Constrained Optimization for Data Mining

Definitely niche, but also a great example

Constrained Optimization for Data Mining

Let's consider a data mining problem for web analytics

- A company wants to analyze user behavior on their web site
- ...With the goal of optimizing its structure
- For privacy reason, the company does not want to resort to tracking
- ...And plan to relies on simple page/link-click counts

Constrained Optimization for Data Mining

Our input consists of page and link counts for multiple time steps

t	0	1	...	0,1	0,3	1,2	...
0	35	12	...	21	7	9	...
1	42	14	...	22	11	10	...
2	38	9	...	17	10	8	...

- Each simple number refers to a page, each pair to a link
- Cells contain presence/link-click counts for different value of the time t

Our output consists of navigation paths on the web site

A path specifies which page is visited at every point of time, e.g.:

$$\{(2, 0), (3, 0), (4, 1), (5, 3)\}$$

- In this case the path starts at time 2, stays at page 0 for two time units
- ...Then moves to 1 and then 3

Constrained Optimization for Data Mining

How would you tackle the problem?

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The main issue is representing and handling paths

- A path is combinatorial object ($\Rightarrow$ not differentiable)
- Nodes in a path must be connected

In other words, the main issue is dealing with constraints

We will see how to tackle the problem directly via Constrained Optimization

- The approach will work well (though it will not be necessarily SotA)
- ...But more importantly we will see many CO methods in action!

Constrained Optimization for Data Mining

This is a very challenging problem!

- There are many viable paths!
- ...And we start with quite poor information

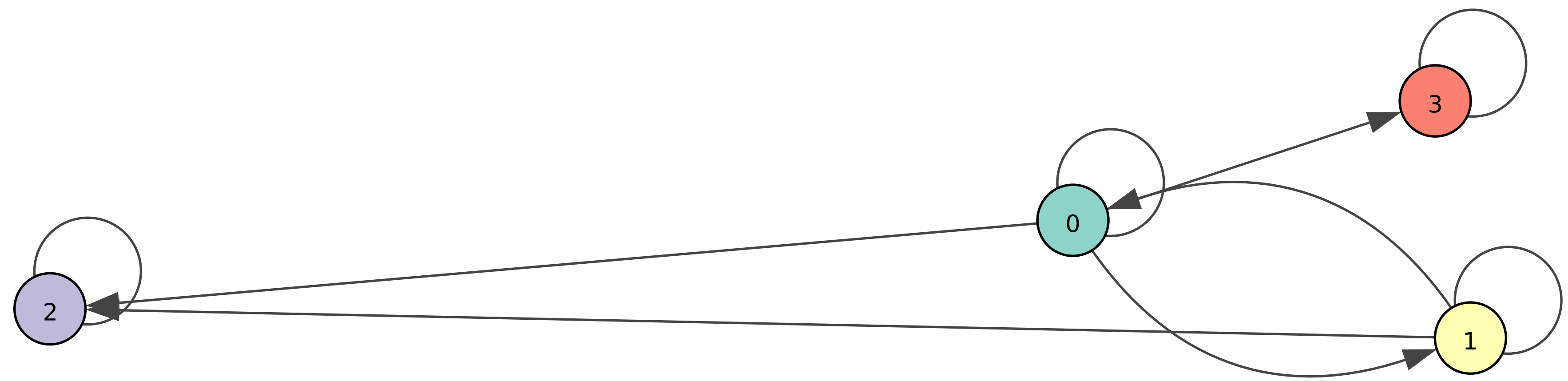
Web Site as Graph

Our web site can be represented as a directed graph

We will generate one at random, with a realistic structure

In [20]:
```
g = util.build_website_graph(nnodes=4, rate=3, extra_arc_fraction=0.25, seed=42)
ig.plot(g, **util.get_visual_style(g), bbox=(700, 200), margin=50)
```

Out[20]:



- The method generates `nnodes` vertexes in a tree structure as a base
- The #children per vertex follows a Poisson distribution with specified rate
- ...Then a fraction of the missing arcs is added at random

Web Site as Graph

Our web site can be represented as a directed graph

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In [13]:
```
g = util.build_website_graph(nnodes=4, rate=3, extra_arc_fraction=0.25, seed=42)
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```
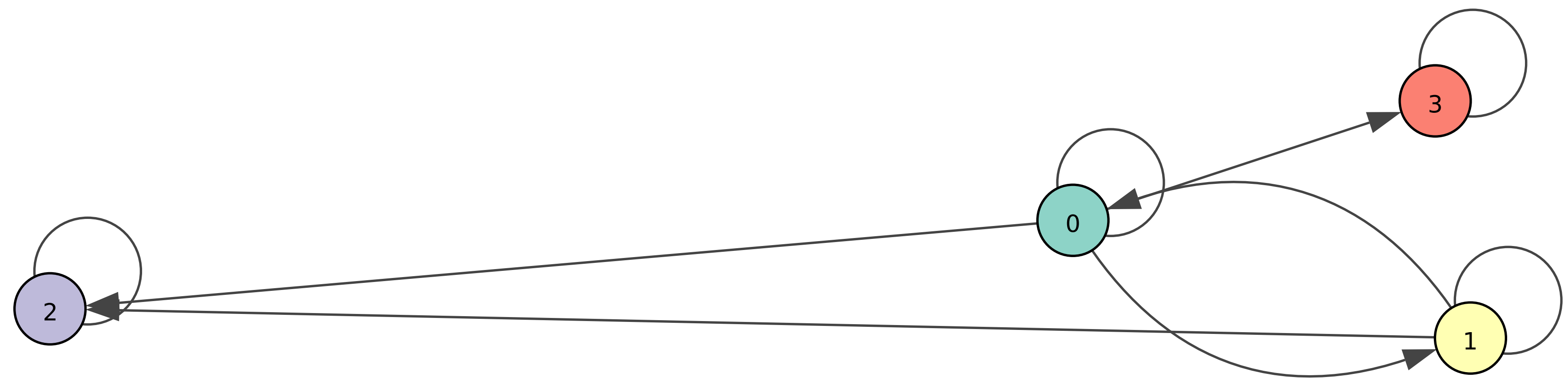

Out[13]:



- The graph is handled via the python-igraph library
- ...Which provides a fast C++ implementation of many graph primitives
- The library also include a good selection of graph algorithms

Ground Truth Generation

We obtain realistic counts by routing "flow" along random paths

For one path, this can be done via a function from the utility module:

```
In [21]: home = g.vs[0] # Home page
         eoh = 4 # End of Horizon

         flow, path = util.route_random_flow(home, min_units=1, max_units=10, eoh=eoh, seed=10)
         print(f'{flow:.2f}: {">".join(str(v) for v in path)}')

3.69: (1, 0)>(2, 3)>(3, 3)
```

- The first vertex represents the home page
- The "flow" represents the amount of users that traverse the path
- `eoh` is the number of time units over which we assume to have counts

Ground Truth Generation

A second function performs random routing for multiple paths

We will start from a simple example with a very small number of paths:

```
In [22]: flows, paths = util.build_random_paths(g, min_paths=3, max_paths=5,
                                                min_units=1, max_units=10, eoh=eoh, seed=42)
         print('FLOW: PATH')
         util.print_ground_truth(flows, paths, sort='descending')
```

```
FLOW: PATH
8.17: 2,3 > 3,3
5.47: 0,2 > 1,2 > 2,2 > 3,2
4.89: 0,1 > 1,1 > 2,0 > 3,0
3.74: 3,3
3.32: 1,0 > 2,0 > 3,2
```

- Paths may start from any page
- Paths may start at any time step within the horizon

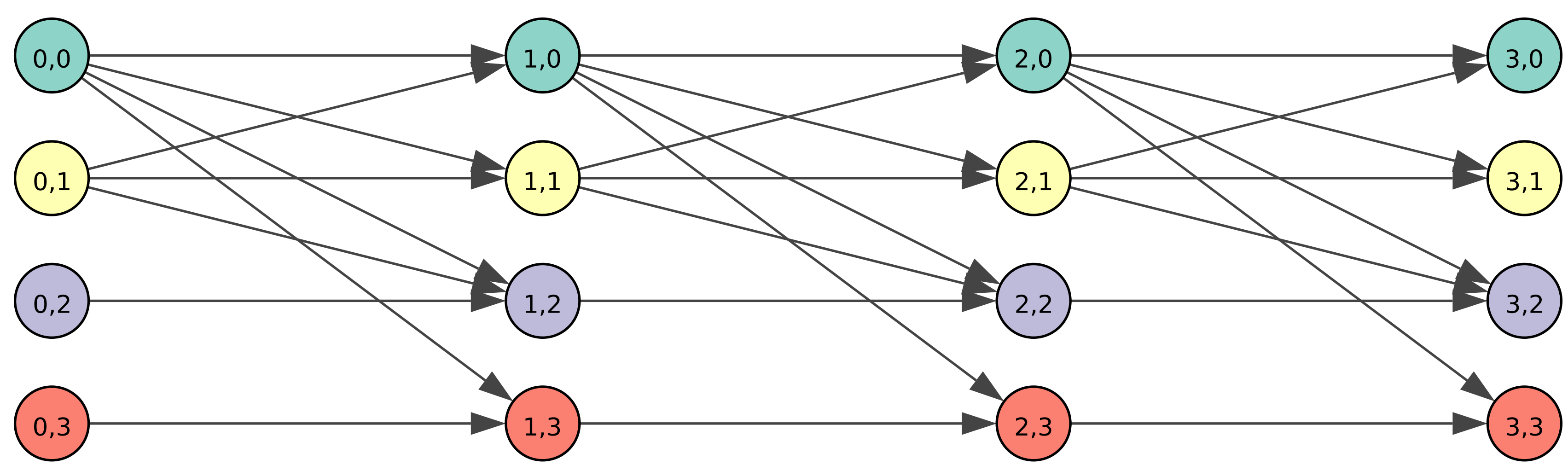
The generated paths represent our ground truth

Time-Unfolded Graph

Our paths may be see as traversal of a time-unfolded version of the graph

In [16]:
```
tug = util.build_time_unfolded_graph(g, eoh=eoh)
ig.plot(tug, **util.get_visual_style(tug), bbox=(700, 250), margin=50)
```

Out[16]:



- We create `eoh` replicas of the vertexes, each referring to a specific time step
- We create `eoh` replicas of the edges, linking vertexes in adjacent time step

This representation is referred to as Time Unfolded Graph

Computing Counts

We can now compute counts for all vertexes and edges in the TUG

In [23]:
```
node_counts, arc_counts = util.get_counts(tug, flows, paths)
print('NODE COUNTS')
print('\t'.join(f'{k}:{v:.2f}' for k, v in node_counts.items()))
print('ARC COUNTS')
print('\t'.join(f'{k}:{v:.2f}' for k, v in arc_counts.items()))
```

```
NODE COUNTS
(0, 0):0.00     (0, 1):4.89     (0, 2):5.47     (0, 3):0.00     (1, 0):3.32     (1, 1):4.89
(1, 2):5.47     (1, 3):0.00     (2, 0):8.22     (2, 1):0.00     (2, 2):5.47     (2, 3):8.17
(3, 0):4.89     (3, 1):0.00     (3, 2):8.79     (3, 3):11.91
ARC COUNTS
(1, 0, 0):0.00  (1, 0, 1):0.00  (1, 1, 1):4.89  (1, 0, 2):0.00  (1, 2, 2):5.47  (1, 0, 3):0.00
(1, 3, 3):0.00  (1, 1, 0):0.00  (1, 1, 2):0.00  (2, 0, 0):3.32  (2, 0, 1):0.00  (2, 1, 1):0.00
(2, 0, 2):0.00  (2, 2, 2):5.47  (2, 0, 3):0.00  (2, 3, 3):0.00  (2, 1, 0):4.89  (2, 1, 2):0.00
(3, 0, 0):4.89  (3, 0, 1):0.00  (3, 1, 1):0.00  (3, 0, 2):3.32  (3, 2, 2):5.47  (3, 0, 3):0.00
(3, 3, 3):8.17  (3, 1, 0):0.00  (3, 1, 2):0.00
```

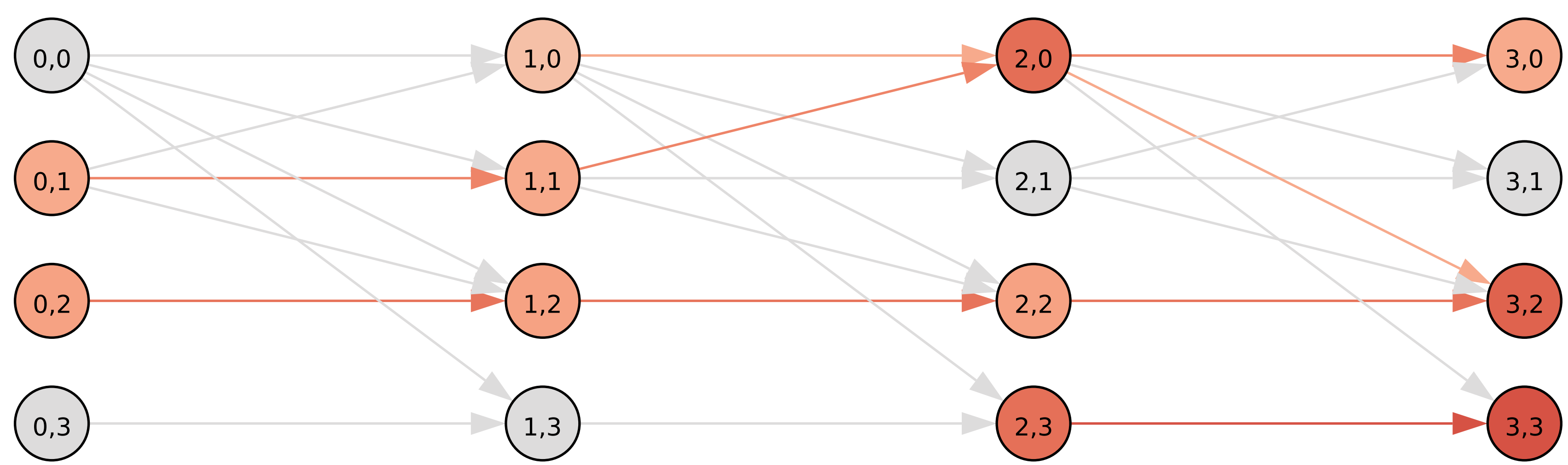
- TUG nodes/vertexes are labeled with $(time, node)$ pairs
- TUG ares are labeled with $(time, source, destination)$ triplets

Computing Counts

We can inspect the arc counts visually on the TUG

In [24]:
```
visual_style = util.get_visual_style(tug, vertex_weights=node_counts, edge_weights=arc_counts)
ig.plot(tug, **visual_style, bbox=(700, 250), margin=50)
```

Out[24]:



- A grey shade corresponds to lower counts
- A red shade corresponds to higher counts

These counts are our available information

Problem Formulation

By far the most important step of any solution process

Problem Formulation

Every good approach starts with a problem formulation

- If you don't have a formulation
- Odds are that you will come up with a patched-up solution

Let's try to come up with a formulation for our problem!

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Let's try to come up with a formulation for our problem!

We can introduce a variable x_j for each path

- The value of x_j represents the flow associated to the path
- Then we can compute the estimated count per TUG node/arc
- ...By simply summing the x_j values of paths that pass through the node/arc

Problem Formulation

Every good approach starts with a problem formulation

- If you don't have a formulation
- Odds are that you will come up with a patched-up solution

Let's try to come up with a formulation for our problem!

This approach is remarkably simple

- Computing counts is easy
- Connectivity constraints are safisfied by construction

Basically, we handle some constraints in the problem formulation itself

This is a first, powerful, and underestimated method to deal with constraints

Path Formulation

We will call this approch the path formulation

Formally, our problem can be stated as:

$$\arg\min_x \left\{ \|Vx - \hat{v}\|_2^2 + \|Ex - \hat{e}\|_2^2 \mid x \geq 0 \right\}$$

- For simplicity, here we use linear indexes for TUG nodes and arcs
- V is a matrix such that $V_{ij} = 1$ iff path j passes through node i
- E is a matrix such that $E_{kj} = 1$ iff path j passes through arc k

Path variables cannot be negative (it would make no sense)

- Hence the path formulation is itself a constrained optimization problem
- ...Though the constraints are in this case very simple

Problem Reduction

For an squared L2 norm in the form $\|Ax - b\|_2^2$ we have that:

$$\begin{aligned}
\|Ax - b\|_2^2 &= (Ax - b)^T(Ax - b) \\
&= x^T A^T A x - x^T A^T b - b^T A x + b^T b \\
&\propto \frac{1}{2} x^T (A^T A) x - \frac{1}{2} x^T A^T b - \frac{1}{2} b^T A x \\
&= \frac{1}{2} x^T (A^T A) x + (-A^T b)^T x
\end{aligned}$$

- This is true since $x^T A^T b$ and $b^T A x$ are scalar
- ...And $y^T x = x^T y$ if the quantity is a scalar
- The scaling factor $1/2$ will become convenient later

This reduction is valid for any least squares problem

Problem Reduction

We can use the relation to reduce our problem to a more compact form

In particular, we have that:

$$
\begin{aligned}
&\|Vx - \hat{v}\|_2^2 + \|Ex - \hat{e}\|_2^2 \\
&\propto \frac{1}{2}\|Vx - \hat{v}\|_2^2 + \frac{1}{2}\|Ex - \hat{e}\|_2^2 \\
&= \frac{1}{2}x^T(V^TV)x + (-V^T\hat{v})^T x + \frac{1}{2}x^T(E^TE)x + (-E^T\hat{e})^T x \\
&= \frac{1}{2}x^T P x + q^T x
\end{aligned}
$$

- Where $P = V^TV + E^TE$
- ...And $q = -V^T\hat{v} - E^T\hat{e}$

Path Formulation as Convex Quadratic Programming

Therefore, the path formulation can be reduced to:

$$\arg\min_x \left\{ \frac{1}{2} x^T P x + q^T x \mid x \geq 0 \right\}$$

...Which is a quadratic program

- I.e. a problem where we want to minimize a quadratic form
- ...Subject to linear constraints

Our problem is also convex

- This is true since $P = V^T V + E^T E$
- ...And it is therefore guaranteed semi-definite positive

Convex quadratic programs can be solved in polynomial time