MCSX 2022 Warmup - Python for Network Analysis

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1 Network analysis with Python

Overview of the most used Python Libraries for Data and Network Analysis.

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1.0.2 This notebook is available at https://bit.ly/3u2S2Li

https://marcograssia.com/talk/mscx_2022_warmup/

2 *Python*

2.1 What is *python*

> Python is an *interpreted*, *object-oriented*, *high-level* programming language with dynamic semantics. [...]
>
> It is suitable for **rapid development** and for use as a "**glue language**" to connect various components (e.g., written in different languages).

Python is **one of the most used programming languages**[1]

[1]: StackOverflow's 2021 survey

2.1.1 Why is *python* so popular?

Its popularity can be rooted to its characteristics - *Python* is fast to learn, very versatile and flexible - It is very high-level, and complex operations can be performed with few lines of code

And to its large user-base: - **Vast assortment of libraries** - **Solutions to your problems may be already available** (e.g., on StackOverflow)

2.1.2 Some real-world applications

- Data science (loading, processing and plotting of data)
- Scientific and Numeric computing
- Modeling and Simulation
- Web development

- Artificial Intelligence and Machine Learning
- Image and Text processing
- Scripting

2.2 How to get *python*?

Using the **default environment that comes with your OS is not a great idea**: - Usually older *python* versions are shipped - You cannot upgrade the *python* version or the libraries freely - Some functions of your OS may depend on it

You can either: 1. Download *python* 2. Use a distribution like *Anaconda*

2.2.1 Anaconda

Anaconda is a *python* distribution that packs the most used libraries for data analysis, processing and visualization

Anaconda installations are managed through the *conda* package manager

Anaconda "distribution" is free and open source

Anaconda distribution

3 *Python* virtual environments

> A virtual **environment** is a Python environment such that the Python interpreter, libraries and scripts installed into it are isolated from those installed in other virtual environments

Environments are used to freeze specific interpreter and libraries versions for your projects

If you start a new project and need newer libraries, just create a new environment

You won't have to worry about breaking the other projects

Environment creation

> conda create –name [] [–channel]

You can also specify additional channels to search for packages (in order)

Example:

> conda create –name gt python=3.9 graph-tool pytorch torchvision torchaudio cudatoolkit=11.3 pyg seaborn numpy scipy matplotlib jupyter -c pyg -c pytorch -c nvidia -c anaconda -c conda-forge

Switch environment

> conda activate <ENV_NAME>

Example > conda activate gt

Full documentation

3.1 Data analysis and visualization libraries

- NumPy
- SciPy
- Matplotlib
- Seaborn
- Pandas

These libraries are general, and can be used also in Network Analysis

3.2 Network analysis and visualization libraries

- graph-tool
- PyTorch Geometric (PyG)

3.3 NumPy

> ***NumPy*** is the fundamental package for scientific computing in Python.

NumPy offers new data structures: - **Multidimensional array** objects (the ***ndarray***) - Various derived objects (like ***masked arrays***)

And also a **vast assortment of functions**: - **Mathematical functions** (arithmetic, trigonometric, hyperbolic, rounding, …) - **Sorting, searching, and counting** - Operations on **Sets** - Input and output - **Fast Fourier Transform** - Complex numbers handing - (pseudo) random number generation

NumPy is fast: - Its core is written in C/C++ - Arrays are stored in contiguous memory locations

It also offers tools for integrating C/C++ code

Many libraries are built on top of NumPy's arrays and functions.

The *ndarray* Mono-dimensional

Multi-dimensional

NumPy documentation

[6]:
```
import numpy as np
```

[7]:
```
np.random.rand(3)
```

[7]:
```
array([0.23949294, 0.49364534, 0.10055484])
```

[8]:
```
np.random.rand(1, 3)
```

[8]:
```
array([[0.45292492, 0.32975629, 0.53797728]])
```

[9]:
```
np.random.randint(10, size=(2, 2, 2))
```

[9]:
```
array([[[9, 1],
        [9, 9]],
```

```
[[5, 7],
 [3, 3]]])
```

3.4 *SciPy*

SciPy is a **collection of mathematical algorithms** and convenience functions **built on the NumPy library**

SciPy is written in C and Fortran, and provides: - Algorithms for **optimization, integration, interpolation, eigenvalue problems, algebraic equations, differential equations, statistics, etc**. - Specialized data structures, such as **sparse matrices** and k-dimensional trees - Tools for the interactive Python sessions

SciPy's main **subpackages** include:

- Data clustering algorithms
- Physical and mathematical constants
- Fast Fourier Transform routines
- Integration and ordinary differential equation solvers
- Linear algebra
- …
- …
- N-dimensional image processing
- Optimization and root-finding routines
- Signal processing
- Sparse matrices and associated routines
- Spatial data structures and algorithms
- Statistical distributions and functions

[10]:
```
import scipy as sp
```

SciPy documentation

3.4.1 Sparse matrices

There are many sparse matrices implementations, each optimized for different operations.

For instance: - **Coo**rdinate (COO) - **Li**nked **L**ist Matrix (LIL) - **C**ompressed **S**parse **R**ow (CSR) - **C**ompressed **S**parse **C**olumn (CSC)

Check this nice tutorial for more! Sparse matrices tutorial

3.5 Pandas

pandas allows easy data organization, filtering, analysis and plotting

pandas provides **data structures** for **"relational" or "labeled" data**, for instance: - **Tabular data** with **heterogeneously-typed columns**, as in an Excel spreadsheet - Ordered and unordered **time series data** - **Arbitrary matrix data** (even heterogeneous typed) with row and column labels

The two primary data structures provided are the: - **Series** (1-dimensional) - **DataFrame** (2-dimensional)

Series

DataFrame

These structures heavily rely on *NumPy* and its arrays

pandas integrates well with other libraries built on top of *NumPy*

Supported file formas *pandas* can recover data from/store data to SQL databases, Excel, CSVs…

[11]:
```
import pandas as pd
```

pandas documentation

DataFrame example Penguins example dataset from the Seaborn package

[12]:
```
penguins = sns.load_dataset("penguins")
display(penguins)
```

```
    species     island  bill_length_mm  bill_depth_mm  flipper_length_mm  \
0    Adelie  Torgersen            39.1           18.7              181.0
1    Adelie  Torgersen            39.5           17.4              186.0
2    Adelie  Torgersen            40.3           18.0              195.0
3    Adelie  Torgersen             NaN            NaN                NaN
4    Adelie  Torgersen            36.7           19.3              193.0
..      …        …              …              …                 …
339  Gentoo     Biscoe             NaN            NaN                NaN
340  Gentoo     Biscoe            46.8           14.3              215.0
341  Gentoo     Biscoe            50.4           15.7              222.0
342  Gentoo     Biscoe            45.2           14.8              212.0
343  Gentoo     Biscoe            49.9           16.1              213.0

     body_mass_g     sex
0         3750.0    Male
1         3800.0  Female
2         3250.0  Female
3            NaN     NaN
4         3450.0  Female
..           …     …
339          NaN     NaN
340       4850.0  Female
341       5750.0    Male
342       5200.0  Female
343       5400.0    Male

[344 rows x 7 columns]
```

Series of the species

[13]:
```
penguins["species"]
```

[13]:
```
0      Adelie
1      Adelie
2      Adelie
3      Adelie
4      Adelie
       ...
339    Gentoo
340    Gentoo
341    Gentoo
342    Gentoo
343    Gentoo
Name: species, Length: 344, dtype: object
```

Unique species

[14]:
```
penguins["species"].unique()
```

[14]:
```
array(['Adelie', 'Chinstrap', 'Gentoo'], dtype=object)
```

Average bill length

[15]:
```
penguins["bill_length_mm"].mean()
```

[15]:
```
43.9219298245614
```

Standard deviation of the bill length

[16]:
```
penguins["bill_length_mm"].std()
```

[16]:
```
5.4595837139265315
```

Data filtering for male penguins

[17]:
```
penguins["sex"] == "Male"
```

[17]:
```
0       True
1      False
2      False
3      False
4      False
       ...
339    False
340    False
341     True
342    False
343     True
Name: sex, Length: 344, dtype: bool
```

[18]:
```
penguins.loc[                          # .loc property
    penguins["sex"] == "Male"          # Row filter (boolean)
]
```

[18]:
```
     species     island  bill_length_mm  bill_depth_mm  flipper_length_mm  \
0     Adelie  Torgersen            39.1           18.7              181.0
5     Adelie  Torgersen            39.3           20.6              190.0
7     Adelie  Torgersen            39.2           19.6              195.0
13    Adelie  Torgersen            38.6           21.2              191.0
14    Adelie  Torgersen            34.6           21.1              198.0
..       …        …              …              …                 …
333   Gentoo     Biscoe            51.5           16.3              230.0
335   Gentoo     Biscoe            55.1           16.0              230.0
337   Gentoo     Biscoe            48.8           16.2              222.0
341   Gentoo     Biscoe            50.4           15.7              222.0
343   Gentoo     Biscoe            49.9           16.1              213.0

     body_mass_g   sex
0         3750.0  Male
5         3650.0  Male
7         4675.0  Male
13        3800.0  Male
14        4400.0  Male
..           …   …
333       5500.0  Male
335       5850.0  Male
337       6000.0  Male
341       5750.0  Male
343       5400.0  Male

[168 rows x 7 columns]
```

Average bill length for male penguins

[19]:
```
penguins.loc[ penguins["sex"] == "Male",    # Mask (row filter)
              "bill_length_mm",             # Column filter
].mean()
```

[19]:
```
45.85476190476191
```

Average bill length and weight for female penguins

[20]:
```
penguins.loc[penguins["sex"] == "Female",                # Mask (row filter)
             ["bill_length_mm", "body_mass_g"]           # Column filter
            ].mean()
```

[20]:
```
bill_length_mm      42.096970
body_mass_g       3862.272727
dtype: float64
```

3.6 *Matplotlib*

Matplotlib is a comprehensive library for creating static, animated, and interactive visualizations in *Python*

Matplotlib documentation

3.6.1 Some plot examples

From the Matplotlib gallery

Line plots Source

Scatterplots and histograms Source

Barplots

Simple barplot Source

Stacked barplot Source

Grouped barplot Source

Horizontal bar chart Source

3.6.2 (Nested) pie charts

Source

Heatmaps Source

Violin and box plots Source

Stackplots Source

... and many more

[21]:
```
import matplotlib.pyplot as plt
```

3.7 *Seaborn*

Seaborn is a library for making statistical graphics in Python

Thanks to its **high-level interface**, it makes plotting very complex figures easy

Seaborn **builds on top of *matplotlib*** and **integrates** closely **with *pandas* data structures**

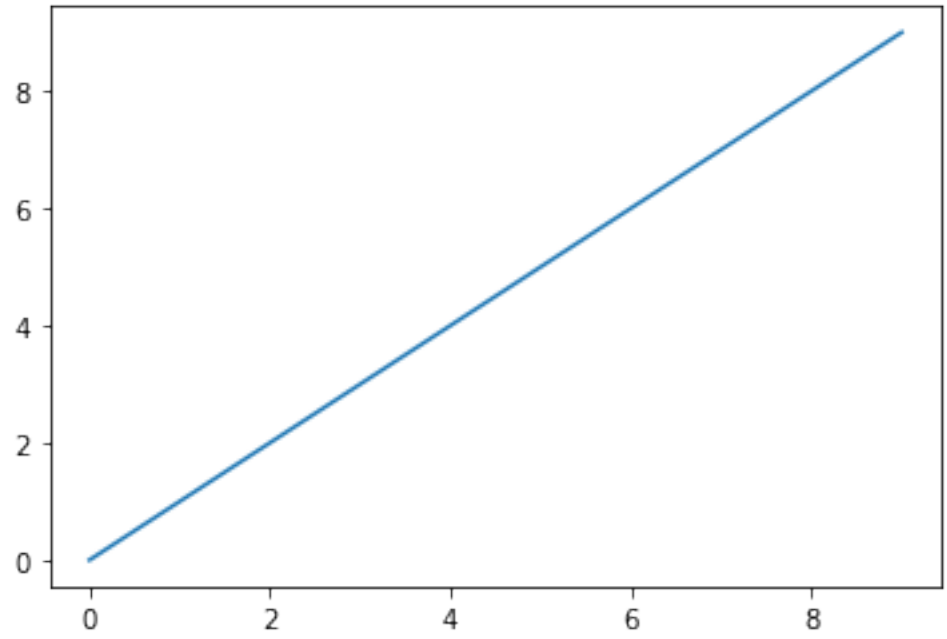
[22]:
```
import seaborn as sns
```

It provides **helpers to improve how all matplotlib plots look**: - Theme and style - Colors (even colorblind palettes) - Scaling, to quickly switch between presentation contexts (e.g., plot, poster and talk)

[23]:
```
sns.reset_defaults()
```

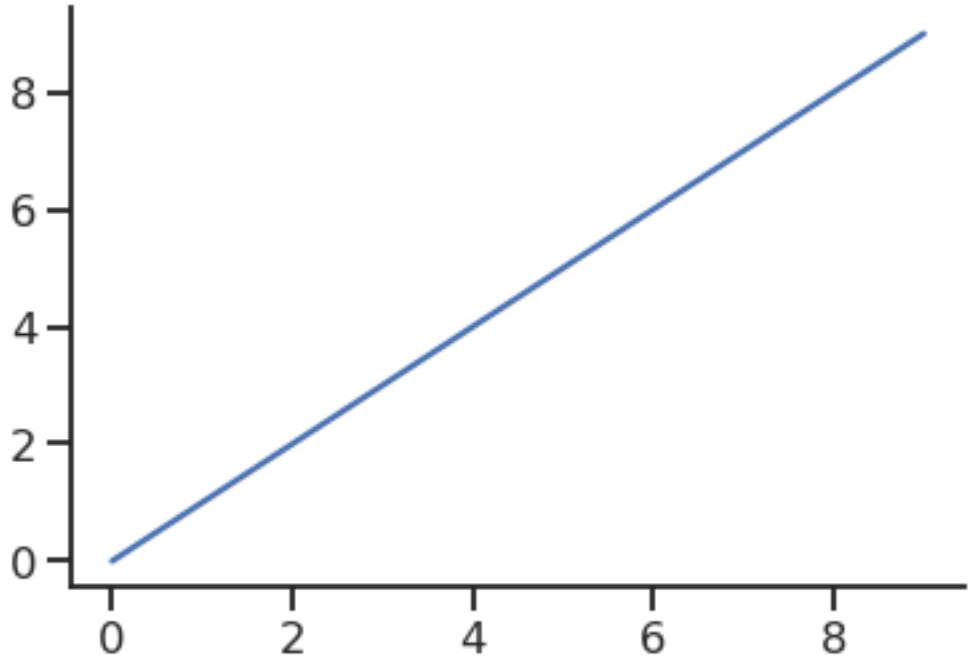
[24]:
```
plt.plot(range(10), range(10))
```

[24]:
```
[<matplotlib.lines.Line2D at 0x7f1ed75972b0>]
```



[25]:
```
sns.set_theme(context="talk",
              style="ticks",
              palette="deep",
              font="sans-serif",
#               font_scale=1,
              color_codes=True,
              rc={
                  'figure.facecolor': 'white'
#                   'figure.figsize': (10, 6),
#                   "text.usetex": True,
#                   "font.family": "sans-serif",
              },

              )
```

[26]:
```
plt.plot(range(10), range(10))
sns.despine()
```



Seaborn's FacetGrid offers a convenient way to visualize multiple plots in grids

They can be drawn with up to three dimensions: rows, columns and hue

Tutorial: Building structured multi-plot grids

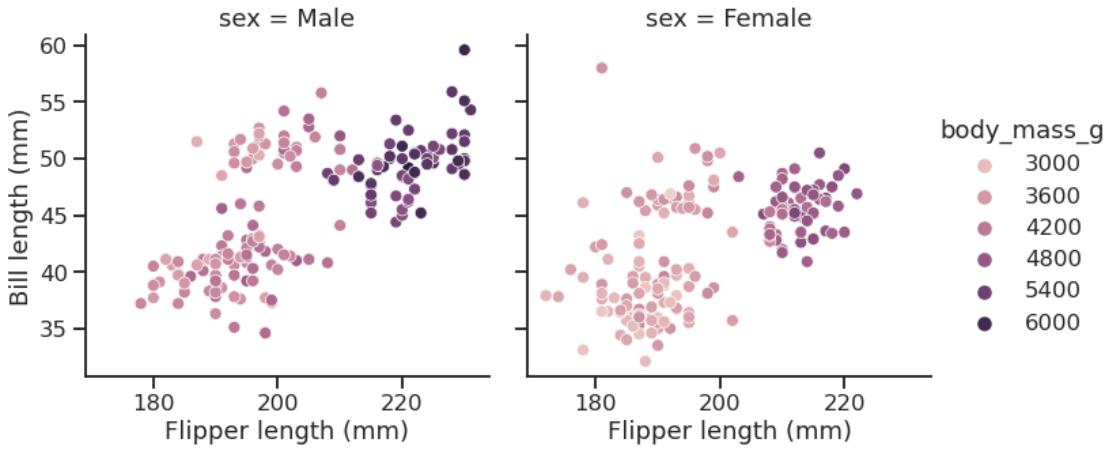
[27]:
```
penguins.head()
```

[27]:

	species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	body_mass_g	sex
0	Adelie	Torgersen	39.1	18.7	181.0	3750.0	Male
1	Adelie	Torgersen	39.5	17.4	186.0	3800.0	Female
2	Adelie	Torgersen	40.3	18.0	195.0	3250.0	Female
3	Adelie	Torgersen	NaN	NaN	NaN	NaN	NaN
4	Adelie	Torgersen	36.7	19.3	193.0	3450.0	Female

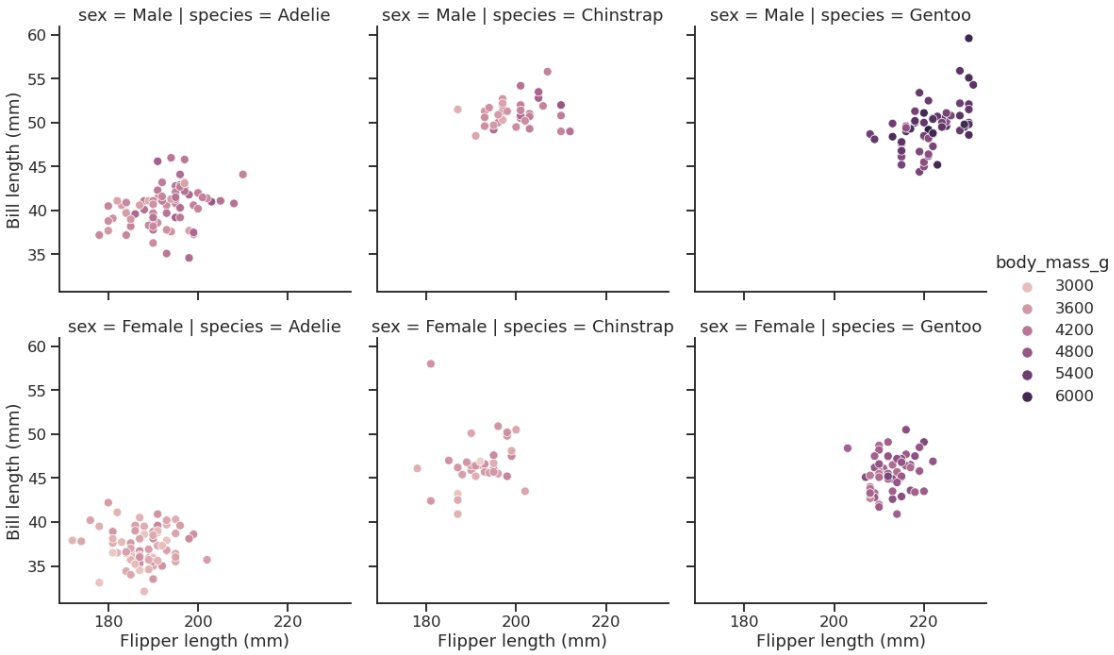
[28]:
```
g = sns.relplot(data=penguins,
                x="flipper_length_mm",
                y="bill_length_mm",
                col="sex",
                hue="body_mass_g"
               )
g.set_axis_labels("Flipper length (mm)", "Bill length (mm)")
```

[28]: <seaborn.axisgrid.FacetGrid at 0x7f1ed7597a90>



[29]:
```
g = sns.relplot(data=penguins,
                x="flipper_length_mm",
                y="bill_length_mm",
                row="sex",
                col="species",
                hue="body_mass_g"
               )
g.set_axis_labels("Flipper length (mm)", "Bill length (mm)")
```

[29]: <seaborn.axisgrid.FacetGrid at 0x7f1ed73a5f10>



Seaborn documentation

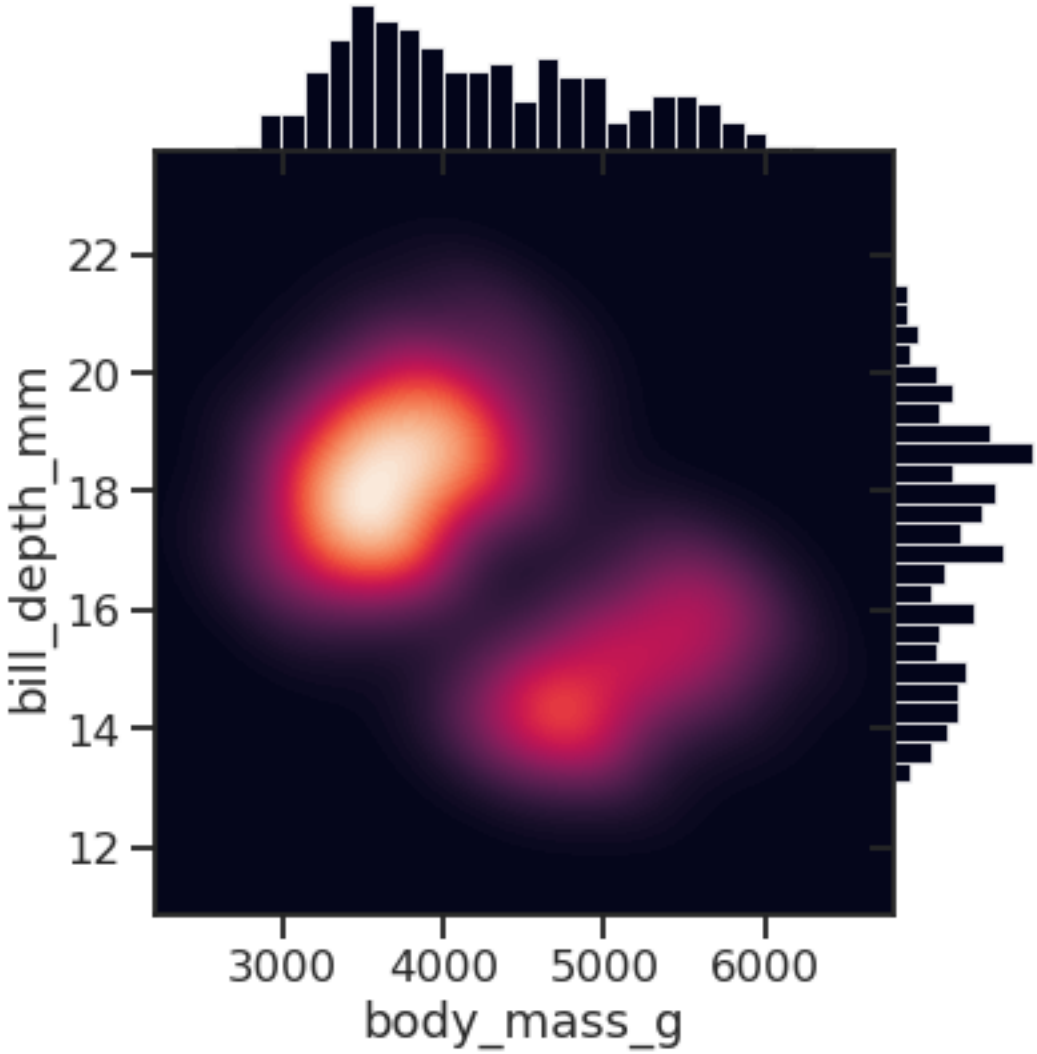
3.7.1 Some more plot examples

From Seaborn example gallery

Smooth kernel density with marginal histograms (source)

[30]:
```
g = sns.JointGrid(data=penguins, x="body_mass_g", y="bill_depth_mm", space=0)
g.plot_joint(sns.kdeplot,
             fill=True, clip=((2200, 6800), (10, 25)),
             thresh=0, levels=100, cmap="rocket")
g.plot_marginals(sns.histplot, color="#03051A", alpha=1, bins=25)
```

[30]:
```
<seaborn.axisgrid.JointGrid at 0x7f1ed5671ca0>
```

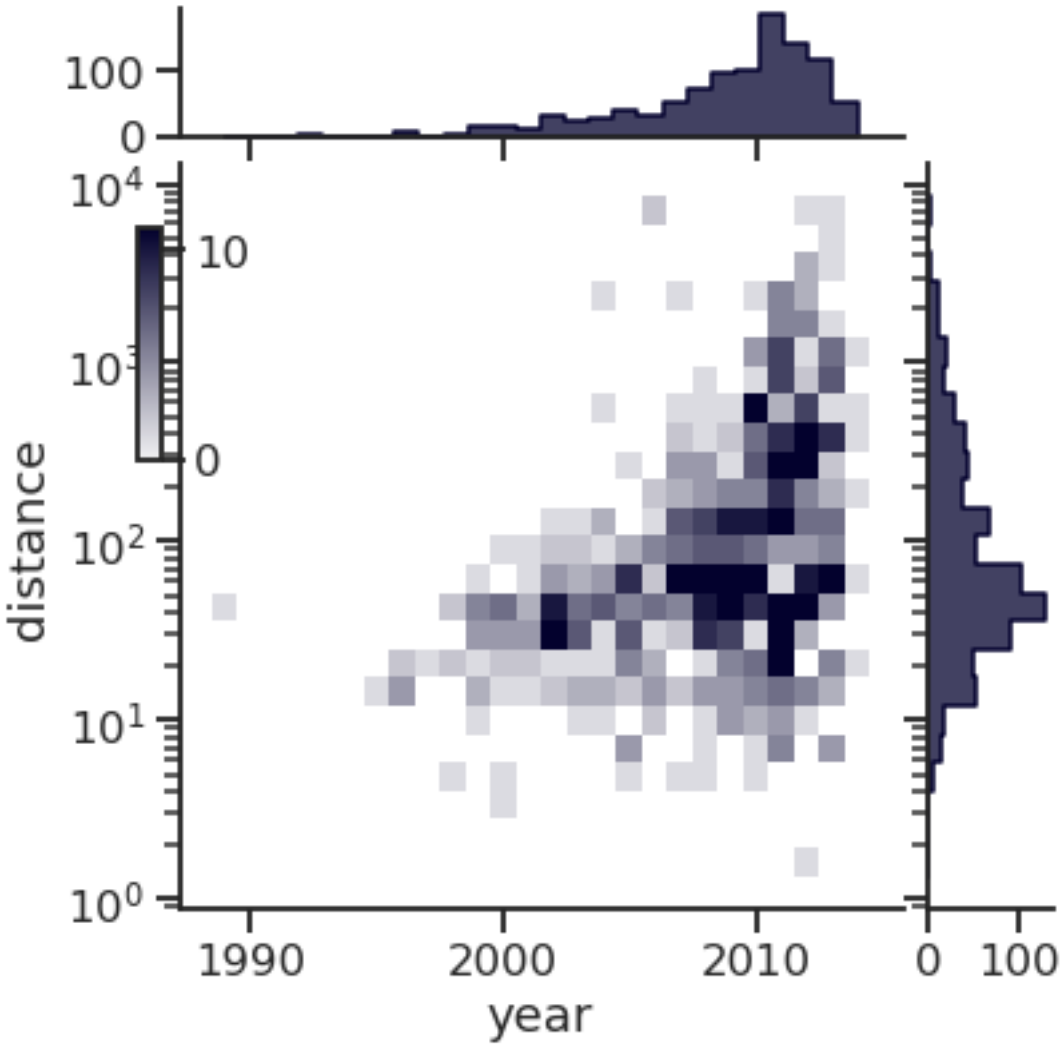


Joint and marginal histograms Source

[31]:
```
g = sns.JointGrid(data=planets, x="year", y="distance", marginal_ticks=True)

# Set a log scaling on the y axis
g.ax_joint.set(yscale="log")

# Create an inset legend for the histogram colorbar
cax = g.figure.add_axes([.15, .55, .02, .2])

# Add the joint and marginal histogram plots
g.plot_joint(
    sns.histplot, discrete=(True, False),
    cmap="light:#03012d", pmax=.8, cbar=True, cbar_ax=cax
```

```
)
g.plot_marginals(sns.histplot, element="step", color="#03012d")
```

[31]: <seaborn.axisgrid.JointGrid at 0x7f1ed4503c70>



Custom projections Source

Discovering structure in heatmap data Source

Bivariate plot with multiple elements Source

4 Network Analysis with Python

Three main libraries: - *graph-tool* - *networkx* - *python-igraph*

4.1 *graph-tool*

graph-tool is a **graph analysis** library for *Python*

It provides the ***Graph*** data structure, and various algorithms

It is mostly written in C++, and based on the Boost Graph Library

It supports multithreading and it is fairly easy to extend

Built in algorithms: - **Topology** analysis tools - **Centrality**-related **algorithms** - **Clustering coefficient** (transitivity) algorithms - **Correlation** algorithms, like the **assortativity** - **Dynamical processes** (e.g., SIR, SIS, …) - Graph **drawing** tools - **Random graph** generation - **Statistical inference of generative network models** - **Spectral properties** computation

Documentation

[32]:
```
import graph_tool.all as gt
```

Performance comparison (source: graph-tool.skewed.de/)

Algorithm	graph-tool (16 threads)	graph-tool (1 thread)	igraph	NetworkX
Single-source shortest path	0.0023 s	0.0022 s	0.0092 s	0.25 s
Global clustering	0.011 s	0.025 s	0.027 s	7.94 s
PageRank	0.0052 s	0.022 s	0.072 s	1.54 s
K-core	0.0033 s	0.0036 s	0.0098 s	0.72 s
Minimum spanning tree	0.0073 s	0.0072 s	0.026 s	0.64 s
Betweenness	102 s (~1.7 mins)	331 s (~5.5 mins)	198 s (vertex) + 439 s (edge) (~ 10.6 mins)	10297 s (vertex) 13913 s (edge) (~6.7 hours)

4.2 How to load a network

0. Choose a graph analysis library. The right one mostly depends on your needs (e.g., functions, performance, etc.)

   In this warm-up, we will use *graph-tool*.

1. To load the network, we need to use the right loader function, which depends on the file format

4.2.1 File formats

Many ways to represent and store graphs.

The most popular ones are: - edgelist - GraphML

For more about file types, check the NetworkX documentation

4.2.2 Edgelist (.el, .edge, ...)

As the name suggests, it is a list of node pairs (source, target) and edge properties (if any). Edgelists cannot store any information about the nodes, or about the graph (not even about the directedness)

Values may be separated by commas, spaces, tabs, etc. Comments may be supported by the reader function.

Example file:

```
# source, target, weight
0,1,1
0,2,2
0,3,2
0,4,1
0,5,1
0,6,1
1,18,1
1,3,1
1,4,2
2,0,1
2,25,1
#...
```

4.2.3 GraphML (.graphml, .xml)

Flexible format based on XML.

It can store hierarchical graphs, information (i.e., attributes or properties) about the graph, the nodes and the edges.

Main drawback: heavy disk usage (space, and IØtime)

Example of the file:

```
<?xml version="1.0" encoding="UTF-8"?>
<graphml xmlns="http://graphml.graphdrawing.org/xmlns"
         xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
         xsi:schemaLocation="http://graphml.graphdrawing.org/xmlns http://graphml.graphdrawing

  <!-- property keys -->
  <key id="key0" for="node" attr.name="_pos" attr.type="vector_float" />
  <key id="key1" for="graph" attr.name="citation" attr.type="string" />
  <key id="key2" for="graph" attr.name="description" attr.type="string" />
  <!-- [...] -->
  <key id="key8" for="edge" attr.name="weight" attr.type="short" />

  <graph id="G" edgedefault="directed" parse.nodeids="canonical" parse.edgeids="canonical" pars

   <!-- graph properties -->
   <data key="key1">[&apos;J. S. Coleman. &quot;Introduction to Mathematical Sociology.&quot; I
   <data key="key2">A network of friendships among male students in a small high school in Ill
```

```
  <!-- [...] -->

  <!-- vertices -->
   <node id="n0">
     <data key="key0">0.92308158331278289, 12.186082864409657</data>
   </node>
   <node id="n1">
     <data key="key0">1.2629064355495019, 12.213213242633238</data>
   </node>
   <node id="n2">
     <data key="key0">1.1082744694986855, 12.190211909578192</data>
   </node>

   <!-- [...] -->

   <!-- edges -->
   <edge id="e0" source="n0" target="n1">
     <data key="key8">1</data>
   </edge>
   <edge id="e1" source="n0" target="n2">
     <data key="key8">2</data>
   </edge>
   <edge id="e2" source="n0" target="n3">
     <data key="key8">2</data>
   </edge>
   <edge id="e3" source="n0" target="n4">
     <data key="key8">1</data>
   </edge>

   <!-- [...] -->

  </graph>
</graphml>
```

5 How to load a network

0. Choose a graph analysis library. The right one mostly depends on your needs (e.g., features, performance, etc.)

   In this warm-up, we will use *graph-tool*.

1. To load the network, we need to use the right loader function, which depends on the file format

2. After identifying the file format and the right loader function, we load the network

[33]:
```
g = gt.load_graph("highschool.graphml")

display(g)
```

```
<Graph object, directed, with 70 vertices and 366 edges, 1 internal vertex␣
 ↪property, 1 internal edge property, 7 internal graph properties, at␣
 ↪0x7f1ed41879d0>
```

[34]:
```
display(g.graph_properties)
```

```
{'citation': <GraphPropertyMap object with value type 'string', for Graph␣
 ↪0x7f1ed41879d0, at 0x7f1ed4187220>, 'description': <GraphPropertyMap object␣
 ↪with value type 'string', for Graph 0x7f1ed41879d0, at 0x7f1ed4187130>,␣
 ↪'konect_meta': <GraphPropertyMap object with value type 'string', for Graph␣
 ↪0x7f1ed41879d0, at 0x7f1ed4187070>, 'konect_readme': <GraphPropertyMap object␣
 ↪with value type 'string', for Graph 0x7f1ed41879d0, at 0x7f1ed41b80a0>, 'name':
 ↪ <GraphPropertyMap object with value type 'string', for Graph 0x7f1ed41879d0,␣
 ↪at 0x7f1ed4225070>, 'tags': <GraphPropertyMap object with value type␣
 ↪'vector<string>', for Graph 0x7f1ed41879d0, at 0x7f1ed4225040>, 'url':␣
 ↪<GraphPropertyMap object with value type 'string', for Graph 0x7f1ed41879d0,␣
 ↪at 0x7f1ed4256d00>}
```

[35]:
```
display(g.vertex_properties)
```

```
{'_pos': <VertexPropertyMap object with value type 'vector<double>', for Graph␣
 ↪0x7f1ed41879d0, at 0x7f1ed4187730>}
```

[36]:
```
display(g.edge_properties)
```

```
{'weight': <EdgePropertyMap object with value type 'int16_t', for Graph␣
 ↪0x7f1ed41879d0, at 0x7f1ed4291130>}
```

5.1 Some network analysis

Get the number of nodes

[37]:
```
number_of_nodes = g.num_vertices()
display(f"Number of nodes: {number_of_nodes}")
```

```
'Number of nodes: 70'
```

Get the number of edges

[38]:
```
number_of_edges = g.num_edges()
display(f"Number of edges: {number_of_edges}")
```

```
'Number of edges: 366'
```

Get the in and out degrees

[39]:
```
in_degree = g.get_in_degrees(g.get_vertices(), eweight=None)
```

[40]:
```
average_in_degree = np.mean(in_degree)

display("Average in degree", average_in_degree)
```

```
'Average in degree'
```

```
5.228571428571429
```

[41]:
```
out_degree = g.get_out_degrees(g.get_vertices(), eweight=None)
```

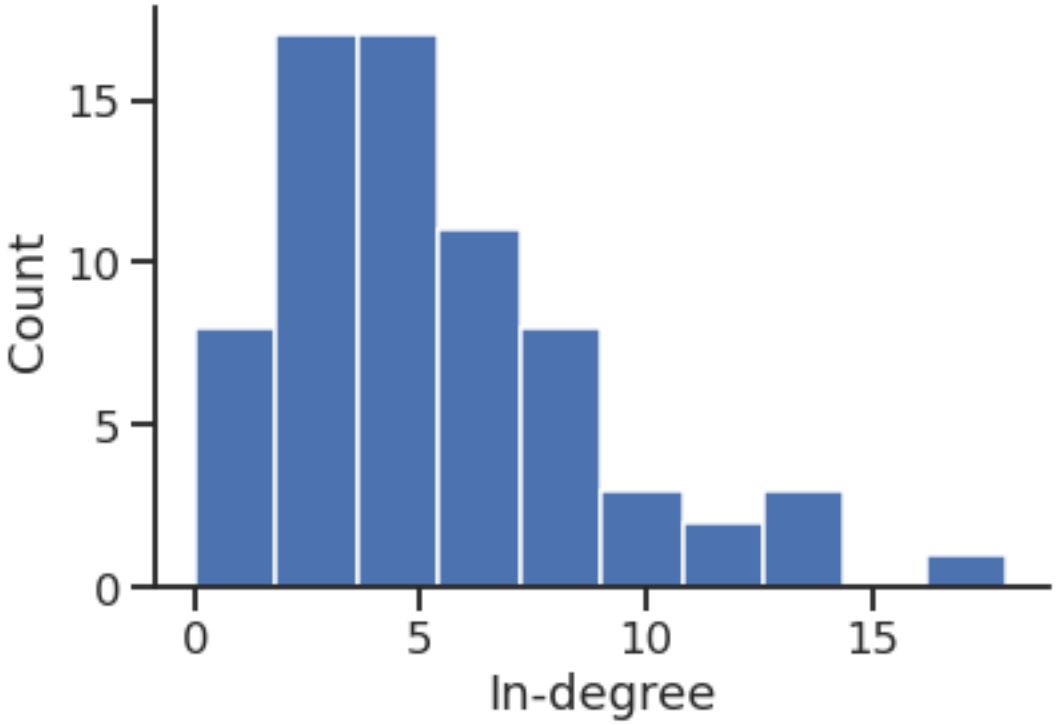
[42]:
```
average_out_degree = np.mean(out_degree)
display("Average out degree", average_out_degree)
```

```
'Average out degree'
```

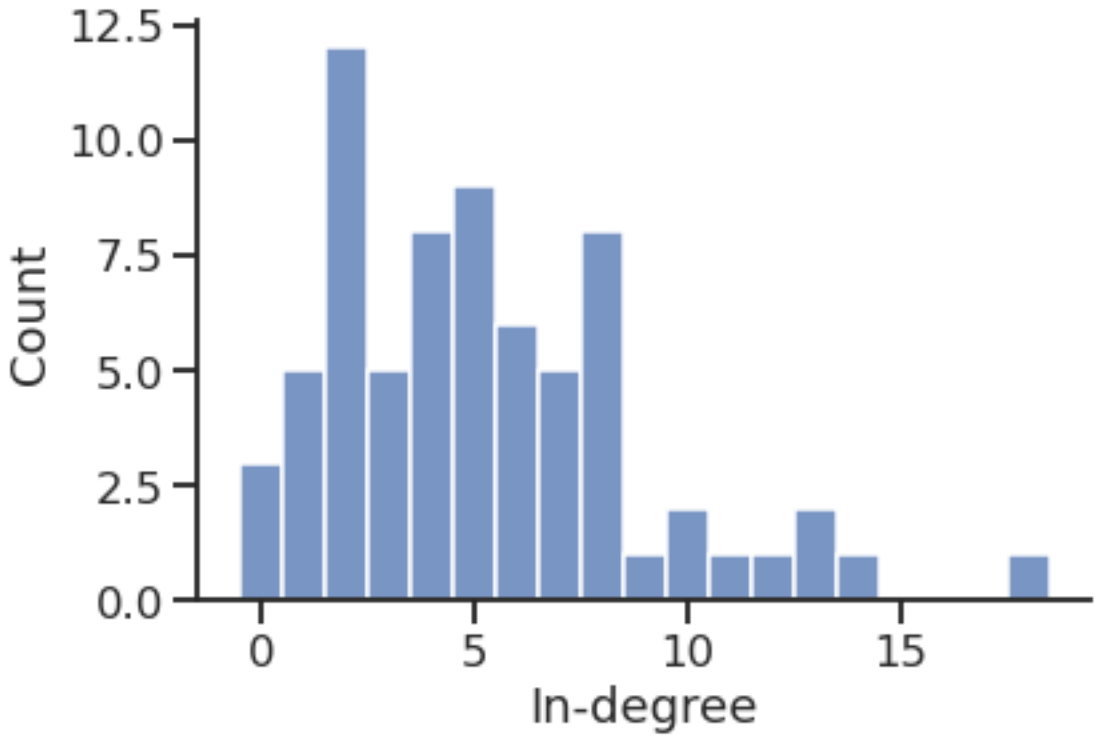
```
5.228571428571429
```

In-degree distribution

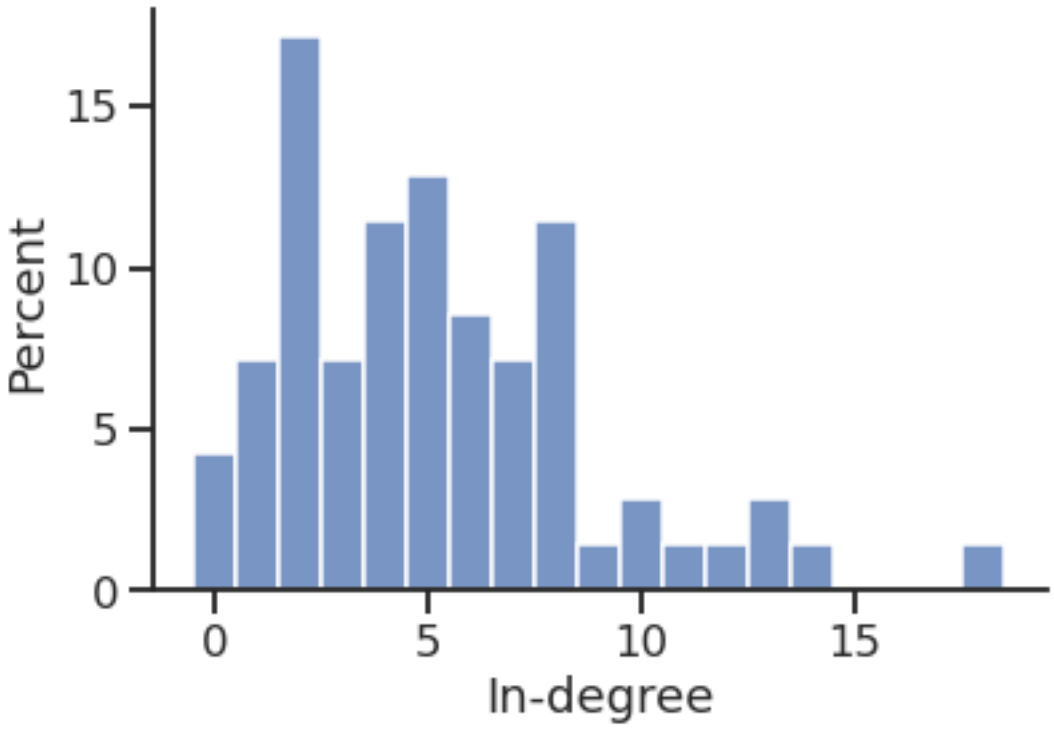
[43]:
```
p = plt.hist(in_degree)

plt.ylabel("Count")
plt.xlabel("In-degree")
sns.despine()
```



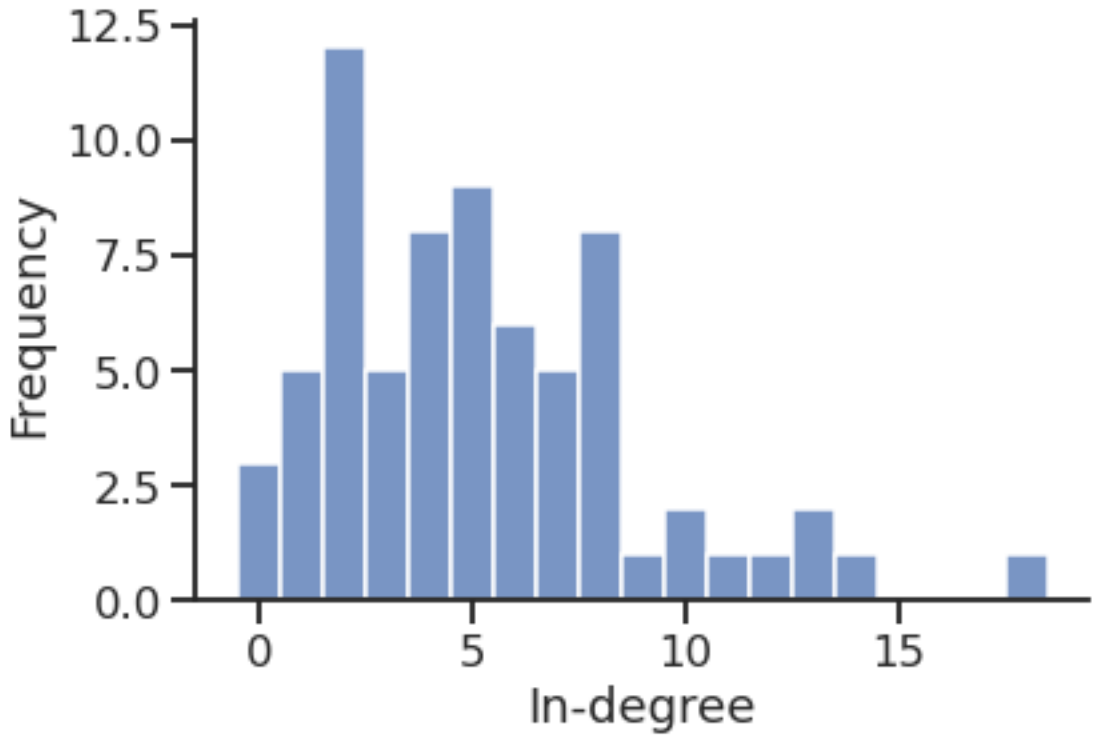
[44]:
```
p = sns.histplot(in_degree,
                 stat="count",
                 discrete=True,
)
p.set_xlabel("In-degree")
sns.despine()
```



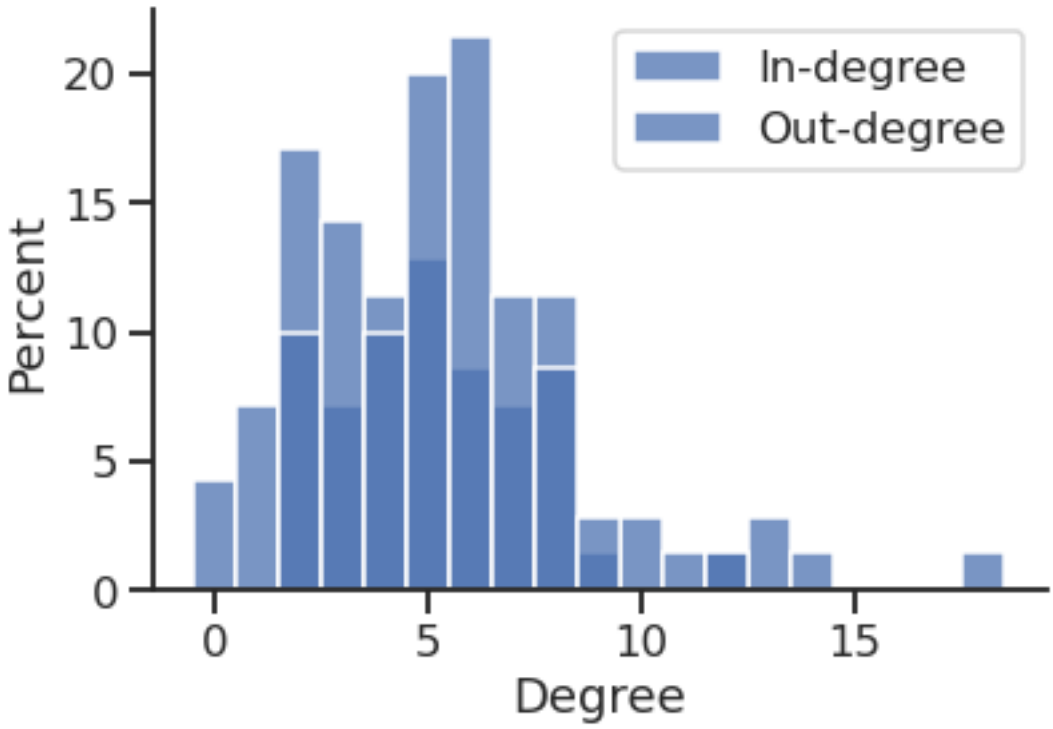
[45]:
```
p = sns.histplot(in_degree,
                 stat="percent",
                 discrete=True,
)
p.set_xlabel("In-degree")
sns.despine()
```



[46]:
```
sns.histplot(in_degree,
             stat="frequency",
             discrete=True,
)
plt.xlabel("In-degree")
sns.despine()
```



[47]:
```
sns.histplot(in_degree,
             stat="percent",
             discrete=True,
             label="In-degree",
             legend=True,

)
sns.histplot(out_degree,
             stat="percent",
             discrete=True,
             label="Out-degree",
             legend=True,
)

plt.xlabel("Degree")
plt.legend()
sns.despine()
```

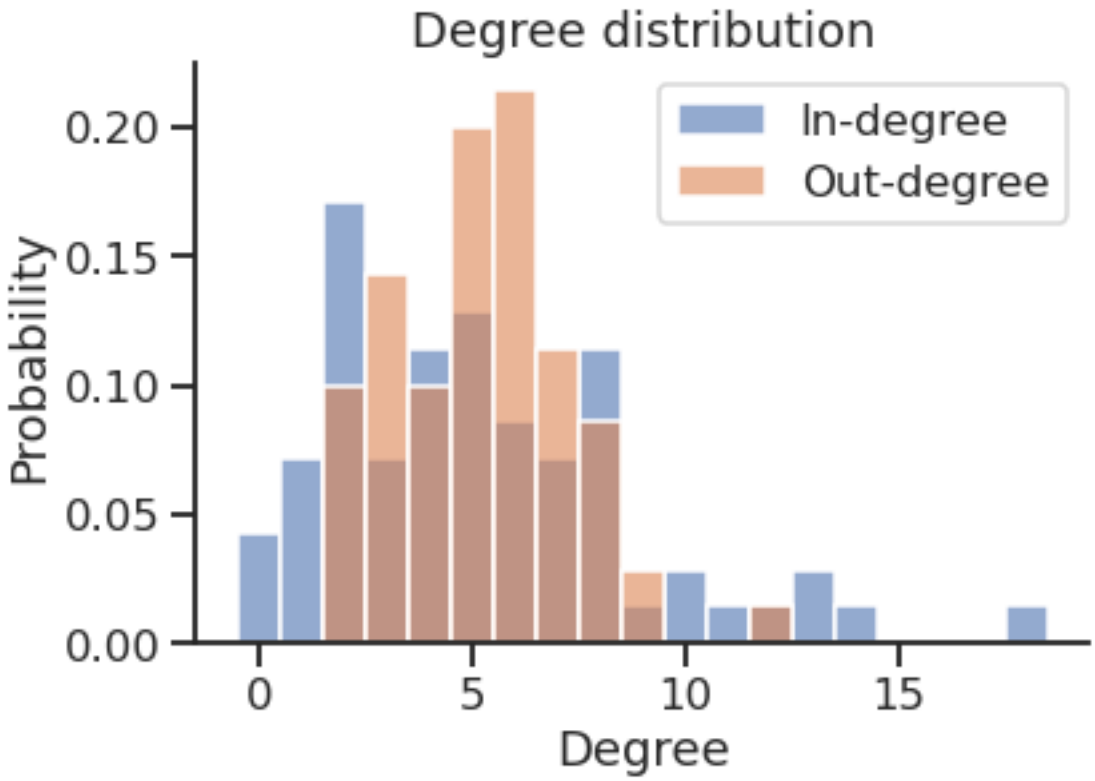


[48]:
```
cmap = sns.color_palette("deep", n_colors=2)

cmap
```

[48]:
```
[(0.2980392156862745, 0.4470588235294118, 0.6901960784313725),
 (0.8666666666666667, 0.5176470588235295, 0.3215686274509804)]
```

[49]:
```
sns.histplot(in_degree,
             stat="probability",
             discrete=True,
             label="In-degree",
             legend=True,
             color=cmap[0],
             alpha=0.6,
)
sns.histplot(out_degree,
             stat="probability",
             discrete=True,
             label="Out-degree",
             legend=True,
             color=cmap[1],
             alpha=0.6,
)
```

```
plt.title("Degree distribution")
plt.xlabel("Degree")
plt.legend()
sns.despine()
```

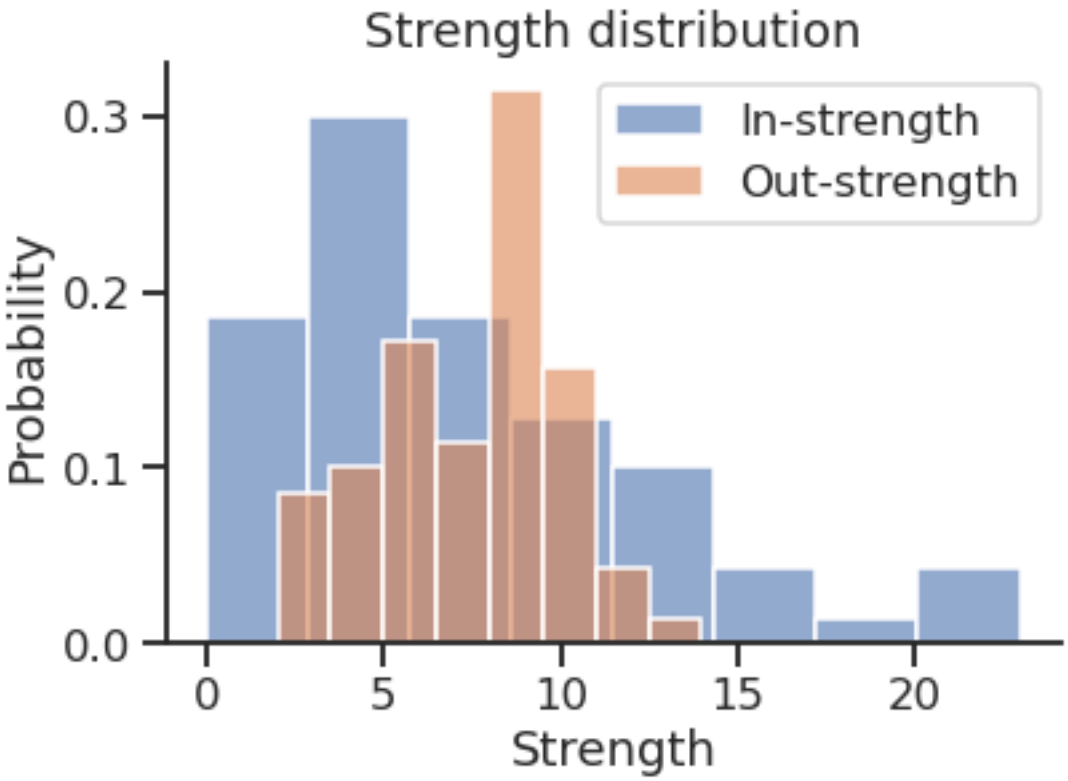


Get the in and out strength

[50]:
```
weight = g.edge_properties["weight"]

in_strength = g.get_in_degrees(g.get_vertices(), eweight=weight)

out_strength = g.get_out_degrees(g.get_vertices(), eweight=weight)
```

[51]:
```
sns.histplot(in_strength,
             stat="probability",
             discrete=False,
             label="In-strength",
             legend=True,
             color=cmap[0],
             alpha=0.6,
)
```

```
sns.histplot(out_strength,
             stat="probability",
             discrete=False,
             label="Out-strength",
             legend=True,
             color=cmap[1],
             alpha=0.6,
)

plt.title("Strength distribution")
plt.xlabel("Strength")
plt.legend()
sns.despine()
```



5.1.1 Store the values as a DataFrame

[52]:
```
df = pd.DataFrame(
    data={
        ("Degree", "In"): in_degree,
        ("Degree", "Out"): out_degree,
```

```
        ("Strength", "In"): in_strength,
        ("Strength", "Out"): out_strength,
    },
)

df.head()
```

[52]:

	Degree		Strength	
	In	Out	In	Out
0	2	6	2	8
1	2	3	3	4
2	2	4	3	5
3	12	6	19	9
4	13	5	21	9

5.1.2 ... and plot the DF using *Seaborn*

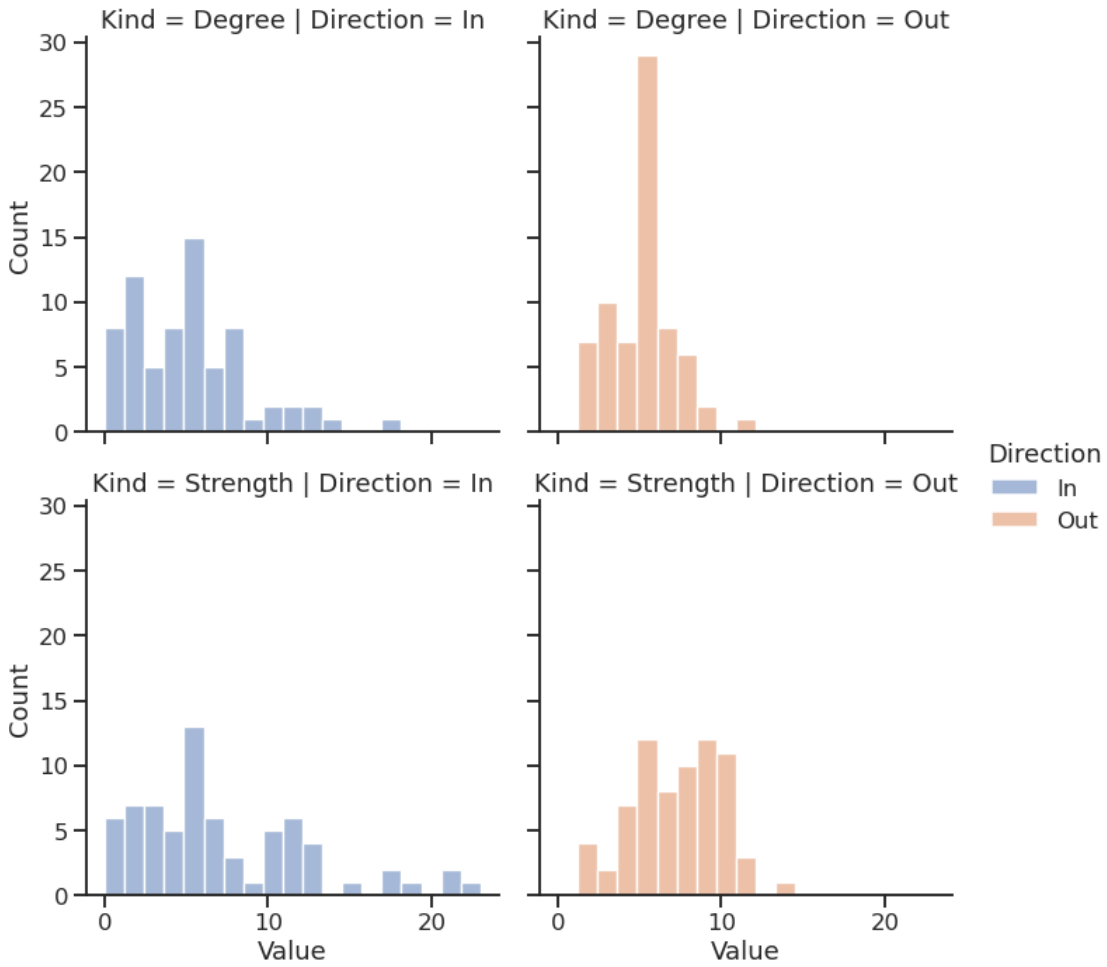
[53]:
```
melted_df = pd.melt(df, var_name=["Kind", "Direction"], value_name="Value")

melted_df
```

[53]:

	Kind	Direction	Value
0	Degree	In	2.0
1	Degree	In	2.0
2	Degree	In	2.0
3	Degree	In	12.0
4	Degree	In	13.0
..	…	…	…
275	Strength	Out	7.0
276	Strength	Out	10.0
277	Strength	Out	10.0
278	Strength	Out	4.0
279	Strength	Out	5.0

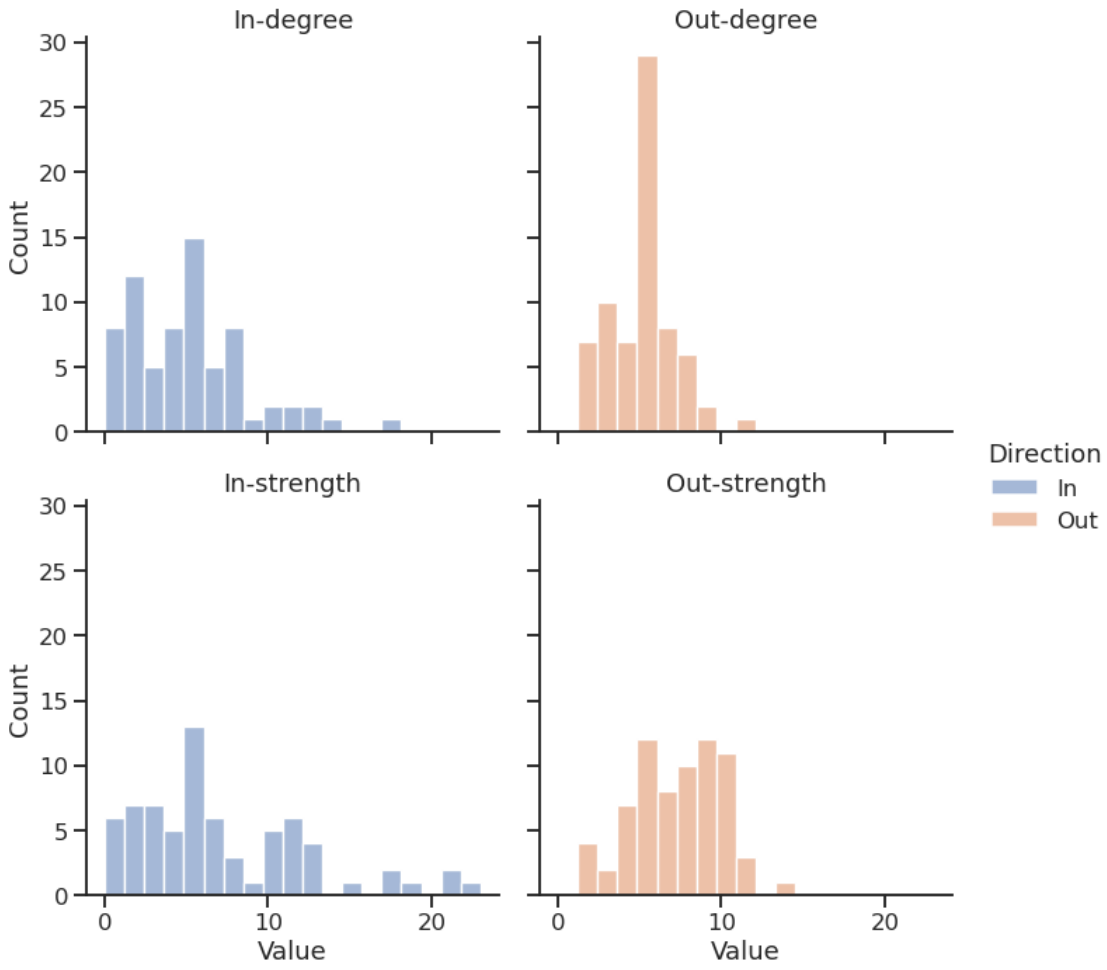
[280 rows x 3 columns]

[54]:
```
facet = sns.displot(melted_df,
                    x="Value",
                    kind="hist",
                    row="Kind",
                    col="Direction",
                    hue="Direction",
                    )
```



[55]:
```
melted_df["Kind"] = melted_df["Kind"].apply(str.lower)

facet = sns.displot(melted_df,
                    x="Value",
                    kind="hist",
                    row="Kind",
                    col="Direction",
                    hue="Direction",
                    )

facet.set_titles(template="{col_name}-{row_name}")
```

[55]: <seaborn.axisgrid.FacetGrid at 0x7f1ecf5c6610>



5.2 Graph visualization

1. Compute the node layout

[56]:
```
pos = gt.fruchterman_reingold_layout(g, n_iter=1000)
```

2. Plot the network

[57]:
```
gt.graph_draw(g, pos=pos,
              bg_color="#111",
              )
```

[57]: <VertexPropertyMap object with value type 'vector<double>', for Graph 0x7f1ed41879d0, at 0x7f1ed41312b0>

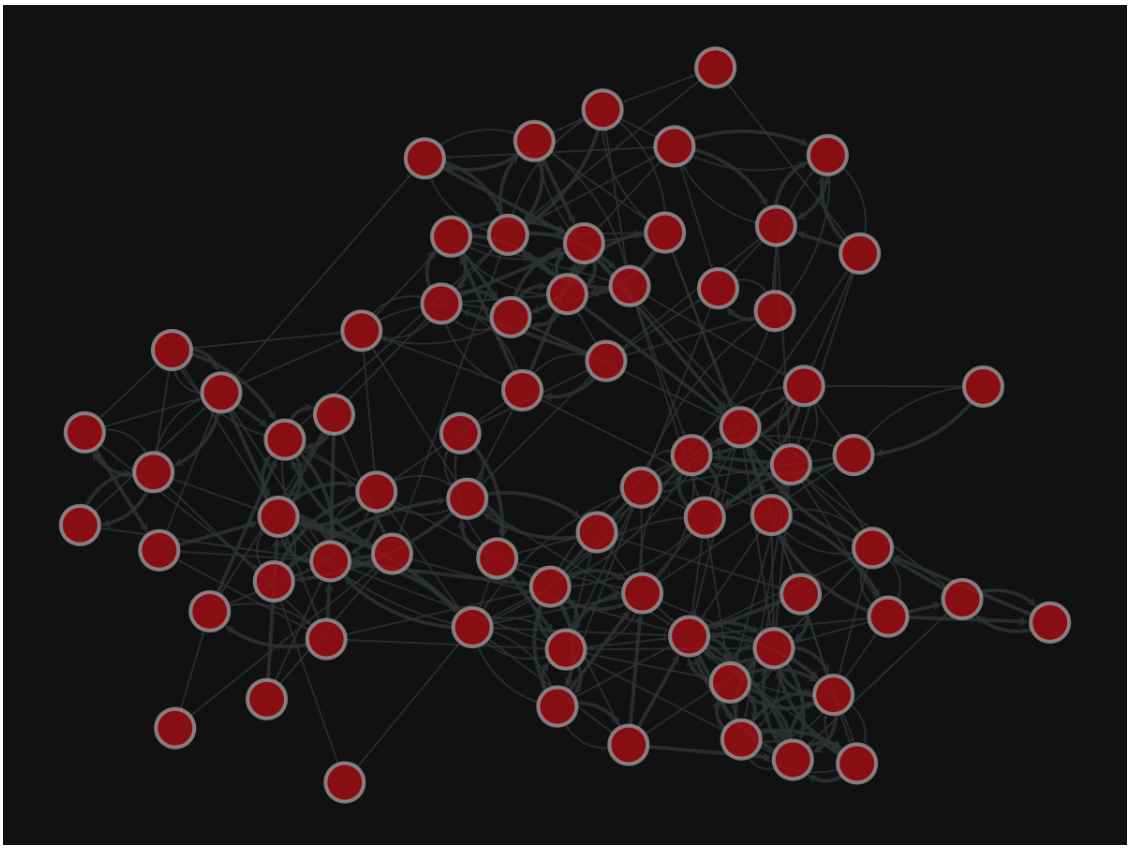
Add the edge weight

[58]:
```
gt.graph_draw(g,
              pos=pos,
              edge_pen_width=g.edge_properties["weight"],
              bg_color="#111",
              )
```

[58]:
```
<VertexPropertyMap object with value type 'vector<double>', for Graph
0x7f1ed41879d0, at 0x7f1ecf79e910>
```

More layouts

[59]:
```
pos = gt.sfdp_layout(g)

gt.graph_draw(g, pos=pos,
              edge_pen_width=g.edge_properties["weight"],
              bg_color="#111",
              )
```

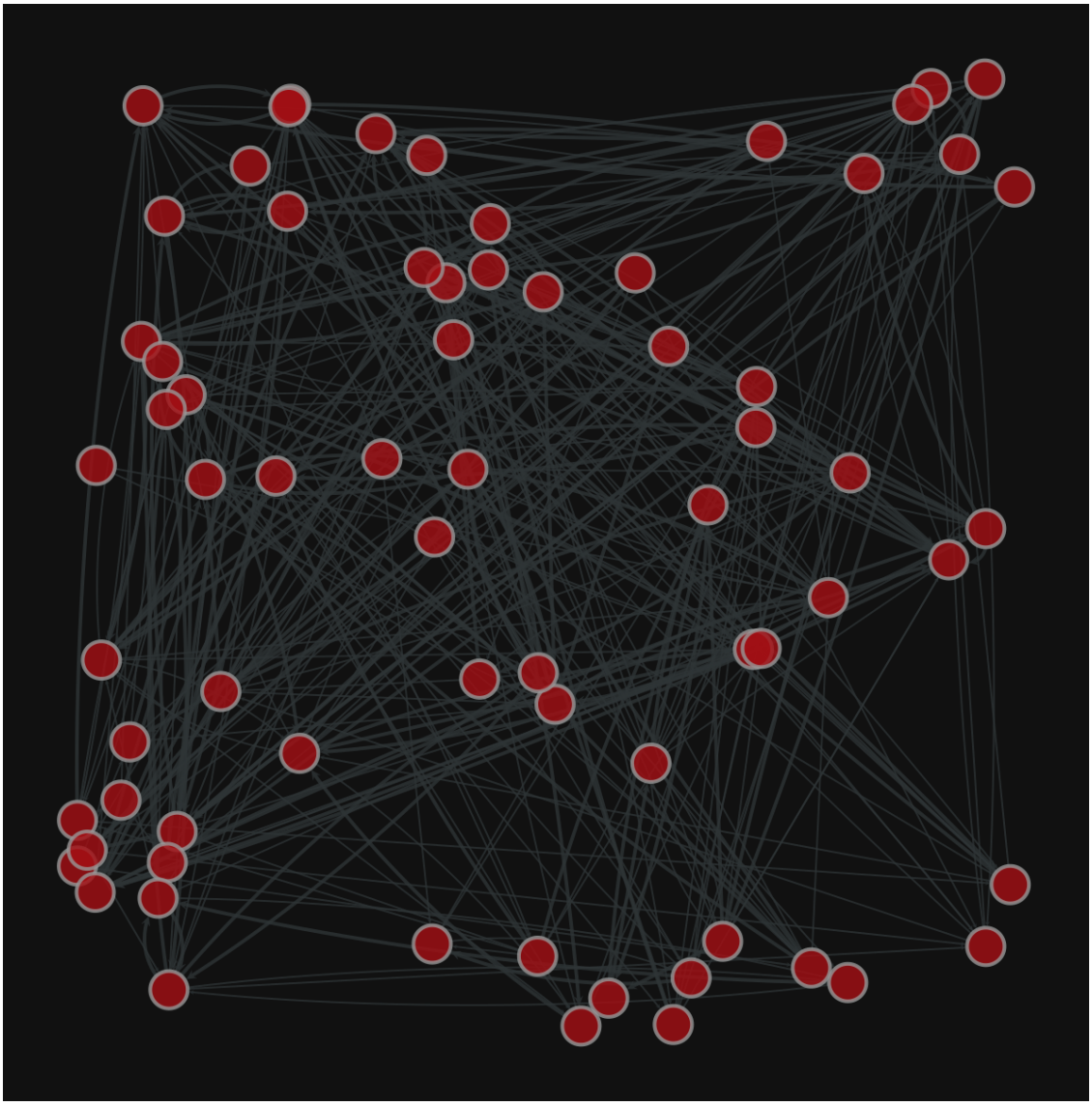


[59]:
```
<VertexPropertyMap object with value type 'vector<double>', for Graph
0x7f1ed41879d0, at 0x7f1ecf79eca0>
```

[60]:
```
pos = gt.arf_layout(g)

gt.graph_draw(g,
              pos=pos,
              bg_color="#111",
              )
```

[60]:
```
<VertexPropertyMap object with value type 'vector<double>', for Graph
0x7f1ed41879d0, at 0x7f1ed411b9a0>
```

[61]:
```
pos = gt.random_layout(g)

gt.graph_draw(g,
              pos=pos,
              edge_pen_width=g.edge_properties["weight"],
              bg_color="#111",
              )
```



[61]:
```
<VertexPropertyMap object with value type 'vector<double>', for Graph
0x7f1ed41879d0, at 0x7f1ecf645ac0>
```

5.3 Centrality computation

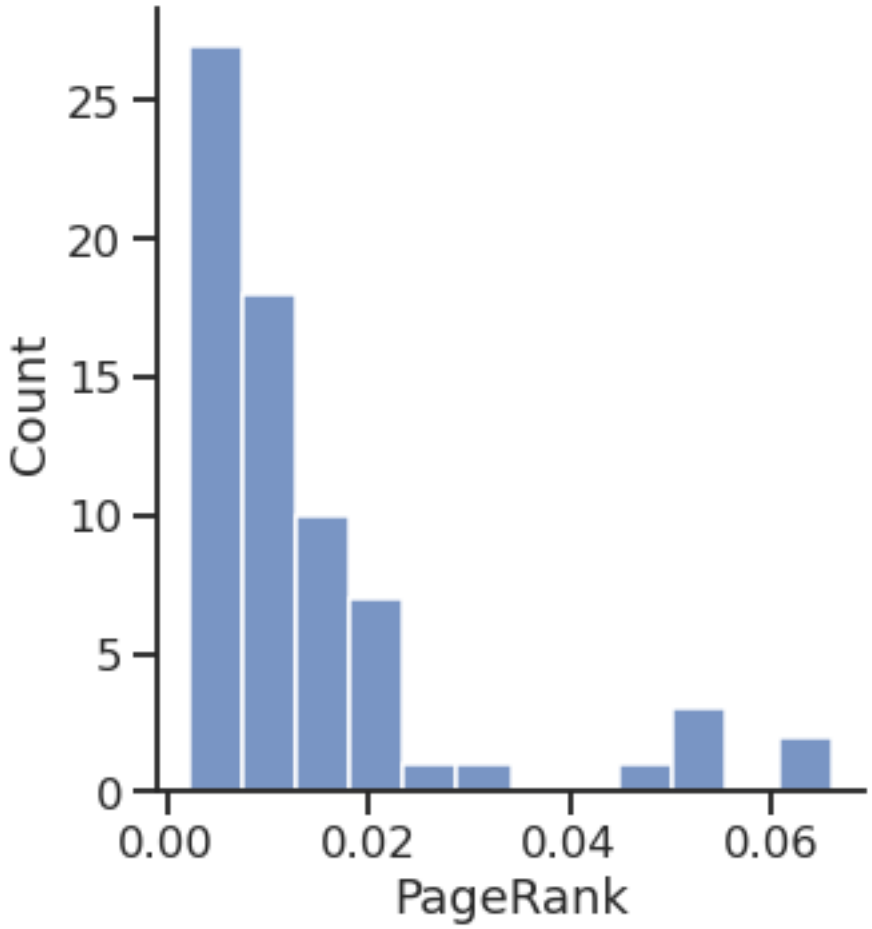
[62]:
```
gw = gt.GraphView(g, vfilt=gt.label_largest_component(g))
```

PageRank

[63]:
```
pr = gt.pagerank(g)
```

[64]:
```
sns.displot(pr.a)
plt.xlabel("PageRank")
```

[64]: Text(0.5, 15.439999999999998, 'PageRank')

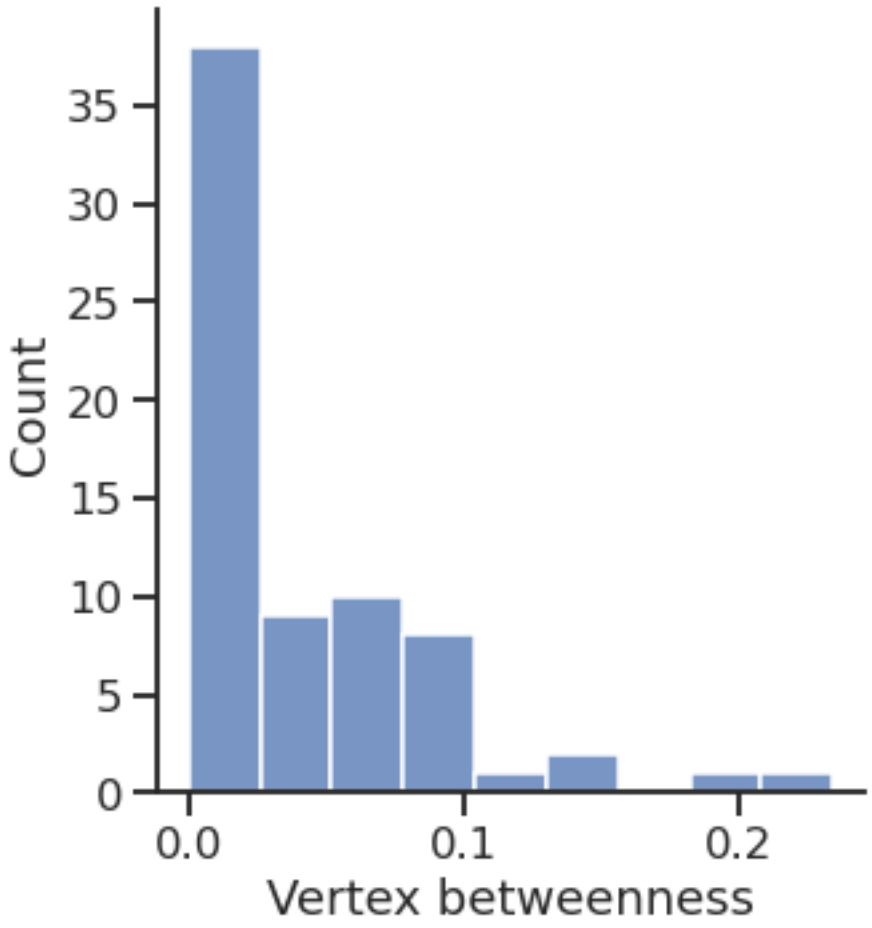


Betweenness

[65]:
```
vertex_betweenness, edge_betweenness =  gt.betweenness(g)
```

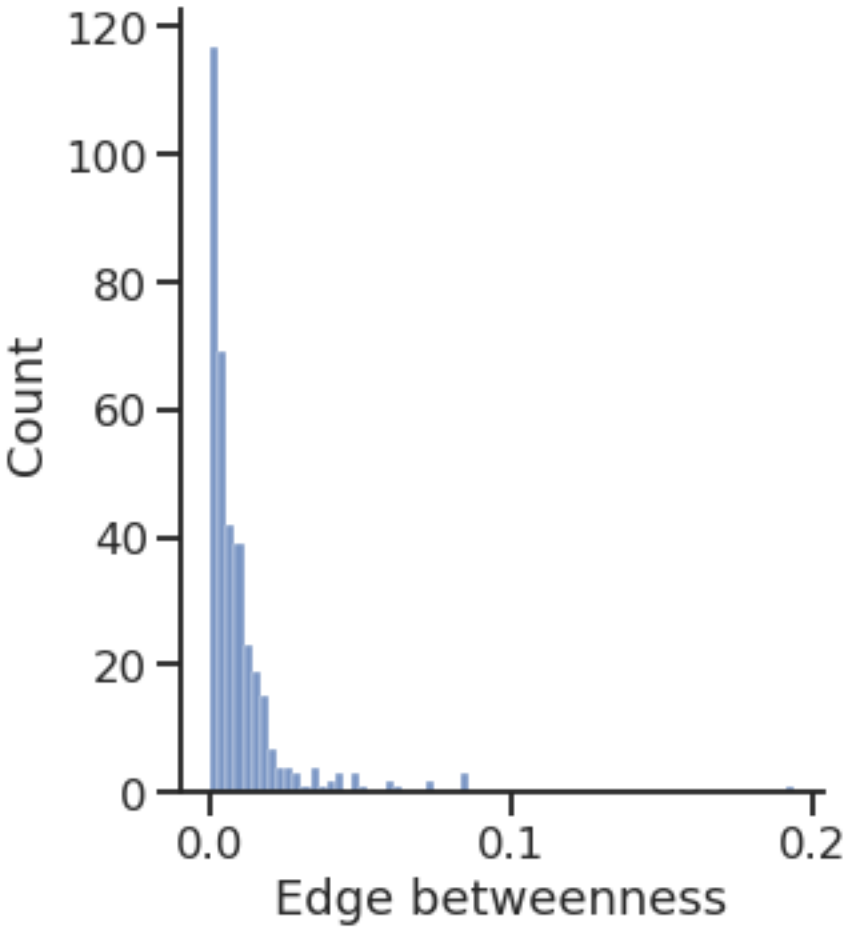
[66]:
```
sns.displot(vertex_betweenness.a)
plt.xlabel("Vertex betweenness")
```

[66]: Text(0.5, 15.439999999999998, 'Vertex betweenness')

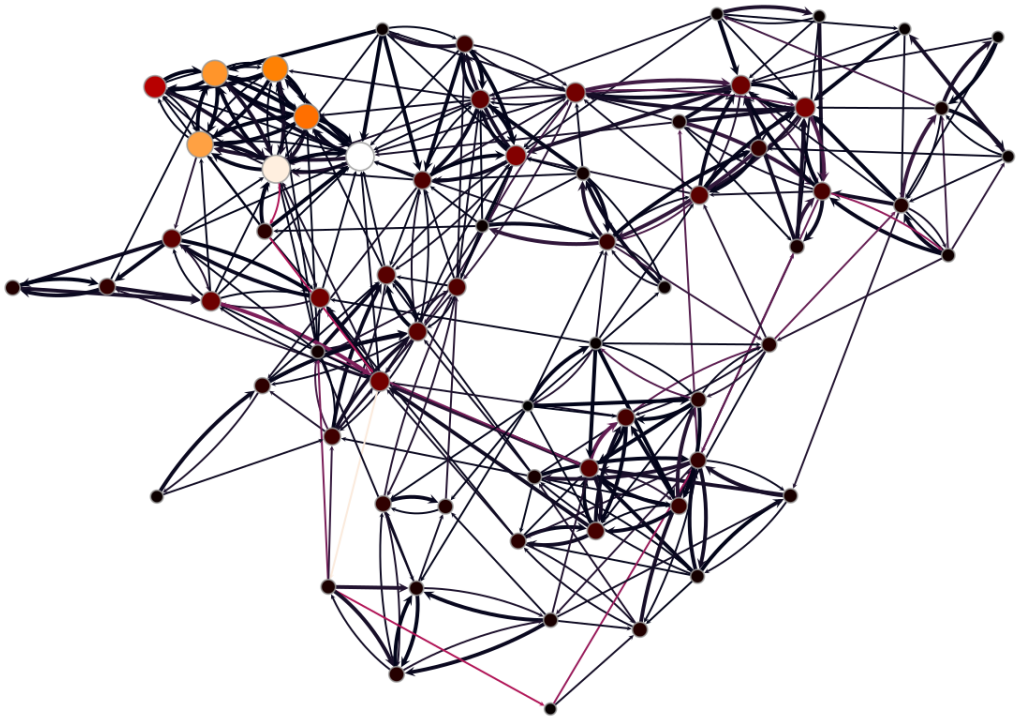


[67]:
```
sns.displot(edge_betweenness.a)
plt.xlabel("Edge betweenness")
```

[67]:
```
Text(0.5, 15.439999999999998, 'Edge betweenness')
```



[68]:
```
gt.graph_draw(gw,
              pos=g.vp["_pos"],
              vertex_fill_color=pr, vorder=pr,
              edge_color=edge_betweenness,
              vertex_size=gt.prop_to_size(pr, mi=5, ma=15),
              vcmap=sns.color_palette("gist_heat", as_cmap=True),
              ecmap=sns.color_palette("rocket", as_cmap=True),
              edge_pen_width=g.edge_properties["weight"],
              bg_color="white",
              )
```

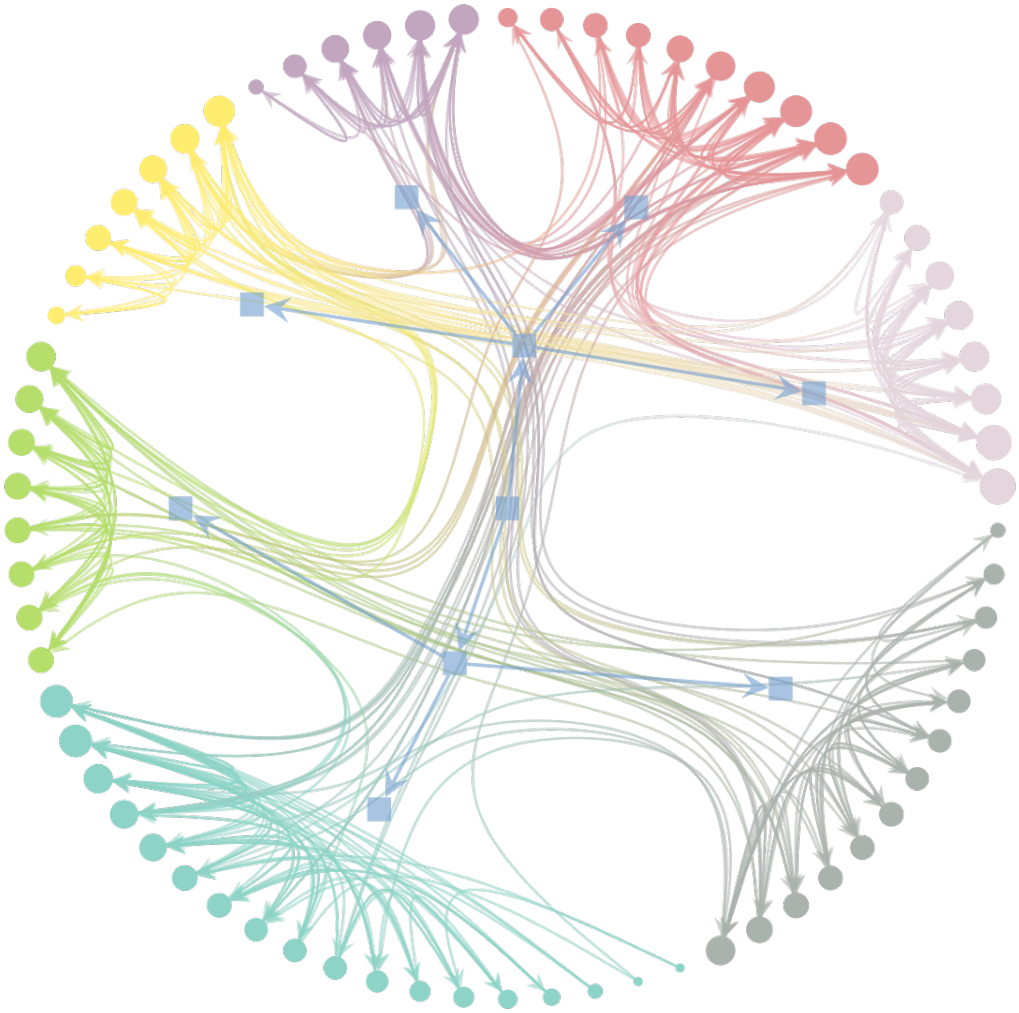


[68]:
```
<VertexPropertyMap object with value type 'vector<double>', for Graph
0x7f1ed4113fa0, at 0x7f1ed40db340>
```

5.4 Inferring modular structure

[69]:
```
# state = gt.minimize_blockmodel_dl(g)
state = gt.minimize_nested_blockmodel_dl(g)
```

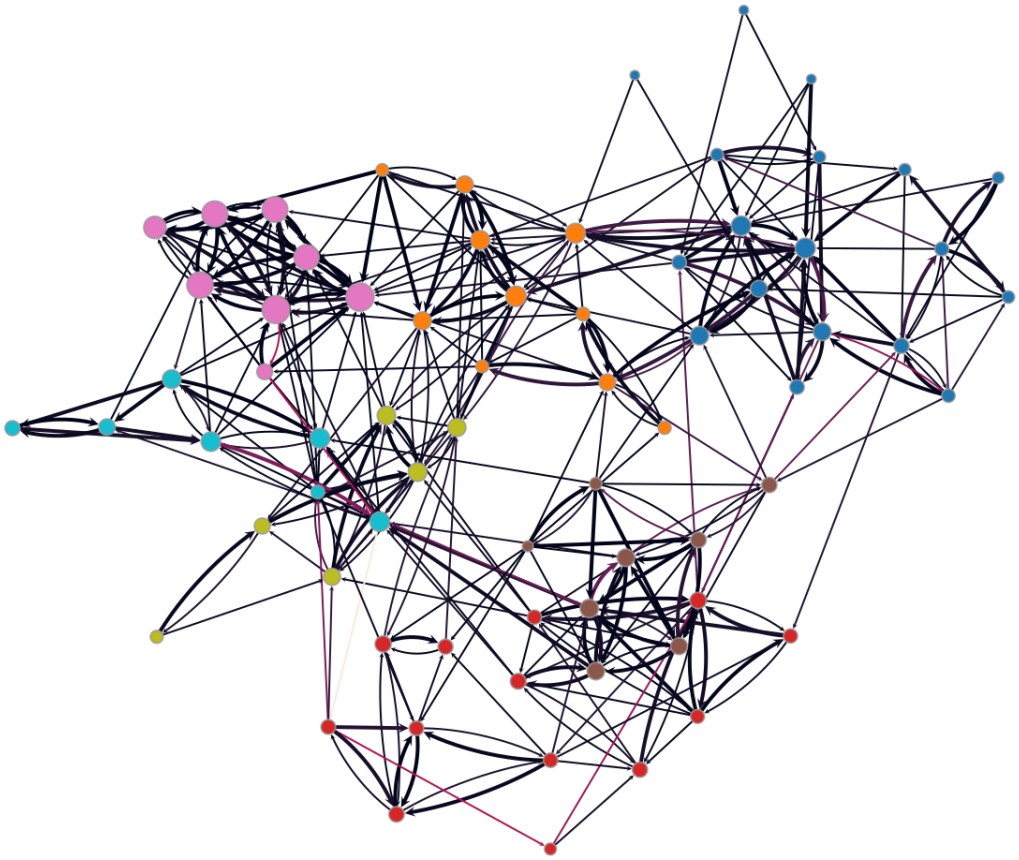
[70]:
```
state.draw()
```



[70]:
```
(<VertexPropertyMap object with value type 'vector<double>', for Graph
0x7f1ed41879d0, at 0x7f1ecf7d77c0>,
 <GraphView object, directed, with 80 vertices and 79 edges, edges filtered by
(<EdgePropertyMap object with value type 'bool', for Graph 0x7f1ecf32dfa0, at
0x7f1ecf338040>, False), vertices filtered by (<VertexPropertyMap object with
value type 'bool', for Graph 0x7f1ecf32dfa0, at 0x7f1ecf330ee0>, False), at
0x7f1ecf32dfa0>,
 <VertexPropertyMap object with value type 'vector<double>', for Graph
0x7f1ecf32dfa0, at 0x7f1ecf330eb0>)
```

[71]:
```
levels = state.get_levels()
```

[72]:
```
gt.graph_draw(g,
              pos=g.vp["_pos"],
              vertex_fill_color=levels[0].get_blocks(),
              edge_color=edge_betweenness,
              vertex_size=gt.prop_to_size(pr, mi=5, ma=15),
              vorder=pr,
              vcmap=sns.color_palette("tab10", as_cmap=True),
              ecmap=sns.color_palette("rocket", as_cmap=True),
              edge_pen_width=g.edge_properties["weight"],
              bg_color="white",
              )
```



[72]:
```
<VertexPropertyMap object with value type 'vector<double>', for Graph
0x7f1ed41879d0, at 0x7f1ecf3c9310>
```

5.4.1 Add some columns to our DataFrame

[73]:
```
df["PageRank"] = pr.a

df["Betweenness"] = vertex_betweenness.a

df["Block"] = levels[0].get_blocks().a

df.head()
```

[73]:

	Degree		Strength		PageRank	Betweenness	Block
	In	Out	In	Out			
0	2	6	2	8	0.003871	0.024913	44
1	2	3	3	4	0.003502	0.002819	44
2	2	4	3	5	0.003602	0.005649	44
3	12	6	19	9	0.020530	0.081323	44
4	13	5	21	9	0.022862	0.079074	44

5.4.2 Save the DataFrame

To CSV (Comma Separated Values)

[74]:
```
df.to_csv("dataframe.csv")
```

To Excel

[75]:
```
df.to_excel("dataframe.xlsx")
```

5.5 PyTorch Geometric (PyG)

> *PyG* is a library built upon *PyTorch* to easily write and train *Graph Neural Networks* (GNNs) for a wide range of applications related to structured data.

Library for Deep Learning on graphs

It provides a large collection of GNN and pooling layers

New layers can be created easily

It offers: - Support for Heterogeneous and Temporal graphs - Mini-batch loaders - Multi GPU-support - DataPipe support - Distributed graph learning via Quiver - A large number of common benchmark datasets - The GraphGym experiment manager

PyTorch Geometric documentation

5.5.1 Introduction by example

Each network is described by an instance of *torch_geometric.data.Data*, which includes: - *data.**x***: **node feature matrix**, with shape [num_nodes, num_node_features] - *data.**edge_index***: **edge list in COO format**, with shape [2, num_edges] and type *torch.long* - *data.**edge_attr***: *edge feature matrix*, with shape [num_edges, num_edge_features] - *data.**y***: target to train against (may have arbitrary shape)

[76]:
```
import torch

from torch_geometric.data import Data
```

Let's build our Data object

Node features We do not have any node feature

We can use a constant for each node, e.g., 1

[77]:
```
x = torch.ones(size=(g.num_vertices(), 1),
               dtype=torch.float32
    )

display(x.shape)

display(x.T)
```

```
torch.Size([70, 1])
```

```
tensor([[1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.,
         1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.,
         1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.,
         1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.]])
```

Connectivity matrix and edge attributes

[78]:
```
edge_index = torch.empty(size=(2, g.num_edges()),
                         dtype=torch.long,
)

display("edge_index", edge_index.shape)

edge_attr = torch.empty(size=(g.num_edges(),),
                        dtype=torch.float32,
)
display("edge_attr", edge_attr.shape)
```

```
'edge_index'
```

```
torch.Size([2, 366])
```

```
'edge_attr'
```

```
torch.Size([366])
```

[79]:
```
for i, (source, target, weight) in enumerate(g.iter_edges(eprops=[g.
 ↪edge_properties["weight"]])):
    edge_index[0, i] = source
    edge_index[1, i] = target
```

```
    edge_attr[i] = weight


display("edge_index", edge_index[:, :10])

display("edge_attr", edge_attr[:10])
```

```
'edge_index'
```

```
tensor([[ 0,  0,  0,  0,  0,  0,  1,  1,  1,  2],
        [ 1,  2,  3,  4,  5,  6, 18,  3,  4,  0]])
```

```
'edge_attr'
```

```
tensor([1., 2., 2., 1., 1., 1., 1., 1., 2., 1.])
```

Create the *Data* instance

[80]:
```
network_data = Data(
    x=x,
    edge_index=edge_index,
    edge_attr=edge_attr,
)

display(network_data)
```

```
Data(x=[70, 1], edge_index=[2, 366], edge_attr=[366])
```

5.5.2 Create the train and test set

For link prediction, we need positive (existent) and negative (non-existent) edges

We can use the *RandomLinkSplit* class, that does the *negative sampling* for us

[81]:
```
from torch_geometric.transforms import RandomLinkSplit

transform = RandomLinkSplit(num_val=0,
                            num_test=0.2,
                            disjoint_train_ratio=0.2,
                            split_labels=False,
                            add_negative_train_samples=True,
                            neg_sampling_ratio=1.0,
                            is_undirected=False,
)
train_data, _, test_data = transform(network_data)
```

[82]:
```
display(train_data)
```

```
Data(x=[70, 1], edge_index=[2, 235], edge_attr=[235], edge_label=[116],␣
↪edge_label_index=[2, 116])
```

[83]:
```
display(test_data)
```

```
Data(x=[70, 1], edge_index=[2, 293], edge_attr=[293], edge_label=[146],␣
↪edge_label_index=[2, 146])
```

Create the model Model architecture: - 2x GINE convolutional layers - 1x Multi-Layer Perceptron (MLP)

The GINE layers will compute the ***node embedding***

We can build the ***edge embedding*** by, e.g., concatenating the source and target nodes' embedding

The MLP will take the edge embeddings and return a probability for each

[84]:
```
from torch_geometric.nn import MLP

class MLP(MLP):

    def __getitem__(self, item):
        return self.lins[item]
```

[85]:
```
import torch.nn.functional as F
from torch_geometric.nn import GINEConv
from torch.nn import Sequential, Linear, ELU

class GINEModel(torch.nn.Module):
    def __init__(self, in_channels, hidden_channels, out_channels, edge_dim):
        super().__init__()
        self.conv1 = GINEConv(nn=MLP([in_channels, hidden_channels,␣
↪hidden_channels]),
                              train_eps=False, edge_dim=edge_dim,)

        self.conv2 = GINEConv(nn=MLP([hidden_channels, hidden_channels,␣
↪out_channels]),
                              train_eps=False, edge_dim=edge_dim,)

        self.edge_regression = MLP(channel_list=[2 * out_channels,␣
↪out_channels, 1],
                                   batch_norm=False, dropout=0.3)


    def forward(self, x, edge_index, target_edges):
        x = self.conv1(x=x, edge_index=edge_index, edge_attr=edge_attr)
        x = F.relu(x)
        x = self.conv2(x=x, edge_index=edge_index, edge_attr=edge_attr)
        x = F.relu(x)

        x = torch.hstack((
            x[target_edges[0, :]],
            x[target_edges[1, :]],
        ))
```

```
        x = self.edge_regression(x)

        return x
```

Let's create the model instance

[86]:
```
model = GINEModel(in_channels=network_data.x.shape[1],
                  hidden_channels=20,
                  out_channels=20,
                  edge_dim=network_data.edge_attr.shape[0],
)

display(model)
```

```
GINEModel(
  (conv1): GINEConv(nn=MLP(1, 20, 20))
  (conv2): GINEConv(nn=MLP(20, 20, 20))
  (edge_regression): MLP(40, 20, 1)
)
```

Create the optimizer and loss instances

[87]:
```
optimizer = torch.optim.Adam(params=model.parameters(), lr=0.005,␣
 ↪weight_decay=1e-4)
criterion = torch.nn.BCEWithLogitsLoss()
# criterion = torch.nn.MSELoss()

epoch = 0
```

Define the train function and train the model

[88]:
```
def train():
    model.train()
    optimizer.zero_grad()

    edge_probability = model(train_data.x, train_data.edge_index, train_data.
 ↪edge_label_index).squeeze()
    loss = criterion(edge_probability, train_data.edge_label)
    loss.backward()
    optimizer.step()

    return loss
```

Define the test function

[89]:
```
@torch.no_grad()
def test():
    model.eval()

    edge_probability = model(test_data.x, test_data.edge_index, test_data.
 ↪edge_label_index).squeeze()
```

```
    edge_probability = torch.sigmoid(edge_probability)

    return edge_probability, test_data.edge_label
```

5.5.3 Training and testing

[93]:
```
from tqdm import tqdm

for _ in tqdm(range(2001)):
    loss = train()

    if epoch % 500 == 0:
        display(f'Epoch: {epoch:03d}, Loss: {loss:.4f}')

    epoch += 1
```

```
 24%|
| 489/2001 [00:02<00:05, 262.96it/s]
'Epoch: 2500, Loss: 0.0881'
 50%|
| 991/2001 [00:04<00:04, 211.13it/s]
'Epoch: 3000, Loss: 0.1207'
 75%|
| 1495/2001 [00:06<00:01, 271.06it/s]
'Epoch: 3500, Loss: 0.0798'
 99%|
                    | 1973/2001 [00:08<00:00, 291.01it/s]
'Epoch: 4000, Loss: 0.0769'
100%|
                   | 2001/2001 [00:08<00:00, 241.67it/s]
```

[94]:
```
edge_probability, test_y = test()
```

5.5.4 Evaluate the model performance

The *torchmetrics* package provides many performance metrics for various tasks

It is inspired by *scikit-learn*'s *metrics* subpackage

[96]:
```
from torchmetrics import Accuracy, AUROC

accuracy = Accuracy(threshold=0.5)

auroc = AUROC()

display("Accuracy", accuracy(edge_probability, test_y.to(torch.int)).item())
display("AUROC", auroc(edge_probability, test_y.to(torch.int)).item())
```

```
'Accuracy'
```

```
0.6095890402793884
```

```
'AUROC'
```

```
0.6100582480430603
```