Constraints for Regularization

Where there's room for one elephant, there's room for two

Something Fishy is Going On

Notice how we are consistently getting 0 RSSE?

```
In [2]: rflows, rpaths = util.solve_path_selection_full(tug, node_counts, arc_counts, verbose=0, so
        print('FLOW: PATH')
        util.print_solution(tug, rflows, rpaths, sort='descending')
        sse = util.get_reconstruction_error(tug, rflows, rpaths, node_counts, arc_counts)
        print(f'\nRSSE: {np.sqrt(sse):.2f}')
```

```
FLOW: PATH
8.17: 2,3 > 3,3
5.47: 0,2 > 1,2 > 2,2 > 3,2
3.74: 3,3
3.10: 0,1 > 1,1 > 2,0 > 3,0
1.79: 1,0 > 2,0 > 3,0
1.79: 0,1 > 1,1 > 2,0 > 3,2
1.53: 1,0 > 2,0 > 3,2

RSSE: 0.00
```

Something Fishy is Going On

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```
In [2]: rflows, rpaths = util.solve_path_selection_full(tug, node_counts, arc_counts, verbose=0, so
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```

```
FLOW: PATH
8.17: 2,3 > 3,3
5.47: 0,2 > 1,2 > 2,2 > 3,2
3.74: 3,3
3.10: 0,1 > 1,1 > 2,0 > 3,0
1.79: 1,0 > 2,0 > 3,0
1.79: 0,1 > 1,1 > 2,0 > 3,2
1.53: 1,0 > 2,0 > 3,2

RSSE: 0.00
```

How can that be the case?

The Must be Some Noise in Your Dataset

So far, we have implicitly assumed noiseless data

We will fix that by adding some proportional noise

- Which we picked since it is reasonably realistic
- ...Even if it causes issues for our MSE loss

This is done in the `add_proportional_noise` function:

```
# Add noise to the node counts
for k, v in node_counts.items():
    node_counts[k] = max(0, v * (1 + np.random.normal(0, sigma)))
# Add noise to the arc counts
for k, v in arc_counts.items():
    arc_counts[k] = max(0, v * (1 + np.random.normal(0, sigma)))
```

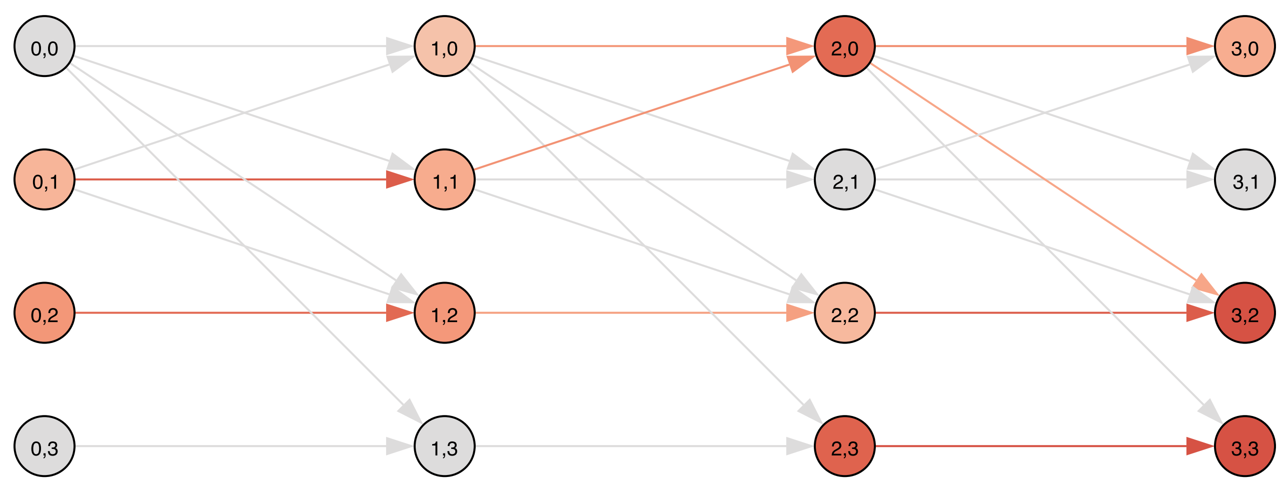
- The `sigma` parameter controls the noise level

There Must be Some Noise in Your Dataset

Let's inject a lot of noise and inspect the results

In [3]:
```
node_counts_n, arc_counts_n = util.add_proportional_noise(node_counts, arc_counts, sigma=0.
visual_style = util.get_visual_style(tug, vertex_weights=node_counts_n, edge_weights=arc_co
ig.plot(tug, **visual_style, bbox=(700, 300), margin=50)
```

Out[3]:



Solving the Noisy Path Formulation

Let's try to solve the path formulation with noisy data

In [4]:
```
rflows_n, rpaths_n = util.solve_path_selection_full(tug, node_counts_n, arc_counts_n, verbos
print('FLOW: PATH')
util.print_solution(tug, rflows_n, rpaths_n, sort='descending', max_paths=15)
sse = util.get_reconstruction_error(tug, rflows_n, rpaths_n, node_counts_n, arc_counts_n)
print(f'RSSE: {np.sqrt(sse):.2f}')
```

```
FLOW: PATH
7.28: 2,3 > 3,3
4.49: 3,3
3.02: 0,2 > 1,2 > 2,2 > 3,2
2.22: 0,1 > 1,1 > 2,0 > 3,0
2.19: 0,2 > 1,2
2.08: 3,2
1.48: 1,0 > 2,0 > 3,2
1.47: 1,0 > 2,0 > 3,0
1.43: 2,3
1.28: 2,2 > 3,2
1.27: 0,1 > 1,1 > 2,0 > 3,2
0.90: 0,1 > 1,1
0.84: 0,2
0.60: 3,0
0.45: 1,0 > 2,0
...
RSSE: 1.64
```

Solving the Noisy Path Formulation

There some very noticeable differences w.r.t. the baseline

- The RSSE is a bit higher, which could be expected
- But there are also many more paths, and they tend to be shorter

What is going on?

Solving the Noisy Path Formulation

There some very noticeable differences w.r.t. the baseline

- The RSSE is a bit higher, which could be expected
- But there are also many more paths, and they tend to be shorter

What is going on?

We have overfitting issues

- Our data-mining model is almost free of bias (we can use any possible path)
- Hence, the model tries to cover all nodes with many, short, paths

Can we do something about it?

L1 Regularization, Put to Its Purpose

We know that we can use an L1 regularizer to encourage longer paths

...After all, L1 and L2 regularization were born to counter overfitting

In [5]:
```
rflows_n2, rpaths_n2 = util.solve_path_selection_full(tug, node_counts_n, arc_counts_n, alpl
print('FLOW: PATH')
util.print_solution(tug, rflows_n2, rpaths_n2, sort='descending')
sse = util.get_reconstruction_error(tug, rflows_n2, rpaths_n2, node_counts_n, arc_counts_n)
print(f'RSSE: {np.sqrt(sse):.2f}')
```

```
FLOW: PATH
7.92: 2,3 > 3,3
4.80: 0,2 > 1,2 > 2,2 > 3,2
2.04: 0,1 > 1,1 > 2,0 > 3,0
1.87: 0,1 > 1,1 > 2,0 > 3,2
1.35: 1,0 > 2,0 > 3,2
1.35: 1,0 > 2,0 > 3,0
0.55: 0,1 > 1,1 > 2,0 > 3,3
0.46: 1,0 > 2,0 > 3,3
RSSE: 4.96
```

We get fewer, longer paths, at the expense of a higher RSSE

L1 Regularization, Put to Its Purpose

As usual, we can try to improve our results via consolidation

In [6]:
```
node_counts_r, arc_counts_r = util.get_counts(tug, rflows_n2, rpaths_n2)
cflows, cpaths, cflag = util.consolidate_paths(tug, rpaths_n2, node_counts_r, arc_counts_r)
print('FLOW: PATH')
util.print_solution(tug, cflows, cpaths, sort='descending', max_paths=5)
```

```
FLOW: PATH
7.92: 2,3 > 3,3
4.80: 0,2 > 1,2 > 2,2 > 3,2
3.39: 0,1 > 1,1 > 2,0 > 3,0
2.16: 1,0 > 2,0 > 3,2
1.07: 0,1 > 1,1 > 2,0 > 3,2
...
```

In [7]:
```
util.print_ground_truth(flows, paths, sort='descending')
```

```
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
```

- We got many of the ground truth paths correctly, but we are still using many spurious ones

Minimum Cover Constraints

Perhaps we could try to counter the adverse effects of the L1 term

...Without loosing all of its benefits

- If the L1 weight is too low, the regularizer has little effect
- ...But if it is too high, the solver stops focusing on the count reconstruction

What can we do?

Minimum Cover Constraints

Perhaps we could try to counter the adverse effects of the L1 term

...Without loosing all of its benefits

- If the L1 weight is too low, the regularizer has little effect
- ...But if it is too high, the solver stops focusing on the count reconstruction

What can we do?

One way to achieve this consists in introducing new constraints

- For example, we could require for each vertex
- ...To recover a minimum fraction γ of the total count, i.e.

$$Vx \geq \gamma v$$

Minimum Cover Constraints

The path formulation then becomes

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

With $P = V^T V + E^T E$ and $q = -V^T v - E^T \hat{e} + \alpha$

- We have incorporated both the L1 term (them α term)
- ...And the minimum cover constraints

When calling the OSQP solver

- We need to include α in the definition of q
- Then we need to extend the constraint matrix/vectors A, l, u
- ...So as to account for $V x \geq \gamma v$

Solving the Modified Path Formulation

Let's try to solve the problem for $\alpha = 3$ and $\gamma = 0.8$

In [8]:
```
rflows_n3, rpaths_n3 = util.solve_path_selection_full(tug, node_counts_n, arc_counts_n, alpl
                                                      min_vertex_cover=0.95, solver='piqp')
print('FLOW: PATH')
util.print_solution(tug, rflows_n3, rpaths_n3, sort='descending', max_paths=10)
sse = util.get_reconstruction_error(tug, rflows_n3, rpaths_n3, node_counts_n, arc_counts_n)
print(f'RSSE: {np.sqrt(sse):.2f}')
```

```
FLOW: PATH
8.28: 2,3 > 3,3
5.23: 0,2 > 1,2 > 2,2 > 3,2
2.62: 3,3
2.42: 0,1 > 1,1 > 2,0 > 3,0
1.87: 0,1 > 1,1 > 2,0 > 3,2
1.78: 1,0 > 2,0 > 3,0
1.52: 1,0 > 2,0 > 3,2
0.63: 3,2
0.41: 0,2 > 1,2
0.14: 0,1 > 1,1 > 2,0 > 3,3
...
RSSE: 3.13
```

```
/Users/michelelombardi/Library/Caches/pypoetry/virtualenvs/mining-with-co-eC0Z9-8k-py3.11/
lib/python3.11/site-packages/scipy/sparse/_index.py:108: SparseEfficiencyWarning: Changing
the sparsity structure of a csc_matrix is expensive. lil_matrix is more efficient.
  self._set_intXint(row, col, x.flat[0])
```

Solving the Modified Path Formulation

Let's see what happens with consolidation

In [9]:
```
node_counts_r, arc_counts_r = util.get_counts(tug, rflows_n3, rpaths_n3)
cflows, cpaths, cflag = util.consolidate_paths(tug, rpaths_n3, node_counts_r, arc_counts_r)
print('FLOW: PATH')
util.print_solution(tug, cflows, cpaths, sort='descending', max_paths=5)
```

```
FLOW: PATH
8.28: 2,3 > 3,3
5.23: 0,2 > 1,2 > 2,2 > 3,2
4.28: 0,1 > 1,1 > 2,0 > 3,0
3.40: 1,0 > 2,0 > 3,2
2.62: 3,3
...
```

In [10]:
```
util.print_ground_truth(flows, paths, sort='descending')
```

```
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
```

We got all paths right, and the flows are closer to their real value

Column Generation with Constraints in the Master

Where we make our first acquaintance with the KKT conditions

CG and Modified Path Formulation

The new formulation requires to add new constraints in the master

This is is a problem for Column Generation. Due to the constraints:

- Just looking at the gradient may now be misleading
- ...Since changing a variable may force to change others

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

We need a "constraint-aware gradient"

One way to achieve that is to rely on a Lagrangian approach

- The idea is to turn the constraints in to cost terms
- ...And control their satisfaction by adjusting weights (multipliers)

We will discuss this approach in a general setting

Lagrangian Approach

Let's consider an optimization in the form

$$\text{argmin}_x \{f(x) \mid g(x) \leq 0\} \qquad \textbf{(P1)}$$

where $\boldsymbol{x}$ belongs to $\mathbb{R}^n$ (i.e. this is numeric optimization)

From this, we can obtain a related, unconstrained optimization problem

...By moving the constraints in to the cost function, with weights/multipliers $\boldsymbol{\lambda}$:

$$\text{argmin}_x \mathcal{L}(x, \lambda) = f(x) + \lambda^T g(x) \qquad \textbf{(P2)}$$

The term $\mathcal{L}(x, \lambda)$ is called a Lagrangian

- If a constraint $g_i(x)$ is violated, $\mathcal{L}$ gets a penalty w.r.t. $f(x)$
- If a constraint $g_i(x)$ is satisfied, $\mathcal{L}$ gets a reward w.r.t. $f(x)$

We want to solve (P1) by controlling the multipliers in (P2)

...And KKT Conditions

Let's assume that x is an local optimum for the original problem

...If we want to reach it via (P2), the multipliers should be just right:

- They should make the Lagrangian gradient null, i.e.

$$\nabla_x \mathcal{L}(x, \lambda) = 0$$

- They should be non-negative (or a penalty may turn into a reward):

$$\lambda \geq 0$$

- They should be 0 for all satisfied constraints (or $\mathcal{L}$ would be "inflated")

$$\lambda \odot g(x) = 0$$

Additionally, x should be feasible, i.e. $g(x) \leq 0$

...And KKT Conditions

If certain constraint qualifications apply, these are necessary conditions

If a point $\boldsymbol{x}$ is a local optimum, then we have:

$$\begin{aligned} \nabla_x \mathcal{L}(x, \lambda) &= 0 && \text{(null gradient)} \\ \lambda &\geq 0 && \text{(dual feasibility)} \\ \lambda \odot g(x) &= 0 && \text{(complementary slackness)} \\ g(x) &\leq 0 && \text{(primal feasibility)} \end{aligned}$$

They are known as Karush-Kuhn-Tucker (KKT) first order optimality conditions

Some comments:

- If $f(x)$ and $g(x)$ are convex, the KKT conditions are also sufficient
- Equality constrains are equivalent to $g(x) \leq 0$ and $-g(x) \leq 0$
- ...Which can be manipulated to obtain (slighly) simpler formulas

How to Use the KKT Conditions

We can use the KKT conditions to constrain x to be an optimum

- This is useful in bi-level optimization, i.e.:

$$\text{argmax}_y \left\{ f(z) \mid z = \text{argmin}_{x \in X}\, g(x, y) \right\}$$

- If X and g are convex, we can use the KKT conditions are constraints
- ...And replace the optimization step $\text{argmin}_{x \in X}\, g(x, y)$
- Typically, this is useful only the conditions reduce to a simple form

We can use the KKT conditions to check whether x is a local optimum

...Assuming we are in convex optimization and constraint qualifications are met

- If we fix x, then the KKT conditions reduce to a linear system
- ...If we can solve it, then x is a local optimum
- ...And we have found the corresponding optimal multipliers

How to Use the KKT Conditions in CG

As a by-product of the previous use case...

If we know that x is an optimum, we can obtain the optimal λ

This is the application we care about

- If we have constraints in the master problem
- ...Rather than searching for variables such that:

$$\frac{\partial}{\partial x_j} f(x) < 0$$

- ...We search instead for variables such that:

$$\frac{\partial}{\partial x_j} \mathcal{L}(x, \lambda) < 0$$

CG for the Modified Path Formulation

The modified Path Formulation can be rewritten as:

$$\arg\min_{x} \left\{ \frac{1}{2}(\|Vx - v\|_2^2 + \|Ex - e\|_2^2) + \alpha x \mid Vx \geq \gamma v, x \geq 0 \right\}$$

From which we obtain:

$$\mathcal{L}(x, \lambda, \mu) = \frac{1}{2}(\|Vx - v\|_2^2 + \|Ex - e\|_2^2) + \alpha x + \lambda^T(\gamma v - Vx) - \mu^T x$$

And finally:

$$\frac{\partial}{\partial x_j}\mathcal{L}(x, \lambda, \mu) = \sum_{i=1}^{n_v} r_i^v V_{ij} + \sum_{k=1}^{n_e} r_k^e E_{kj} - \sum_{i=1}^{n_v} \lambda_i V_{ij} + \alpha - \mu_j$$

CG for the Modified Path Formulation

Therefore, we can modify our pricing problem so that we minimize:

$$\sum_{i=1}^{n_v} (r_i^v - \lambda_i) V_{ij} + \sum_{k=1}^{n_e} r_k^e E_{kj} + \alpha - \mu_j$$

Whenever we include an arc k in the path we are constructing:

- We accumulate a gradient term equal to r_k^e
- ...Exactly the same as before

Whenever we include a node i in the path we are constructing:

- We accumulate a gradient term equal to $r_i^v - \lambda_i$
- I.e. we subtract the multiplier associated to the i-th min cover constraint

Then, for every path, we add α and we subtract μ_j

But how do we get the multipliers?

CG for the Modified Path Formulation

Every λ_i is associated to a (min cover) constraint:

...And we have all of those in our problem!

- Hence, we could compute λ for the current optimal solution
- In practice, the OSQP sover can compute λ for us

Every μ_j is associated to $x_j \geq 0$ constraint:

...And unfortunately we have those only for the paths in the pool

- However, we know that $\mu_j \geq 0$ (by dual feasibility)
- ...And we would have $\mu_j > 0$ only having $x_j < 0$ was beneficial
- ...But we are looking for paths with exactly the opposite property
- Hence, we can just assume $\mu_j = 0$ when generating new paths

Full CG In Action

This is Column Generation as it was meant to be

Obtaining the Duals

We start by solving again the master problem

...But this time we retrieve the optimal (dual) multipliers

- They are the same weights λ used in the ADMM
- ...And can be obtain from the OSQP solution object

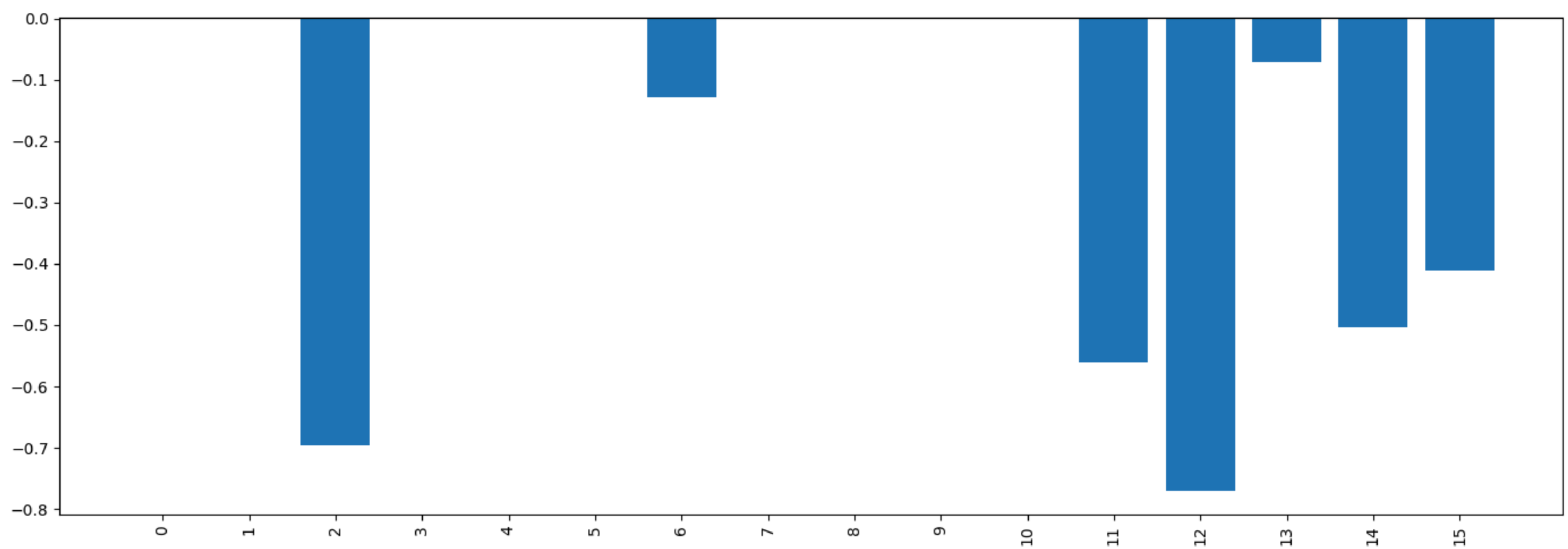
In [11]:
```
mvc, alpha = 0.95, 1
rflows_n3, rpaths_n3, nneg_duals3, mvc_duals3 = util.solve_path_selection_full(tug, node_cou
                                                    alpha=alpha, verbose=0, min_vertex_cove
print('FLOW: PATH')
util.print_solution(tug, rflows_n3, rpaths_n3, sort='descending', max_paths=6)
sse = util.get_reconstruction_error(tug, rflows_n3, rpaths_n3, node_counts_n, arc_counts_n)
print(f'RSSE: {np.sqrt(sse):.2f}')
```

```
FLOW: PATH
8.28: 2,3 > 3,3
4.36: 0,2 > 1,2 > 2,2 > 3,2
2.62: 3,3
2.45: 0,1 > 1,1 > 2,0 > 3,0
1.68: 1,0 > 2,0 > 3,0
1.68: 0,1 > 1,1 > 2,0 > 3,2
...
RSSE: 2.54
```

Inspecting the Duals

Let's inspect the multipliers for the minimum cover constraints

In [12]:
```
util.plot_dict({i:v for i, v in enumerate(mvc_duals3)}, figsize=figsize)
```

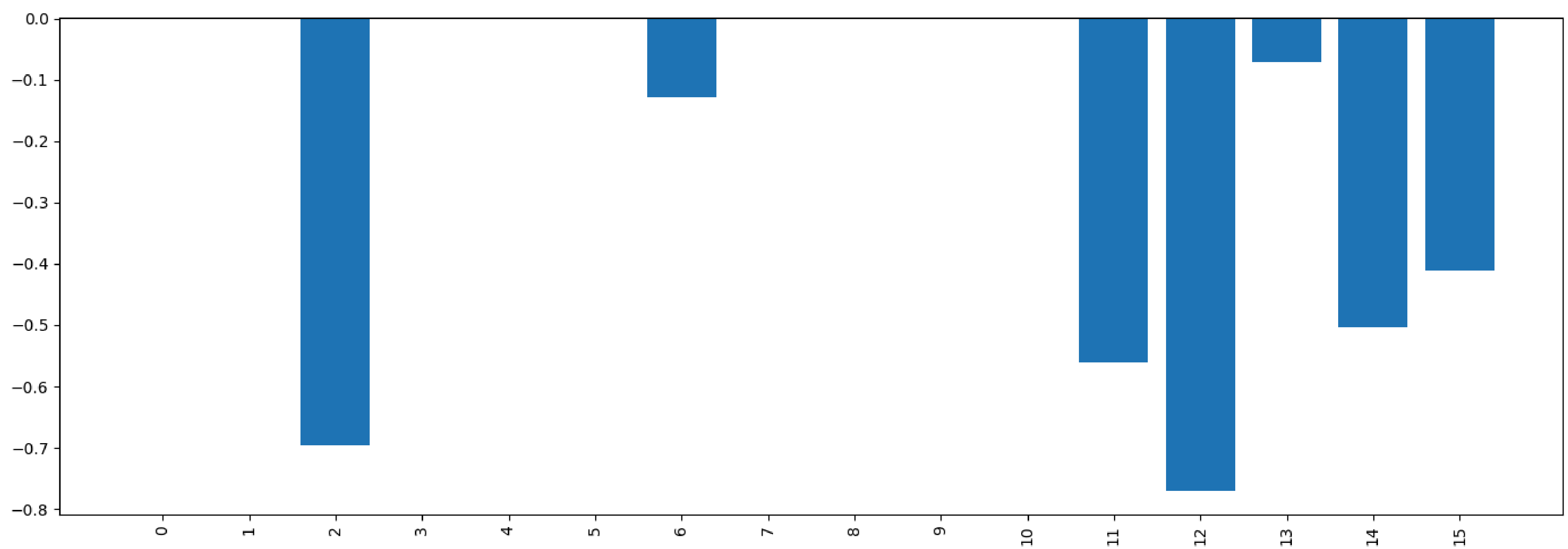


- Some values are 0 (when the constraint is satisfied with a slack)
- ...And some (unexpectedly, are negative)

Inspecting the Duals

Let's inspect the multipliers for the minimum cover constraints

In [13]:
```
util.plot_dict({i:v for i, v in enumerate(mvc_duals3)}, figsize=figsize)
```

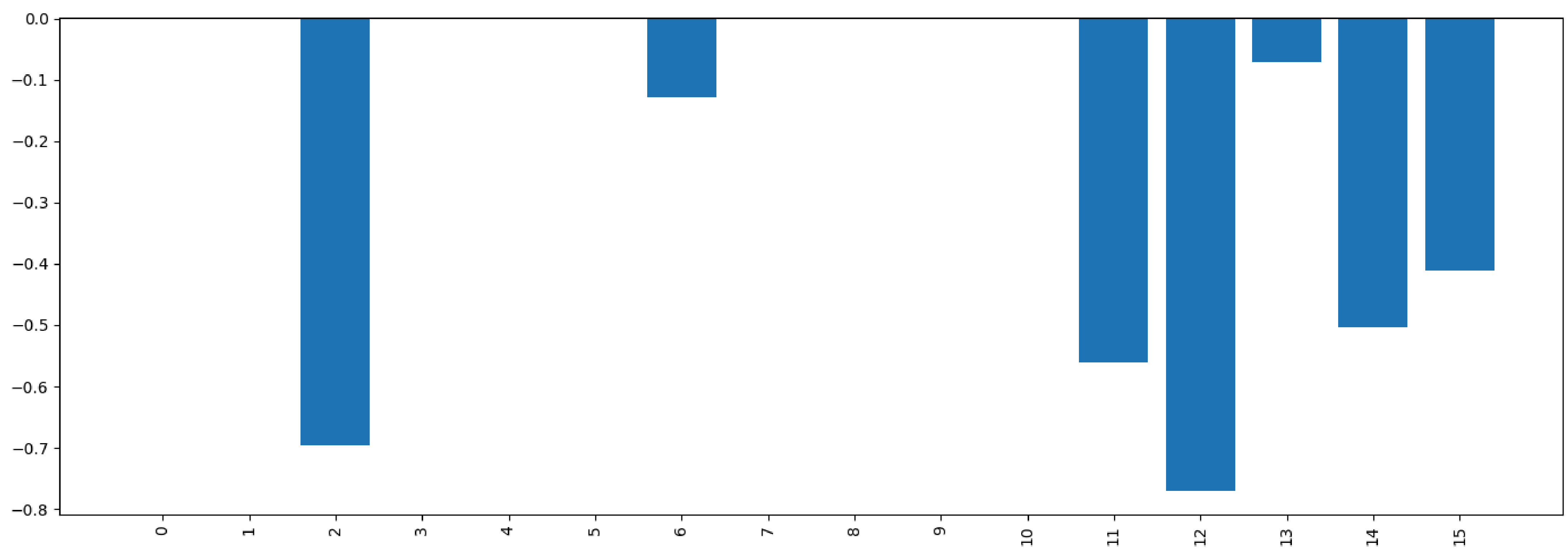


- The reason is the constraint direction: we have $Vx \geq \gamma\hat{v}$ and not $-Vx \leq -\gamma\hat{v}$
- We could fix by switching the constraint direction

Inspecting the Duals

Let's inspect the multipliers for the minimum cover constraints

In [14]:
```
util.plot_dict({i:v for i, v in enumerate(mvc_duals3)}, figsize=figsize)
```



- ...Or by reworking the change though the KKT formulas
- In our case, when we include a node we add λ_i instead of subtracting it

Checking the Pricing Solution

Our pricing problem code can handle both the duals and the L1 weight

We modify node residuals by adding the cover multipliers:

```
if cover_duals is not None:
    for i, v in enumerate(tug.vs):
        nk = v['time'], v['index_o']
        nres[nk] += cover_duals[i]
```

- This provides an incentive to select paths
- ...That traverse a node whose cover constraint is satisfied with a slack

And we add the constant α to the final path weights:

```
    spw = [v + alpha for v in spw]
```

- This a uniform disincentive so select paths

The shortest paths problem is solved as usual

Running the CG Approach

We can now run the CG approach

```
In [15]: rflows_cg, rpaths_cg = util.trajectory_extraction_cg(tug, node_counts_n, arc_counts_n,
                                             alpha=alpha, min_vertex_cover=mvc, max_iter=30,
                                             verbose=1, max_paths_per_iter=10, solver='piqp')
         sse = util.get_reconstruction_error(tug, rflows_cg, rpaths_cg, node_counts_n, arc_counts_n)
         print(f'RSSE: {np.sqrt(sse):.2f}')
```

```
It.0, sse: 209.13, #paths: 26, new: 10
It.1, sse: 83.13, #paths: 34, new: 8
It.2, sse: 67.39, #paths: 41, new: 7
It.3, sse: 42.31, #paths: 45, new: 4
It.4, sse: 7.24, #paths: 47, new: 2
It.5, sse: 6.46, #paths: 49, new: 2
It.6, sse: 6.46, #paths: 49, new: 0
RSSE: 2.54
```

```
/Users/michelelombardi/Library/Caches/pypoetry/virtualenvs/mining-with-co-eC0Z9-8k-py3.11/
lib/python3.11/site-packages/scipy/sparse/_index.py:108: SparseEfficiencyWarning: Changing
the sparsity structure of a csc_matrix is expensive. lil_matrix is more efficient.
  self._set_intXint(row, col, x.flat[0])
```

- Indeed, we obtain the same RSSE as the approach using all paths

We now know how to use CG with constraints in the master problem

Some References

CG is main studied in the context of Linear Optimization

- "Column Generation", by Lübbecke
- "Column Generation", by Desaulniers, Desrosiers, and Solomon