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

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

Main Features

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

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

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

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

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

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

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

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

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 some of the main features outlined in the previous section.

Let's begin by importing the necessary dependencies and setting the relevant constants.

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

# Set the number of nodes: objects represented by multilayer vertices
const n_nodes = 100
# Create a list of nodes
const node_list = [Node(”node_$i”) for i in 1:n_nodes]
```

Layers and Interlayers

We will instantiate layers and interlayers with randomly-selected edges and vertices adopting a variety of techniques. Layers and Interlayers are not immutable, and mostly behave like normal graphs. The reader is invited to consult the API for more information.

Here we define a layer with an underlying simple directed graph using a graph generator-like (or "configuration model"-like) constructor which allows us to specify both the **indegree** and the **outdegree sequences**. Before instantiating each layer we sample the number of its vertices and, optionally, of its edges.

```julia
n_vertices = rand(1:100)                          # Number of vertices
layer_simple_directed = layer_simpledigraph(      # Layer constructor
    :layer_simple_directed,                       # Layer name
    sample(node_list, n_vertices; replace=false), # Nodes represented in the layer
    Truncated(Normal(5, 5), 0, 20), # Indegree sequence distribution
    Truncated(Normal(5, 5), 0, 20)  # Outdegree sequence distribution
)
```

Then we define a layer with an underlying simple weighted directed graph. This is another kind of constructor that allows the user to specify the number of edges to be randomly distributed among vertices.

```julia
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_simple_directed_weighted,                           # Layer name
    sample(node_list, n_vertices; replace=false), # Nodes represented in the layer
    n_edges;                                 # Number of randomly distributed edges
    default_edge_weight=(src, dst) -> rand() # Function assigning weights to edges
)
```

Similar constructors, more flexible at the cost of ease of use, enable a finer tuning. The constructor we use below should be necessary only in rare circumstances, e.g. if the equivalent simplified constructor `layer_simplevaldigraph` is not able to infer the correct return types of default_vertex_metadata or default_edge_metadata, or to use and underlying graph structure that isn't currently supported.

```julia
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_simple_directed_value,                                    # Layer name
    sample(node_list, n_vertices; replace=false), # Nodes represented in the layer
    n_edges,                                      # Number of randomly distributed edges
    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
)

# Create a list of layers
layers = [layer_simple_directed, layer_simple_directed_weighted, layer_simple_directed_v
```

There are many more constructors the user is encouraged to explore in the package documentation.

The interface of interlayers is very similar to that of layers. It is very important to notice that, in order to define a `Multilayer(Di)Graph`, interlayers don't need to be explicitly constructed by the user since they are automatically identified by the `Multilayer(Di)Graph` constructor, but for more complex interlayers the manual instantiation is required.

Here we define an interlayer with an underlying simple directed graph.

```julia
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 1
n_vertices_2 = nv(layer_simple_directed_value)      # Number of vertices of layer 2
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 vertex metadata inheritance
)
```

```julia
# Create a list of interlayers
interlayers = [interlayer_simple_directed, interlayer_simple_directed_meta]
```

Multilayer Graphs

In what follows we construct a directed multilayer graph (`MultilayerDiGraph`).

```julia
multilayerdigraph = MultilayerDiGraph( # Constructor
    layers,                     # The (ordered) collection of layers
    interlayers;                # The manually specified interlayers
                                # The interlayers that are left unspecified
                                # will be automatically inserted according
                                # to the keyword argument below
    default_interlayers_structure="multiplex"
    # The automatically specified interlayers will have only diagonal couplings
)

# Layers and interlayer can be accessed as properties using their names
multilayerdigraph.layer_simplevaldigraph
```

Then we proceed by showing how to add nodes, vertices and edges to a directed multilayer graph. The user may add vertices that do or do not represent nodes which are already present in the multilayergraph. In the latter case, we have to create a node first and then add the vertex representing such node to the multilayer graph. The vertex-level metadata are effectively considered only if the graph underlying the relevant layer or interlayer supports them, otherwise they are discarded. The same holds for edge-level metadata and/or weight.

```julia
# Create a node
new_node_1 = Node("new_node_1")
# Add the node to the multilayer graph
add_node!(multilayerdigraph, new_node_1)
# Create a vertex representing the 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
)

# Create another node in another layer
new_node_2 = Node("new_node_2")
# Create another vertex representing the new node
new_vertex_2 = MV(new_node_2, :layer_simpledigraph)
# Add the new vertex
add_vertex!(
    multilayerdigraph,
    new_vertex_2;
    add_node=true # Add the associated node before adding the vertex
)
# Create an edge
new_edge = MultilayerEdge( # Constructor
```

```julia
        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
    )
```

Finally we illustrate how to compute a few multilayer metrics such as the global clustering coefficient, the overlay clustering coefficient, the multilayer eigenvector centrality, and the multilayer modularity as defined in M. D. Domenico et al. (2013).

```julia
# Compute the global clustering coefficient
multilayer_global_clustering_coefficient(multilayerdigraph)
# Compute the overlay clustering coefficient
overlay_clustering_coefficient(multilayerdigraph)
# Compute the multilayer eigenvector centrality
eigenvector_centrality(multilayerdigraph)
# Compute the multilayer modularity
modularity(
    multilayerdigraph,
    rand([1, 2, 3, 4], length(nodes(multilayerdigraph)), length(multilayerdigraph.layers
)
```

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).

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