Dynamics *in* and dynamics *of* networks using DyNSimF

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Abstract

Advancements of formal theories, network science, and data collection technologies make network analysis and simulation an increasingly crucial tool in complexity science. We present **DyNSimF**; the first open-source package that allows for the modeling of complex interacting dynamics *on* a network as well as dynamics *of* (the structure of) a network. The package can deal with weighted as well as directional connections, is scalable and efficient, and includes a utility-based edge-altering framework. **DyNSimF** includes visualization methods and tools to help analyze models. It is designed to be easily extendable and makes use of **NetworkX** graphs. It aims to be easy to learn and to work with, enabling non-experts to focus on the development of models, while at the same time being highly customizable and extensible to allow for complex custom models.

Keywords: dynamic networks, Python, software package, simulation, Agent-Based Models, ABM, social networks, Complex Agent Networks, CAN.

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1. Introduction

The field of complexity science has witnessed significant growth over the past decades, partly due to its ability to help understand the complex behavior seen in many systems in nature (CAN; Mei, Zarrabi, Lees, and Sloot 2015). It provides a way to use surrogate reasoning (Swoyer 1991) and to enable collaboration of different fields to solve complex multidisciplinary problems (Cohen and Havlin 2010; Forsman, Moll, and Linder 2014; Fortunato 2011; Fan, Meng, Ludescher, Chen, Ashkenazy, Kurths, Havlin, and Schellnhuber 2020; Arthur 2014).

Complex systems can be characterized as consisting of many interacting components, each adapting and interacting in a non-linear way. The behavior of these systems is driven by feedback loops where macroscopic patterns of the system impact the microscopic interactions which in turn lead to new macroscopic dynamics. To represent and reason about these systems it is necessary to view the system holistically, capturing the interactions between the elements and how those interactions evolve through time Phelan (2001). The field of complexity science has been synonymous with methodologies and paradigms designed to simplify and quantify these interactions. Agent-based models Gilbert (2019) and Complex Networks (Barbati, Bruno, and Genovese 2012; Sloot, Kampis, and Gulyás 2013) are two common approaches to model complexity and have been proven successful in describing the behavior and interactions across many application domains, including protein-protein interactions, social networks, financial networks, and the World Wide Web. While these techniques have helped achieve important scientific breakthroughs, the area of dynamic (or temporal) networks has only recently gained significant attention. Modeling the temporal dynamics of network structure (connectivity) is difficult due to both computational and data requirements. It is only due to advances in computing power that simulating these complex dynamic structures has become feasible. This, coupled with modern data-collection methods capable of obtaining longitudinal, dynamic network data, has led the field of dynamic networks to be rapidly developing. Currently, while there are several software packages available for the simulation of network models, there aren't any designed to deal with dynamic network structure as well.

DyNSimF is the first software package designed to simulate dynamics on a network (e.g., disease spreading, opinion spreading) by modeling 1) dynamics within the nodes, and 2) the dynamics of the network structure (e.g., temporal networks or Complex Agent Networks (Mei *et al.* 2015)). It treats each node as an individual model with multiple continuous internal states interacting with each other as well as interacting with other nodes, able to create and break connections with other nodes. **DyNSimF** is designed to provide modelers with the tools to easily implement and run their temporal network-models. The package aims to make modeling more accessible to modelers who are non-programmers by providing a platform that is easy to work with. We envisage that **DyNSimF** will help accelerate the creation and development of models in this field.

2. Methodology

This section introduces the methodology that **DyNSimF** utilizes to create a model. We show how to work with **DyNSimF** by creating a susceptible-infected-recovered (SIR) model on a network with self-quarantine dynamics, inspired by the work of Lagorio, Dickison, Vazquez, Braunstein, Macri, Migueles, Havlin, and Stanley (2011). More examples can be found in the

documentation as well as the example document on GitHub¹. We recreate a simplified version of their ‘*strategy A*’: every time step each infected node attempts to transmit the disease to a susceptible neighbor. Simultaneously, every node with an infected neighbor has a probability w to self-quarantine and disconnect herself from the infected node. After a fixed period of time infected nodes recover. Depending on the infection rate, recovery time, and especially the self-quarantine probability this can result in an endemic or epidemic state.

A **DyNSimF** model consists of a required ‘nodal model’ and an optional ‘connectivity model’. The nodal model defines how the internal variables—here called ‘states’—of the nodes change, depending on its own characteristics and its surrounding nodes. The connectivity model determines how the nodes change their connections and thus, how the network structure changes. The interaction of these models describes how the network structure reacts (or adapts) to changes in the nodes’ states and how the nodes’ states are affected by the network structure. When only the nodal model is defined, **DyNSimF** operates as a more traditional, non-dynamic, network model.

2.1. Installation

There are multiple ways to install **DyNSimF**. The easiest way is to use **pip**², which can be acquired by installing the **python** **setuptools** or, if using **conda** by running `conda install pip`. Then by running `pip install dynsimf` the package can be installed. The library can also be installed by downloading it from GitHub¹. After it has been unpacked to the desired directory, the package can be installed by running `python setup.py install`.

2.2. Setup

To set up a model we need to import the necessary dependencies. Every model that is created using **DyNSimF** uses a **NetworkX** (Hagberg, Swart, and S Chult 2008) graph. Each nodes’ states and relations are tracked using this graph object. With **Numpy** (Harris, Millman, van der Walt, Gommers, Virtanen, Cournapeau, Wieser, Taylor, Berg, Smith, Kern, Picus, Hoyer, van Kerkwijk, Brett, Haldane, del R’io, Wiebe, Peterson, G’erard-Marchant, Sheppard, Reddy, Weckesser, Abbasi, Gohlke, and Oliphant 2020) imported, **DyNSimF** can implement its array operation routines, increasing speed when working with big networks. Finally, to set up a **DyNSimF** model, it is required to import the `Model` class. When modeling a static network, `dynsimf.models.Model` can be used. For dynamic networks one should use `UtilityCostModel`, explained in Section 2.4.

```
import numpy as np
import networkx as nx
from dynsimf.models.Model import Model
```

Next, we define the initial graph. This should be a **NetworkX** `Graph` object. **DyNSimF** can work with undirected and directed, weighted and unweighted edges, and with both graphs as well as multigraphs. The graph can be defined manually or be created with **NetworkX** graph generators. An example would be: `g = nx.erdos_renyi_graph(n=1000, p=0.1)`, which would store an Erdős-Rényi graph (Erdős and Rényi 1960) (i.e., a binomial graph with 1000

¹<https://github.com/Tensaiz/DyNSimF>

²<https://pypi.org/project/dynsimf/>

nodes and a 0.1 probability for edge creation). The example below creates a graph with small-world properties by using `watts_strogatz_graph`.

Once the network has been defined, the `Model` class object can be defined. This model requires the previously defined **NetworkX** graph and takes this as an argument to its constructor. When constructing the model it also possible to specify a random `seed`, as well a configuration object which defines the data to keep track of for use in analysis, discussed in Section 3.1.

```
g = nx.watts_strogatz_graph(n = 25, k = 5, p = 0.2)
model = Model(g)
```

2.3. Nodal model

The nodal model defines the behavior of each node. It describes how the internal variables—here called ‘states’—of the nodes change over time, depending on its past states and its local network. As each node can have its own internal dynamics, each node can be seen as a model by itself, similar to the agents of an agent-based model. Depending on the nodal model’s states discussed in this section, the nodes can change their connections as discussed in Section 2.4.

Initialization

To create an nodal model we define the constants and the states it uses and set their initial values. **DyNSimF** implements the constants as a dictionary. This dictionary is the input to the `model.constants` object. The constants can be of any type, and they can be either a single value, where each node has this same constant, or, when each node has a different constant, they can be a list of the same size as the number of nodes.

To tell the package which state variable names are used in the model, the `model.set_states()` function should be used. It takes a list of strings with the states’ names as input. Their initial values can then be set using `model.set_initial_state()`. The first argument of this function is a dictionary, with as keys the state variable names and as value a list of their initial value for each node. As with constants, the initial value for the states can be a single communal value or a list with an individual value for each node. The argument can also be a function which returns this list. If it is a function, there is another argument: a dictionary that specifies the arguments passed to this user-defined function. This can be seen in the example code below.

```
constants = {
    'n': n,
    'initial_infected': 2,
    'beta' : 0.2,
    'recovery_time': 5
}

def initial_phase(constants):
    # Initialize everyone as Susceptible, value 0
    phase = np.zeros(constants['n'])
```

```

# Give the initial Infected I value 1
phase[np.random.choice(
    len(phase), constants['initial_infected'])] = 1
return phase

model.constants = constants
model.set_states(['phase', 'toi'])
model.set_initial_state(
    {'phase': initial_phase},
    {'constants': model.constants}
)
# time of infection
model.set_initial_state(
    {'toi': np.zeros(n)})

```

In this example, we use ‘phase’ to indicate in which phase of Susceptible: 0, Infected: 1 and Recovered: 2 each node is. Further, there is a state called ‘toi’ (time of infection), keeping track of how many time steps a node is infected. This is 0 for each node but will increase every time step for an infected node.

Update functions

The way the nodes’ internal states are changed during the course of the simulation is defined by *update* functions. These functions calculate the value of all nodes’ states of the current timestep by using information from the previous time-step. This means that by default **DyNSimF** uses Euler’s method to solve differential-equation-based models. This can have implications on accuracy depending on chosen timestep and time-sensitivity of the system. If any other solver needs to be used, one can utilize the `get_previous_nodes_states()` discussed in Section 4.1 to implement their own. This quarantine model has a simple forward-time scheme, but more intricate examples based on differential equations with multiple states interacting with each other can be found in the supplementary materials.

The user-defined update functions should return a dictionary where the keys refer to the state, and the values are lists, ordered by node id, indicating the new values for that state per node. This means it is possible for one function to update all of the states of all nodes at once, or to have multiple functions updating different states. The update functions can be added to the model using the `model.add_update()`. Again, the first argument of this function is the update function created by the user. The second argument is a dictionary that contains key/value pairs of the argument to be passed to the function. Should this update function only apply to a selection of nodes, a third argument, a boolean called `get_nodes`, can be set. Then only the list of nodes passed as an argument will be updated using that function.

When the update function is created and is added to the model, a simulation with a static network can already be performed. This can be done with `model.simulate(N)`, where N is the number of iterations the model should be ran for.

```
def update_states(constants):
```

```

SIR = model.get_state('phase')
infected_time = model.get_state('toi')
I = np.where(SIR == 1)[0]

# Infected nodes have beta chance to infect neighbors
for infected_node in I:
    nbs = model.get_neighbors(infected_node)
    for nb in nbs:
        if np.random.rand(1) < constants['beta']:
            SIR[nb] = 1

# Heal after certain time
infected_time[infected_node] += 1
if infected_time[infected_node] > constants['recovery_time']:
    SIR[infected_node] = 2

return {'state': SIR, 'toi': infected_time}

model.add_update(update_states, {'constants': constants})

model.simulate(50)

```

2.4. Connectivity model

DyNSimF provides methods designed to model dynamic networks: nodes can be removed or added, and their connections—also called ‘ties’, or ‘edges’—changed. This can be done in two ways: by manually changing the **NetworkX** graph, or by defining a *utility-cost* function and letting **DyNSimF** handle changes in the network structure. Changing the network manually is explained in Section 4.4. Here we explain the *utility-cost* methodology, which is another generic way to define how nodes change their edges.

Utility-Cost

The *utility-cost* methodology is based on the idea that agents behave strategically: agents make rational decisions based on the estimated costs of an action against its potential benefits, or utility (Myerson 2013). In network-formation, this means that agents assess the utility and cost of their current and possible future connections, and adjust their edges accordingly (Mele 2013). While the ‘utility’ nomenclature is based on behavioral economics, social science approaches are similar, such as the work of Snijders, van de Bunt, and Steglich (2010). They describe in-depth the different ‘effects’ that can impact the attractiveness for individuals to connect to each other. These effects depend both on the involved agents’ internal states as well as on their position in the network and their local topology.

In **DyNSimF**, every node in the network can be seen as an agent that aims to maximize its total utility: the sum of the utility from its connections. Each node can gain a certain utility by forming new connections, but, maintaining or creating these connections could come with a certain ‘cost’. In social networks, this cost can represent the amount of effort or time that an individual spends making and maintaining friendships. Each node is limited

in this resource; it is limited in its ability to make and maintain connections. Thus the sum of the cost associated with all the node's connections may not exceed a certain level. When passing this threshold, nodes are forced to remove connections, presumably those with a high cost and low utility. Lastly, the information available to the agents when choosing their new connections has a high impact on the network dynamics, and this needs to be specified within **DyNSimF** to finalize the connectivity model.

In **DyNSimF**, by default, updates are calculated each timestep for each node and state. Following the node updates, the network re-configures its connections. To implement the utility-cost methodology in **DyNSimF**, a utility and cost function should be defined by the user. In addition, the information available to agents when assessing possible future connections should be specified.

There are two options available for the definition of the utility and cost functions. These functions can either return a value for two given nodes, or they can return a complete matrix, enabling **Numpy** routines. To tell **DyNSimF** which function is being used, the **FunctionType** enumeration class is used, being either **FunctionType.MATRIX** or **FunctionType.PAIRWISE**. In the case of a pairwise function, the utility or cost function should take 2 arguments, one for node i and the other for agent j . When **MATRIX** is chosen, the utility or cost functions should return a matrix with dimension $n \times n$, where n is the number of nodes in the network. Each entry M_{ij} then represents either the utility that agent i will gain by forming a connection with agent j , or the cost associated with each connection.

The information available to each agent can be defined by setting the argument of the `set_sampling_function()`. By passing **SampleMethod.ALL**, one assumes *complete information*: each node can be eligible to be connected with any other. Alternatively, **SampleMethod.NEIGHBORS_OF_NEIGHBORS** limits a node to only be able to connect with nodes up to a distance of two—'neighbors of neighbors'. Finally, a user-defined sampling function can be chosen using **SampleMethod.CUSTOM**. This user-defined function should be provided to the `set_sampling_function()` as the second argument, returning an $n \times n$ binary matrix g , with entry $g_{ij} = 1$ if agent j is an eligible connection for agent i . To add dynamic network-formation to a model using utility and cost functions, instead of using the previously shown **Model** class, the extended class **UtilityCostModel** should be used instead, with an added argument—`cost_threshold` indicating the threshold for the maximum sum of the cost associated with each nodes' connections.

In the example below, we have added a **MemoryConfiguration** object. This indicates that the adjacencies (an $n \times n$ matrix indicating which nodes are connected) should be stored in memory, which is required for visualization of the dynamic network. More information about this configuration is given in Section 3.1.

The cost threshold in this example represents 1 minus the rewiring probability w of [Lagorio et al. \(2011\)](#). The `cost_calculation` makes it such that a susceptible node removes an edge that connects with an infected neighboring node when a drawn random number is higher than this cost threshold. For simplicity, in this example, we only allow the model to break connections; we give the nodes a custom sampling function returning a matrix of zeros such that no node is eligible to create a connection with. With no eligible connections, it is not needed to calculate which node would have the highest utility, and thus the specific function we give for utility, in this case, does not matter. Lastly, we add these functions to the model, using **FunctionType.MATRIX**, as we return full matrices for cost and utility. After storing the

result of `simulate` we can start to analyze our results.

```

from dynsimf.models.UtilityCostModel import UtilityCostModel
from dynsimf.models.UtilityCostModel import FunctionType
from dynsimf.models.UtilityCostModel import SampleMethod

cfg = {
    'adjacency_memory_config': \
        MemoryConfiguration(MemoryConfigurationType.ADJACENCY, {
            'memory_size': 0
        }),
}

cost_threshold = 0.45
model = UtilityCostModel(g, cost_threshold, \
    config = ModelConfiguration(cfg))

def cost_calculation():
    # Define variables
    SIR = model.get_state('phase')
    I = np.where(SIR==1, 1, 0)
    S = np.where(SIR == 0, 1, 0)

    # Probabilities to disconnect
    p_disconnect = np.random.rand(constants['n'], constants['n'])

    # Only disconnect with infected
    cost = p_disconnect*I

    # Only susceptibles disconnect
    cost = S*cost.T

    return cost

def utility_calculation():
    # No new connections -> placeholder utility
    utility = np.ones((constants['n'], constants['n']))
    return utility

def sampling_method():
    # No new connections, no nodes eligible
    return np.zeros((constants['n'], constants['n']))

model.add_utility_function(utility_calculation, FunctionType.MATRIX)
model.add_cost_function(cost_calculation, FunctionType.MATRIX)
model.set_sampling_function(SampleMethod.CUSTOM, sampling_method)

```



```
output = model.simulate(50)
```

3. Analysis

3.1. Memory Configuration

By default, the output of the `simulate` function returns the data that can be used for analyses. It is a dictionary that can contain four metrics: the states, adjacencies, edge values and utilities³. Its structure is shown in Figure 1. By default, **DyNSimF** only stores the states of each node for every simulation step. However, using the `ModelConfiguration` object, the user can specify which variables **DyNSimF** should keep track of, and how.

Figure 1: A representation of the data structure of the output of the `simulate()` function. Each square is a dictionary, starting with `output`, which has four keys as shown above. Each of those keys (e.g. `'states'`) points to a value which is another dictionary. The keys of this dictionary are the iteration number, and they refer to the matrix of that metric of that iteration. The order of the columns in the `'states'` array matches the order of the states set using the `set_states()` function.

The `ModelConfiguration` object is passed when initiating the `model` object. There are four types of characteristics that the user can configure to be saved into memory during the simulation. They are specified using keys: `state_memory_config` for states, `adjacency_memory_config` for adjacencies, `edge_values_memory_config` for edge values, and `utility_memory_config` for utility.

The value tied to these keys should be an object from the `MemoryConfiguration` class. This class requires two arguments, one indicating which type the configuration is for, which is either `ADJACENCY`, `UTILITY`, `EDGE_VALUES` or `STATE`. The second argument is another dictionary incorporating the actual configuration for that type. These settings are the keys:

³Note that the `'edge values'` are only relevant if using weighted connections and `'utility'` only when using the utility-cost method.

`save_disk`, `memory_size`, `save_interval`, and `memory_interval`. The ‘save disk’ option is a boolean value that allows the user to have its output metric saved to a file on disk during the simulation. This is a `.txt` file with the name of the type, e.g. `STATE.txt`, and is saved in the `./output/` folder. The ‘memory size’ can be used to set the max amount of iterations the values should be stored into the output of the `simulation` function, where `-1` indicates it should not be saved at all. The save and memory interval values determine how many iterations should be between storing.

The example code below creates a model where at each iteration of the simulation the states of the nodes are stored: every iteration they are stored on hard drive, while every 10 iterations they get stored into memory.

```
from dynsimf.models.Model import Model
from dynsimf.models.Model import ModelConfiguration
from dynsimf.models.components.Memory import MemoryConfiguration
from dynsimf.models.components.Memory import MemoryConfigurationType

cfg = {
    'state_memory_config': \
        MemoryConfiguration(MemoryConfigurationType.STATE, {
            'memory_size': 1,
            'save_disk': True,
            'save_interval': 1,
            'memory_interval': 10
        }),
}

model = UtilityCostModel(g, ModelConfiguration(cfg))
```

3.2. Property functions

DyNSimF can keep track of custom, user-defined properties of the model during simulations by using ‘property functions’. This way, different algorithms can be implemented to keep track of network coefficients, network scale metrics, or any other measures. Initializing a property function requires four inputs: its name, the user-defined function to execute, the arguments of that function, and an iteration interval. During the simulation, these property functions will be executed according to their iteration intervals, and their output will be stored as values in a dictionary with each ‘property name’ as key. After running the simulation, this dictionary can be obtained by using `model.get_properties()`. After importing the class, an object can be created by making an instance and adding that instance to the model as follows:

```
from dynsimf.models.components.PropertyFunction import PropertyFunction

prop_1 = PropertyFunction(
    'property name',
    custom_function,
    iteration_interval,
    {'param_1': argument}).
```

```
model.add_property_function(prop_1)
```

3.3. Visualization

DyNSimF provides methods for dynamic visualization of the network and the states of nodes during a simulation. An example of one frame of the quarantine model is given in Figure 2. The network is shown with the nodes colored according to a user-selected state. Underneath the network, bar plots of (a selection of) the states are shown. This animated visualization is rendered as a **Matplotlib** window and can be stored as an animated GIF file.

Figure 2: One frame produced by the visualization tool. It shows the title, current iteration, the network, and bar plots of the model states. To the right of the network, a color bar showing the colorscale of the nodes is displayed. The colors of the nodes represent a specific state of the model, which in this case is the ‘phase’.

The visualization methods offer many configuration options. Here we highlight a few of the most important. These are: the ‘plot interval’, which describes the interval of the iterations that should be shown, the ‘plot variable’, indicating which state the color of the nodes represent, the ‘layout’, specifying the node positioning algorithm to be used, and the ‘plot output’, specifying where the GIF should be stored. If not all states should be shown in the histograms, specific states can be selected using the `histogram_states` key.

A dictionary containing these visualization options should be provided as the first argu-

ment for the `configure_visualization` of a `Model` object, as demonstrated in the example code below. The second argument should be the output from the simulation function. The `visualize('animation')` function on the `Model` object will launch a **Matplotlib** (Hunter 2007) window showing the animation, and if required, save the animation. The code below results in Figure 2.

```
visualization_config = {
    'plot_variable': 'phase',
    'fixed_positions': nx.drawing.layout.spring_layout(g, seed=seed),
    'variable_limits': {'phase': [0, 2]},
    'color_scale': 'Greens',
    'show_plot': True,
    'plot_output': './animations/quarantine.gif',
    'plot_title': 'Quarantine SIR model',
    'directed': False,
    'edge_values': 'no'
}

model.configure_visualization(visualization_config, output)
vis = model.visualize('animation')
```

4. Additional functionalities

4.1. Helper functions

Models combining dynamics *on* and *of* a network require access to different characteristics of the network, such as a node's neighbors or the values for different states of a node during previous iterations. Several functions that allow access to this data have been implemented. The list below shows the most common functions that modelers can use when creating a new model.

- `get_state(state_name)` Gets the values of a state for all nodes. This function is generally used to update the state for all nodes by retrieving the current values and modifying them.
- `get_utility()` This function returns a square $n \times n$ matrix A such that its element A_{ij} shows the currently calculated utility for the edge from vertex u_i to u_j .
- `get_previous_nodes_states(n)` Get all the nodes' states from the n 'th previous saved iteration. If t is the current iteration, then the states from iteration $t - n$ will be returned. Using this function, it becomes possible to use differential equations or get the average state values for the nodes for the past few iterations for example. Note that the memory has to be configured to store at least as many iterations as $t - n$.
- `get_previous_nodes_utility(n)` This function returns the matrix from the function `get_utility()` from a previous iteration, provided as argument n , similar to `get_previous_nodes_states(n)`.

- `get_neighbors(node)` Obtains all neighbors of a node. This function returns a list of the **NetworkX** node indicators that are adjacent to the node provided as the argument to the function.
- `get_neighbors_neighbors(node)` This function can be used to only retrieve the neighbors of neighbors of one node. It returns the row of the neighbors of neighbors adjacency matrix that matches the node given as the argument but provides only a list of the **NetworkX** numbers of the neighbors of neighbors.
- `get_adjacency()` Gets the adjacency matrix. This is a square $n \times n$ matrix A such that its element A_{ij} is 1 when there is an edge from vertex u_i to vertex u_j and 0 when there is no edge (Biggs, Biggs, and Norman 1993, definition 2.1, p. 7).
- `get_neighbors_neighbors_adjacency_matrix()` This function provides an adjacency matrix for neighbors of neighbors. This is also a square $n \times n$ matrix A such that its element A_{ij} is 1 when a vertex u_k that has an edge from u_i to u_k exists and there is an edge from vertex u_k to vertex u_j . It is 0 when there is no such vertex.

4.2. Conditions

Sometimes updates should only occur when specific conditions are met for certain nodes. To achieve this, nodes can be filtered using 'conditions'. Only the nodes that meet all the conditions are updated by its corresponding update function. There are three types of conditions that can be used. The *Stochastic condition* triggers an update for each node based on a given probability P . The *Threshold condition* filters nodes based on a chosen variable, threshold, and operators $\leq, <, >, \text{ and } \geq$. The threshold is a single given value and the variable can be any variable of the model. *Custom conditions* filter nodes by applying a user-defined function. This function should return a list of the identifiers of the nodes satisfying the condition. Custom conditions are executed on every node each time step, just like the other conditions, which means that they can be efficiently implemented. Conditions can be chained; nodes that pass one condition can be passed to the next. This can be done by adding the `chained_condition` argument and passing another condition object.

A condition is implemented by adding them to the `model.add_update` object. In the example below, if a node has two or less connections they add a neighbor; the function `add_neighbor` gets called. Argument `get_nodes` passes the nodes that pass the condition. This is an example of a manual network update, see Section 4.4.

```
from dynsimf.models.components.conditions.Condition import ConditionType
import dynsimf.models.components.conditions.ThresholdCondition as tc

# condition indicating 2 or less than 2
cfg = tc.ThresholdConfiguration(tc.ThresholdOperator.LE, 2)
# passes the adjacency of a node for the input of condition
nb_condition = tc.ThresholdCondition(ConditionType.ADJACENCY, cfg)

# add_neighbor gets called, nodes passed satisfy the condition
model.add_network_update(add_neighbor,\
    condition=nb_condition, get_nodes=True)
```

4.3. Schemes

Schemes are another way **DyNSimF** is able to change the way updates are performed. They allow for ‘outside’ perturbations, such as a ‘labor supply shock’ used in economic models. In our example, it could be a temporary introduction of super-spreaders or a super-spreading event. To do this, they can limit the execution of certain updates to a specified selection of iterations during the simulation. One can set a lower and upper boundary within the definition of the scheme, and the passed updates will only occur when the iteration number is within these bounds. As these perturbations often only apply to a selection of nodes, schemes also allow the user to specify a node-sampling function: a function that returns a selection of nodes for which certain updates should take place.

In the example below a scheme with updates is added to a model. Once the Scheme and Update classes are imported an Update object can be created, which in this case is linked to a previously defined function named `update_fun`. Then a scheme object is created, which takes the sample function as the first argument. The second argument is a dictionary that takes four keys: the arguments for the sample function, the lower and upper iteration-bounds, and a list of updates. When the scheme is created, it can be added to the model using the `add_scheme` function.

```
from dynsimf.models.components.Scheme import Scheme
from dynsimf.models.components.Update import Update

u = Update(update_fun)
s = Scheme(sample_function, {
    'args': {'graph': model.graph},
    'lower_bound': 0,
    'upper_bound': 10,
    'updates': [u]
})
model.add_scheme(s)
```

In the example, the update function `update_fun` would be executed during the first 10 iterations. In this case, the function `sample_function` takes in one argument called `graph`, which is the model’s graph. When creating a scheme, any of the keys except `updates` can be omitted. If the lower bound is missing, it will assume the scheme should be active from iteration zero, while if the upper bound is missing it will be active until the end of the simulation.

4.4. Manual Network Updates

It is possible to directly manipulate the network by adding a network-update function to the model via `model.add_network_update()`. This function should return a dictionary with specific keys indicating what kind of change the values of the dictionary are. Figure 3 shows the changes in a network made by the example code below, showing all possible options.

There are two keys to manipulate nodes: ‘add’ and ‘remove’. The corresponding value to the ‘remove’ key should be a list of the names of all the nodes that should be removed from the network. When using the ‘add’ key, the corresponding value should be a list of dictionaries,

where each dictionary inside the list will serve as the initialization for a new node. As can be seen in the example code below, this dictionary should contain two keys: ‘neighbors’ and ‘states’. The ‘neighbors’ key should have a list for the corresponding value, where each entry in the list should be a name of a neighbor. This way new nodes can immediately be connected to other nodes when they are added to the network. The ‘states’ key contains a dictionary, similar to `set_initial_state`: keys for each state’s name and corresponding value for their initial value. This way, nodes can be added to the network with their connections and states defined.

Finally, it is possible to change the edges of individual nodes by using the ‘edge_change’ key in the `add_network_update()` function. Its value should be a dictionary, where every key corresponds with the name of the node whose connections should be updated in the network. Then for each node in the dictionary, another dictionary with 3 possible keys can be created: ‘add’, ‘remove’ and ‘overwrite’. This allows the user to add or remove connections, or to overwrite the complete set of neighbors with new ones. All three keys should have lists as values, where each list contains identifiers of the nodes to add, remove, or overwrite edges with. If a weight should be added for a certain edge, its value should be a list containing the node name, the in-going weight value, and the outgoing weight value. An example of a network update function can be found below. Note that if we apply manual changes to the network, we do not use `UtilityCostModel` but `Model`.

```
model = Model(g, seed = seed, config = ModelConfiguration(cfg))
```

```
def change_network():
    changes = {
        'add': [{
            'neighbors': [1, 2]
            'states': {
                'phase': 1,
                'toi': 0
            }
        }],
        'remove': [5],
        'edge_change':
            0: {
                'add': [1, 2]
                'remove': [3]
            },
            4: {
                'overwrite': [3, 6]
            }
    }
    return changes
model.add_network_update(change_network)
```

5. Related software

Figure 3: An example update of a network using the manual update function shown in 4.4.

DyNSimF has the novel capability of dealing with dynamic networks as well as complex internal dynamics with multiple continuous states. However, there are several other resources available to facilitate the modeling and simulation of complex network-based models in Python. This section discusses the capabilities of these other solutions available and how **DyNSimF** distinguishes itself from the others, with the help of Table 1.

NDlib (Rossetti, Milli, Rinzivillo, Sîrbu, Pedreschi, and Giannotti 2018) is the package that is most similar to **DyNSimF**. **NDlib** was created to solve major issues of other packages such as **Nepidemicx** (Ahrenberg, Kok, Vasarhelyi, and Rutherford 2016) (Python), and **EpiModel** (Jenness, Goodreau, and Morris (2018) (R). While these packages are able to incorporate custom spreading models on networks, they suffer from steep learning curves, and have limited implementation of recent models as they focus only on SIR-type models. **NDlib** also includes a visual interface, allowing an even wider audience to use the package. **DyNSimF** offers internal dynamics with continuous states, directional edges as well as parallelization capabilities over **NDlib**.

Epidemics on Networks (EoN) (Miller and Ting 2020) is based on the book ‘Mathematics of Epidemics on Networks: from Exact to Approximate Models’ (Kiss, Miller, Simon *et al.* 2017). The package offers tools to reproduce models from this book, focusing less on custom complex models. What it does provide over other network-diffusion packages is many out-of-the-box models, different ODE solvers, stochastic dynamics, and extended visualizations including animations. It also includes analysis tools, although often specifically aimed at the models included.

epydemic (Dobson 2020) aims to be the ‘common platform’ for epidemic simulation. While it allows for custom compartmented models, it mainly focuses on scalability and efficiency for conventional SIR-type models.

5.1. Execution times

Numpy Parallelization

DyNSimF is able to facilitate the use of **Numpy** routines, increasing the speed of simulations significantly, as can be seen in Table 2. **DyNSimF** uses **Numpy** arrays under the hood and if the modeler uses data in the form of arrays as well, **Numpy** routines can be used for them.

	DyNSimF	NDlib	Nepidemicx	EoN	epydemic	EpiModel (R)
Internal Dynamics	✓					
Dynamic Network	✓	✓	✓		✓	✓
Stochastic Dynamics				✓	✓	✓
Edge types	++	+		+		
Visualization	✓	✓	✓	✓		✓
Visual Interface		✓				

Table 1: Similar software compared. The first set of rows are about the internal capabilities while the second set of rows are about the tools provided to use and analyze models. ‘Internal Dynamics’ is the capability of having continuous states of a node influence each other, making each agent more complex. ‘Dynamic Network’ is the ability to add and remove nodes or edges. ‘Stochastic Dynamics’ is the ability to implement discrete event algorithms, such as Gillespie simulations. ‘Visualization’ indicates whether the package has tools to show the dynamic behavior. ‘Visual Interface’ represents a user-friendly, non-programming interface to interact with the package. ‘Edge Types’ shows how complex the edges of the networks can be. Every package has edges between nodes. However, + indicates that these edges can be weighted, and ++ that they can be weighted and directional.

Models are only as fast as their slowest component, so one needs to make sure every operation is performed using matrices. This means, for example, that instead of requesting the neighbors for each node, the adjacency matrix containing each neighbor for each node should be used. Below is an example of how the infection and recovery updates of the quarantine model can be done by using only **Numpy** array calculations.

```
def update_states_numpy(constants):
    # define variables
    SIR = model.get_state('phase')
    I = np.where(SIR==1, 1, 0)
    adjacency = model.get_adjacency()
    random = np.random.rand(constants['n'], constants['n'])

    # infection calculation
    # list of nodes eligible to be infected with probability p
    eligible = I * adjacency * random
    # check whether infection event happened
    bool_to_infect = np.any(eligible, axis = 1, \
        where = eligible > (1-constants['beta']))
    nodes_to_infect = np.where(bool_to_infect)[0]
    SIR[nodes_to_infect] = 1

    # recovery calculation
    infected_time = model.get_state('toi')
    # add time to infected toi
    infected_time[np.where(SIR == 1)[0]] += 1
```

```
# if infected long enough, recover
SIR[np.where(infected_time>constants['recovery_time'])]=2

return {'phase': SIR, 'toi': infected_time}
```

Table 2 shows execution times for simulating a SIR model on a network. The different packages all simulate a SIR model with a random geometric graph using a 0.75 distance threshold value for connecting nearby nodes. The simulations were run 10 times per library and the average execution times are shown in the table for different numbers of nodes. The parameters used for the SIR model are $\beta = 0.001$ and $\gamma = 0.01$, while the initial fraction of infected nodes is 5%. All simulations were run on a workstation with a Ryzen 7 2700X, 16GB of RAM operating on 3000hz, and a GTX 1080TI. The execution times shown, only indicate the time spent on 25 iterations, without taking setup time into account. It can be seen how **DyNSimF** rivals, or even outperforms packages specifically created for epidemic simulations in Python. It is noteworthy that these execution speeds were acquired from simulating a highly connected network, amplifying efficiency gains in dense network calculations.

Package	Graph Size (# nodes)		
	10^2	10^3	10^4
DyNSimF for-loop implementation	0.024s	5.162s	658.79s
DyNSimF matrix implementation	0.005s	0.232s	21.86s
NDlib	0.029s	1.516s	124.57s
EoN	0.009s	1.390s	148.08s
epydemic	0.038s	4.482s	927.16s

Table 2: A table showing the execution times of different packages simulating a network SIR model for 25 iterations. Every simulation was run using $\beta = 0.001$ and $\gamma = 0.01$. The initial fraction of infected was 5%. The network used for the model is a random geometric graph with a 0.75 distance threshold value for connecting nearby nodes. The values shown are averages acquired by the results after 10 simulations.

6. Conclusion

DyNSimF, is an open-source, flexible framework for studying custom complex network-dynamics using Python. It is the first package that facilitates studying both dynamics *on* the network as well as *of* the network, as well as their complex interactions.

Built upon **NetworkX**, its core is familiar to many people in Network Science, making **DyNSimF** highly integrative and suitable for many existing analyses. Created with a focus on consistency, readability, and extendability, it aims to improve ease-of-use over alternatives. Array-based routines of **Numpy** can be leveraged, resulting in very competitive modeling speeds, outperforming most alternatives. **DyNSimF** includes customizable dynamic visualizations, useful especially for early-stage modeling, and supports custom metrics for analyses. We hope **DyNSimF** enables novice modelers to focus less on programming and more on modeling while allowing experienced modelers to build intricate, fast, custom models for a wide range of use-cases. Our aim for **DyNSimF** is to become the new standard in complex dynamic network modeling.

DyNSimF is suitable for Python ≤ 3.9 , available on PyPI at <https://pypi.org/project/dynsimf/>. Documentation can be found at <https://dynsimf.readthedocs.io/en/latest/> and the source code is available from the GitHub repository <https://github.com/Tensaiz/DyNSimF>.

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