of vertices
n_edges = rand(n_vertices:(n_vertices * (n_vertices - 1) - 1)) # Number of edges
default_vertex_metadata = v -> ("vertex_$(v)_metadata")      # Vertex metadata
default_edge_metadata = (s, d) -> (rand(),)                  # Edge metadata
layer_simple_directed_value = Layer(                        # Layer constructor
    :layer_simplevaldigraph,                                # Layer name
    sample(node_list, n_vertices; replace=false),           # Nodes represented in th
    n_edges,                                                 # Number of randomly dist
    ValDiGraph(
        SimpleDiGraph{Int64}();
        vertexval_types=(String,),
        vertexval_init=default_vertex_metadata,
        edgeval_types=(Float64,),
        edgeval_init=default_edge_metadata,
    ),
    Float64;
    default_vertex_metadata=default_vertex_metadata,        # Vertex metadata
    default_edge_metadata=default_edge_metadata             # Edge metadata
)

layers = [layer_simple_directed, layer_simple_directed_weighted, layer_simple_directed_v

#=
There are many more constructors that the user is encouraged to explore in the package d
We may now move to Interlayers. Note that, in order to define a `Multilayer(Di)Graph`,
interlayers do not need to be explicitly constructed by the user,
since they are automatically specified by the `Multilayer(Di)Graph` constructor.
Anyway, more complex interlayers need to be manually instantiated.
The interface is very similar to the layers.
=#

# Interlayer with an underlying simple directed graph and `n_edges` edges
n_vertices_1 = nv(layer_simple_directed)                # Number of vertices of layer 1
n_vertices_2 = nv(layer_simple_directed_weighted)       # Number of vertices of layer 2
n_edges = rand(1:(n_vertices_1 * n_vertices_2 - 1))     # Number of interlayer edges
interlayer_simple_directed = interlayer_simpledigraph(  # Interlayer constructor
    layer_simple_directed,                              # Layer 1
    layer_simple_directed_weighted,                     # Layer 2
    n_edges                                             # Number of edges
)

## The interlayer exports a more flexible constructor too.
n_vertices_1 = nv(layer_simple_directed_weighted)       # Number of vertices of layer
n_vertices_2 = nv(layer_simple_directed_value)          # Number of vertices of layer
n_edges = rand(1:(n_vertices_1 * n_vertices_2 - 1))     # Number of interlayer edges
interlayer_simple_directed_meta = interlayer_metadigraph( # Interlayer constructor
```

```
        layer_simple_directed_weighted,                  # Layer 1
        layer_simple_directed_value,                      # Layer 2
        n_edges;                                          # Number of edges
        default_edge_metadata=(src, dst) ->               # Edge metadata
            (edge_metadata="metadata_of_edge_from_$(src)_to_$(dst)"),
        transfer_vertex_metadata=true                     # Boolean deciding layer verte
    )

    interlayers = [interlayer_simple_directed, interlayer_simple_directed_meta]

    # Layers and Interlayers are not immutable, and mostly behave like normal graphs. The re
    # A MultilayerDiGraph (i.e. a directed multilayer graph, following the naming convention

    multilayerdigraph = MultilayerDiGraph(
        layers,                                  # The (ordered) collection of layers
        interlayers;                             # The manually specified interlayers
                                                 # The interlayers that are left unspecifi
                                                 # will be automatically inserted accordin
                                                 # to the keyword argument below
        default_interlayers_structure="multiplex"  # The automatically specified interlayers
    )

    # Layers and interlayer may be accessed as properties using their names
    multilayerdigraph.layer_simple_directed_value

    # We proceed to show some basic functionality.
    ## Add a vertex
    ### The user may add vertices that do or do not represent node_list already present in t
    new_node_1 = Node("new_node_1")
    ### Before adding any vertex representing such node to the multilayer graph, the user sh
    add_node!(multilayerdigraph, new_node_1)
    ### Define a vertex that represents that node
    new_vertex_1 = MV(              # Constructor (alias for "MultilayerVertex")
        new_node_1,                 # Node represented by the vertex
        :layer_simplevaldigraph,    # Layer containing the vertex
        ("new_metadata")            # Vertex metadata
    )
    ### Add the vertex
    add_vertex!(
        multilayerdigraph, # MultilayerDiGraph the vertex will be added to
        new_vertex_1       # MultilayerVertex to add
    )
    # NB: The vertex-level metadata are considered iff the graph underlying the layer/interl

    ### `add_vertex!` implements multiple interfaces.

    ## Add an edge
    ### Let's represent another node in another layer
    new_node_2 = Node("new_node_2")
    new_vertex_2 = MV(new_node_2, :layer_simpledigraph)
    add_vertex!(
        multilayerdigraph,
        new_vertex_2;
        add_node=true # Add the associated node before adding the vertex
    )
```

```
### Construct a new edge
new_edge = MultilayerEdge( # Constructor
    new_vertex_1,          # Source vertex
    new_vertex_2,          # Destination vertex
    ("some_edge_metadata") # Edge metadata
)
### Add the edge
add_edge!(
    multilayerdigraph, # MultilayerDiGraph the edge will be added to
    new_edge           # MultilayerVertex to add
)
# NB: The edge-level metadata and/or weight are considered iff the graph underlying the

#=
Using the provided `add_layer!`, `rem_layer!` and `specify_interlayer!`,
Layers and Interlayers may be added, removed or specified on the fly.
Since MultilayerGraphs.jl extends Graphs.jl, all metrics from the JuliaGraphs ecosystem
should be available by default. Anyway, some multilayer-specific metrics have been imple
and others required to be re-implemented.

We showcase a few of them here:
=#

## Compute the global clustering coefficient as in @DeDomenico2014
multilayer_global_clustering_coefficient(multilayerdigraph) # A weighted version `multil
## Compute the overlay clustering coefficient as in @DeDomenico2013
overlay_clustering_coefficient(multilayerdigraph)
## Compute the eigenvector centrality (the implementation is sp that it coincides with G
eigenvector_centrality(multilayerdigraph)
## Compute the multilayer modularity as in @DeDomenico2013
modularity(
    multilayerdigraph,
    rand([1, 2, 3, 4], length(nodes(multilayerdigraph)), length(multilayerdigraph.layers
)

## Currently, Von Neumann entropy is available only for undirected multilayer graphs.
# NB: this brief script is far from complete: many more features and functionalities are
```

For a more comprehensive exploration of the package features and functionalities we strongly recommend consulting the tutorial included in the package documentation.

Related Packages

R

Here is a list of software packages for the creation, manipulation, analysis and visualisation of multilayer graphs implemented in the R language:

- muxViz implements functions to perform multilayer correlation analysis, multilayer centrality analysis, multilayer community structure detection, multilayer structural reducibility, multilayer motifs analysis and utilities to statically and dynamically visualise multilayer graphs (D. Domenico et al., 2014);
- multinet implements functions to import, export, create and manipulate multilayer graphs, several state-of-the-art multiplex graph analysis algorithms for centrality measures, layer comparison, community detection and visualization (Magnani et al., 2021);

- mully implements functions to import, export, create, manipulate and merge multilayer graphs and utilities to visualise multilayer graphs in 2D and 3D (Hammoud & Kramer, 2018);
- multinets implements functions to import, export, create, manipulate multilayer graphs and utilities to visualise multilayer graphs (Lazega et al., 2008).

Python

Here is a list of software packages for the creation, manipulation, analysis and visualisation of multilayer graphs implemented in the Python language:

- MultiNetX implements methods to create undirected networks with weighted or unweighted links, to analyse the spectral properties of adjacency or Laplacian matrices and to visualise multilayer graphs and dynamical processes by coloring the nodes and links accordingly;
- PyMNet implements data structures for multilayer graphs and multiplex graphs, methods to import, export, create, manipulate multilayer graphs and for the rule-based generation and lazy-evaluation of coupling edges and utilities to visualise multilayer graphs (Kivela et al., 2014).

Acknowledgements

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