Symmetries

Sometimes metrics are not enough

Unexpected Discrepancy

Our current solution seems apparently perfect

```
In [2]: util.print_solution(tug, rflows, rpaths, sort='descending')
        sse = util.get_reconstruction_error(tug, rflows, rpaths, node_counts, arc_counts)
        print(f'RSSE: {np.sqrt(sse):.2f}')

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
```

...And yet it does not match the ground truth!

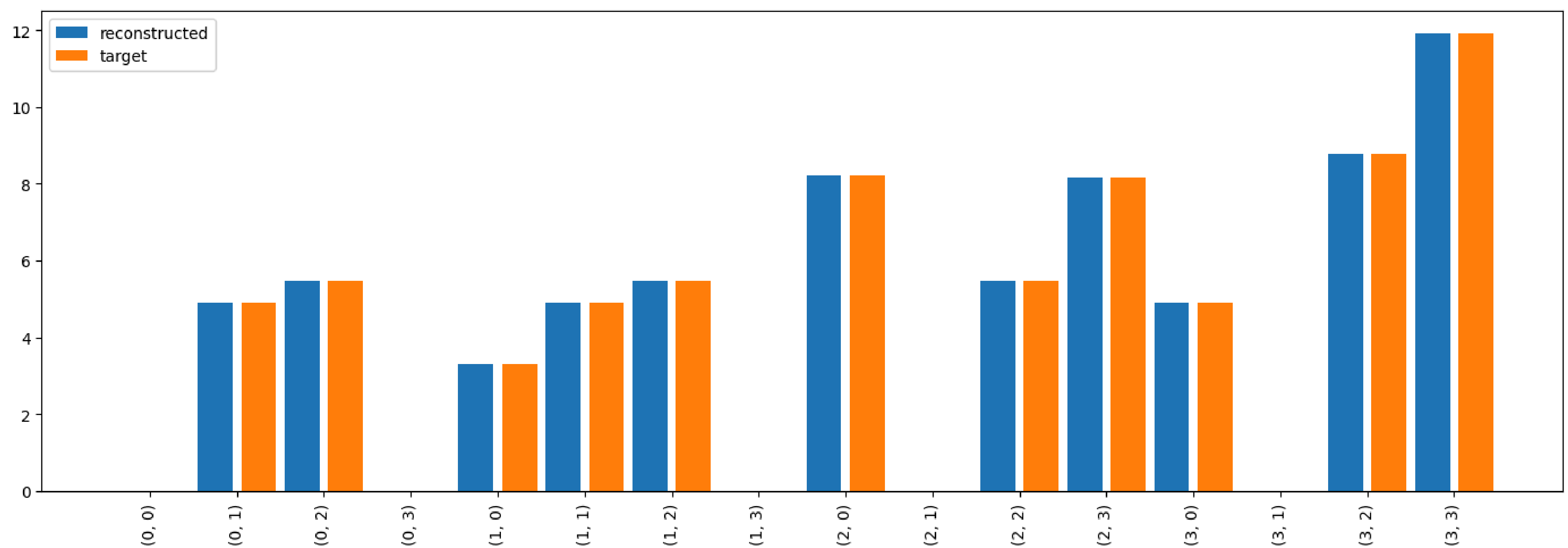
```
In [3]: util.print_ground_truth(flows, paths, sort='descending')

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
```

Unexpected Discrepancy

The discrepancy is unexpected, due to the 0 reconstruction error

Indeed, we can check that the reconstructed counts match the true ones:

```
In [4]: rnc, rac = util.get_counts(tug, rflows, rpaths)
        util.plot_dict(rnc, figsize=figsize, label='reconstructed', data2=node_counts, label2='targe
```



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What is going on?

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We mentioned early on that the available information is poor

- There are many possible paths
- ...And many possible ways to explain the original counts!

How do we fix these symmetries?

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We mentioned early on that the available information is poor

- There are many possible paths
- ...And many possible ways to explain the original counts!

How do we fix these symmetries?

- The only way is adding external information (e.g. a preference on paths)
- We can view this as a form of regularization

Occam's Razor

Intuitively, we could give priority to the simplest explanation

Image credit: xkcd 2541

A reasonable choice may be to use a small number of paths

How do we enforce this?

L1 Regularization and Path Number

We may think of using an L1 regularization

We would just need to add a linear term to the path formulation:

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

...Which would translate into a correction on the $\boldsymbol{q}$ vector:

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

- This trick is implemented in the `solve_path_selection_full` function
- We just need to pass a value for the `alpha` argument

L1 Regularization and Path Number

Let's begin by trying $\alpha = 1$

In [5]:
```
rflows2, rpaths2 = util.solve_path_selection_full(tug, node_counts, arc_counts, verbose=0, a
print('FLOW: PATH')
util.print_solution(tug, rflows2, rpaths2, sort='descending')
sse = util.get_reconstruction_error(tug, rflows2, rpaths2, node_counts, arc_counts)
print(f'\nRSSE: {np.sqrt(sse):.2f}')
```

```
FLOW: PATH
8.10: 2,3 > 3,3
5.37: 0,2 > 1,2 > 2,2 > 3,2
2.97: 0,1 > 1,1 > 2,0 > 3,0
2.36: 3,3
1.66: 0,1 > 1,1 > 2,0 > 3,2
1.61: 1,0 > 2,0 > 3,0
1.40: 1,0 > 2,0 > 3,2
0.21: 0,1 > 1,1 > 2,0 > 3,3
0.17: 1,0 > 2,0 > 3,3
0.06: 1,0 > 2,3 > 3,3

RSSE: 1.32
```

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RSSE: 1.32
```

- The RSSE grows (as it could be expcted)
- But we have more paths!

L1 Regularization and Path Number

What if we make α larger?

In [6]:

```
rflows2, rpaths2 = util.solve_path_selection_full(tug, node_counts, arc_counts, verbose=0, a
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util.print_solution(tug, rflows2, rpaths2, sort='descending')
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print(f'\nRSSE: {np.sqrt(sse):.2f}')
```

```
FLOW: PATH
4.80: 2,3 > 3,3
4.26: 0,2 > 1,2 > 2,2 > 3,2
2.18: 0,1 > 1,1 > 2,0 > 3,0
1.31: 0,1 > 1,1 > 2,0 > 3,2
0.83: 1,0 > 2,3 > 3,3
0.58: 0,1 > 1,1 > 2,0 > 3,3
0.46: 1,0 > 2,0 > 3,0
0.38: 1,0 > 2,0 > 3,2
0.26: 1,0 > 2,0 > 3,3
0.14: 0,1 > 1,0 > 2,3 > 3,3
0.10: 0,1 > 1,0 > 2,0 > 3,0
0.09: 0,1 > 1,0 > 2,0 > 3,2
0.08: 0,1 > 1,0 > 2,0 > 3,3

RSSE: 9.13
```

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0.08: 0,1 > 1,0 > 2,0 > 3,3

RSSE: 9.13
```

- We don't seem to be getting fewer paths, but rather longer ones

L1 Regularization and Path Number

Shouldn't L1 norm work as a sparsifier?

Not exactly: it simply results in a fixed penalty rate for raising a variable

- The solver will try to balance it with a larger reduction of the quadratic loss
- ...Which we can easily improve by including more nodes in each path

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The truth is that when we use an L1 norm as sparsifier...

...We really wished our regularizer to be:

$$N_{paths} = \sum_{j=1}^{n} z_j \quad \text{with: } z_j = \begin{cases} 1 \text{ if } x_j > 0 \\ 0 \text{ otherwise} \end{cases}$$

- Which is inconvenient, since it is non-differentiable
- ...But what if we used an approach for non-differentiable optimization?

Path Consolidation Problem

Let's face an inconvenient truth

Path Consolidation Problem

For example, we could focus on the paths in the current solution:

- ...Minimize the number of used paths
- ...While preserving our reconstruction error

This is form of symmetry breaking (as a post-processing step)

By doing this, we obtain a "path consolidation problem" in the form:

$$
\begin{aligned}
\arg\min_{x} \ & \|z\|_1 \\
\text{subject to: } & Vx = v^* \\
& Ex = e^* \\
& x \leq Mz \\
& x \geq 0 \\
& z \in \{0, 1\}^n
\end{aligned}
$$

Path Consolidation Problem

Let's proceed to examine the formulation a bit better:

$$
\begin{aligned}
\arg\min_{x} \quad & \|z\|_1 \\
\text{subject to:} \quad & Vx = v^* \\
& Ex = e^* \\
& x \leq Mz \\
& x \geq 0 \\
& z \in \{0, 1\}^n
\end{aligned}
$$

- The terms V, E, and x are the same as before
- ...Except in this case we will consider a a subset of the paths
- v^* and e^* are the counts from the optimal path formulation solution
- We are requiring the (reconstructed) counts to be exactly the same

Path Consolidation Problem

Let's proceed to examine the formulation a bit better:

$$\begin{aligned} \arg\min_{x} \quad & \|z\|_1 \\ \text{subject to:} \quad & Vx = v^* \\ & Ex = e^* \\ & x \leq Mz \\ & x \geq 0 \\ & z \in \{0, 1\}^n \end{aligned}$$

- The z variables determine whether a path is used ($z_j = 1$) or not ($z_j = 0$)
- M is a constant large enough to make the constraint trivial if $z_j = 1$
- Constants such as these are often referred to as "big-Ms"
- Basically, $x \leq Mz$ is a linearization of the implication $x > 0 \Rightarrow z = 1$

Path Consolidation Problem

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$$
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\arg\min_{x} \quad & \|z\|_1 \\
\text{subject to:} \quad & Vx = v^* \\
& Ex = e^* \\
& x \leq Mz \\
& x \geq 0 \\
& z \in \{0, 1\}^n
\end{aligned}
$$

- All constraints are linear
- The cost function is linear
- Some variables are integer

This is a Mixed Integer Linear Program (MILP)