From Pricing...

Because there's an elephant in the room, and it's HUGE

Scalability, or Lack Thereof

Our current approach as one, massive, limitations

The number paths in graph scales exponentially on its size

- Meaning that path enumeration becomes quickly very expensive
- ...And the path formulation size grows at the same rate

Let's check the solution time for our small example graph:

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

CPU times: user 7 ms, sys: 1.11 ms, total: 8.12 ms
Wall time: 7.21 ms
```

...And the for a slightly larger graph (8 nodes, 5 time steps):

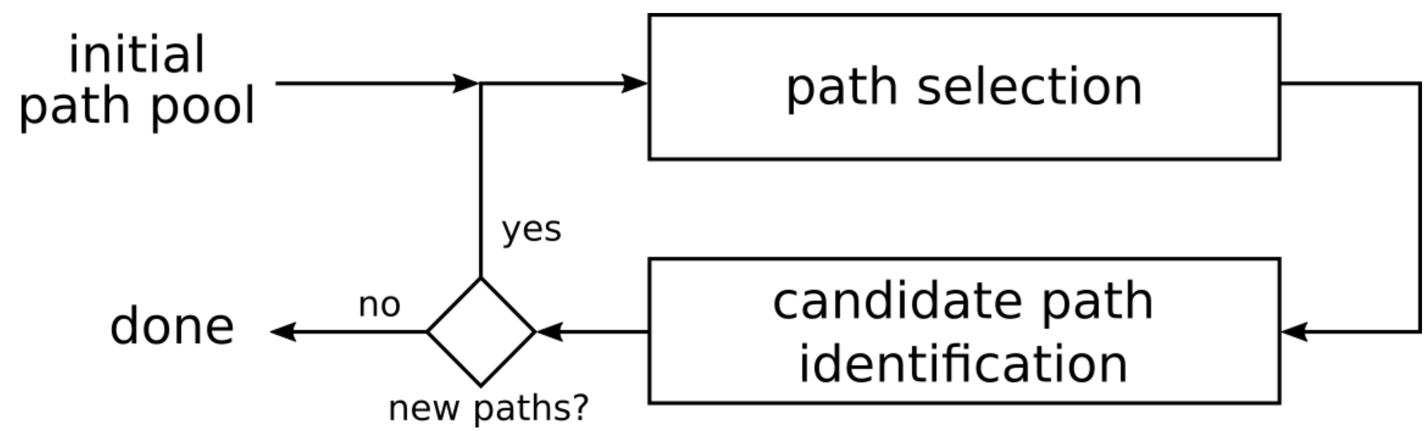
```
In [4]: g8_5, t8_5, f8_5, p8_5, nc8_5, ac8_5 = util.get_default_benchmark_graph(nnodes=8, eoh=5, see
        %time f8_5, p8_5 = util.solve_path_selection_full(t8_5, nc8_5, ac8_5, verbose=0, solver='pi

CPU times: user 5.48 s, sys: 17.2 ms, total: 5.5 s
Wall time: 5.5 s
```

Adding Variables on Demand

What if we had a way to add variables on demand?

Then could think of:

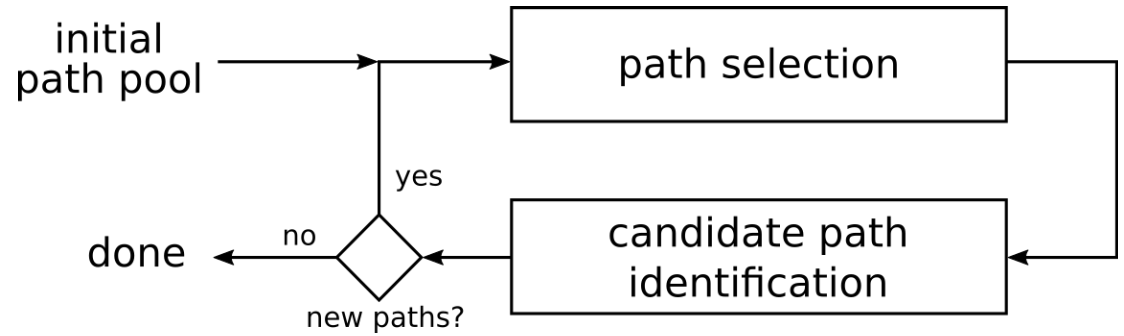


- Solving the Path Formulation with a subset of paths
- ...Then searching for new paths to be added
  - If we find some, we add them to the pool and we repeat
  - If we find none, we are done

An approach such as this may strongly mitigate our scalability issues

Adding Variables on Demand

What do we need to pull this off?



1. The ability to use a limited pool in the path formulation
2. A way to identify new paths to be added

Point 1 is trivial, but what about point 2?

Adding Variables on Demand

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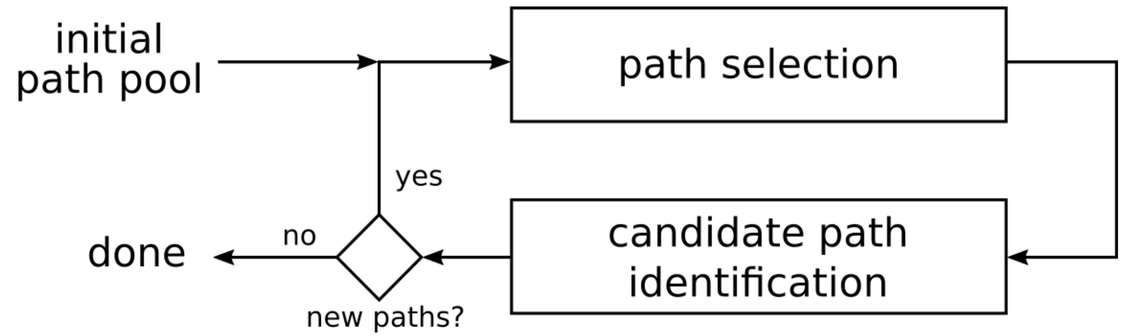


1. The ability to use a limited pool in the path formulation
2. A way to identify new paths to be added

Point 1 is trivial, but what about point 2?

We could split the enumeration in multiple "chunks"

- That would allow to obtain the first solutions more quickly
- But would still need to complete the enumeration to prove optimality

What we need is a way to identify useful paths that are not yet in the pool

Identifying Useful Variables

Let's recall the structure of the Path Formulation

$$\arg\min_x \{ f(x) \mid x \geq 0 \} \qquad \text{with: } f(x) = \frac{1}{2} x^T P x + q^T x$$

- We can view missing variables are having value 0 in the current solution
- So, we are looking for variables that can be raised to reduce error
- Since the problem is convex, we could start by looking at the gradient

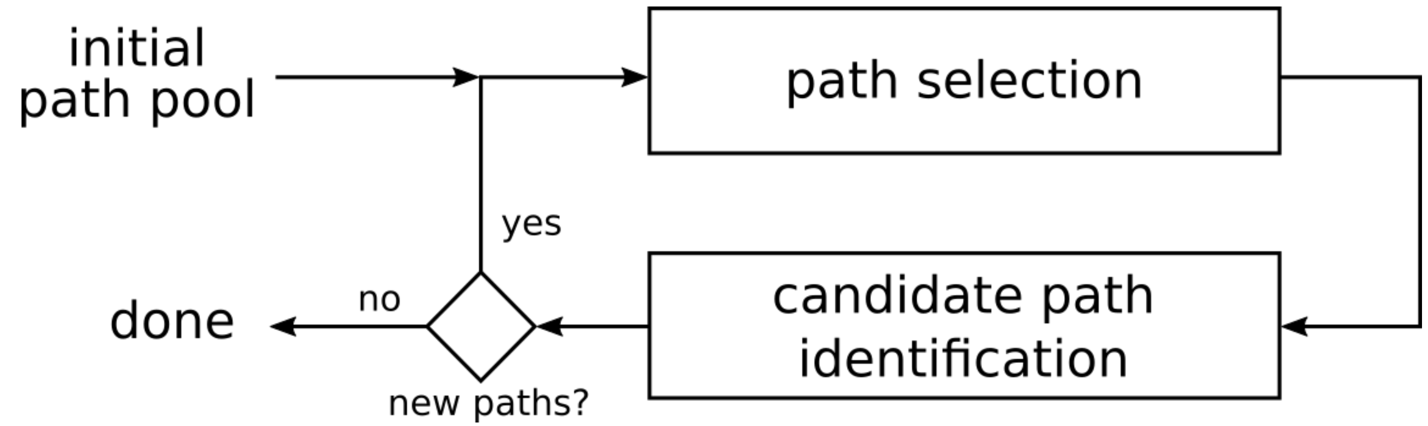
Hence, we could search for variables with a negative gradient term

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

- This a necessary condition in general
- Later in the course we will found out why

Pricing Problem

Let's revisit and generalize our schema



- The "main" problem may not involve paths
  - ...So we will call it just a master problem
- We look for additional variables such that $\frac{\partial}{\partial x_j} f(x) < 0$
  - It's a bit like we are assigning a "price tag" to them
  - If the price is positive, we skip the variable (we know it's useless now)
  - If the price is negative, the variable may be useful
  - For this reasons, we call the second component pricing problem

The Path Selection Gradient

We need to compute gradient terms for variables not yet in the pool

This is easiest if we differentiate our original (equivalent) objective:

$$f(x) = \frac{1}{2}\|Vx - \hat{v}\|_2^2 + \frac{1}{2}\|Ex - \hat{e}\|_2^2$$

- ...Since node contribution mix-up in the $\boldsymbol{P}$ matrix and $\boldsymbol{q}$ vectors

The least square objective can be rewritten as:

$$f(x) = \frac{1}{2}\sum_{i=1}^{n_v}\left(\sum_{j=1}^{n} V_{ij}x_j - \hat{v}_i\right)^2 + \frac{1}{2}\sum_{k=1}^{n_e}\left(\sum_{j=1}^{n} E_{kj}x_j - \hat{e}_k\right)^2$$

- Where $\boldsymbol{n_v}$ is the number of nodes and $\boldsymbol{n_e}$ the number of arcs

The Path Selection Gradient

We can differentiate the expression to obtain

$$\frac{\partial}{\partial x_j} f(x) = \sum_{i=1}^{n_v} \left(\sum_{j=1}^{n} V_{ij} x_j - \hat{v}_i \right) V_{ij} + \sum_{k=1}^{n_e} \left(\sum_{j=1}^{n} E_{kj} x_j - \hat{e}_k \right) E_{kj}$$

Some expressions in the formula are simply the node/edge residuals:

$$r_i^v = \sum_{j=1}^{n} V_{ij} x_j - \hat{v}_i \quad \text{and} \quad r_k^e = \sum_{j=1}^{n} E_{kj} x_j - \hat{e}_k$$

Hence we can rewrite the gradient terms as:

$$\frac{\partial}{\partial x_j} f(x) = \sum_{i=1}^{n_v} r_i^v V_{ij} + \sum_{k=1}^{n_e} r_k^e E_{kj}$$

The Path Selection Gradient

Now, let's parse the meaning of our gradient term:

$$\frac{\partial}{\partial x_j} f(x) = \sum_{i=1}^{n_v} r_i^v V_{ij} + \sum_{k=1}^{n_e} r_k^e E_{kj}$$

- For every (TUG) node $\boldsymbol{i}$ included in the path, we add $\boldsymbol{r_i^v}$
- For every (TUG) arc $\boldsymbol{k}$ included in the path, we add $\boldsymbol{r_k^e}$

This is a simple computation that we can perform on any path

...Including those that are not yet in the path formulation pool

- Just don't forget that this condition identifies (potentially) useful paths
- ...But only w.r.t. the current path formulation solution!

A Look at the Residuals

Let's try it out

First, we enumerate all TUG paths

In [5]:
```
tugs, tugs_source = util._add_source_to_tug(tug)
tug_paths = util.enumerate_paths(tugs, tugs_source, exclude_source=True)
```

Then, we run the path formulation with a limited pool of paths

In [6]:
```
path_pool = tug_paths[:10]
rflows0, rpaths0 = util.solve_path_selection_full(tug, node_counts, arc_counts,
                                                  initial_paths=path_pool, verbose=0)
sse = util.get_reconstruction_error(tug, rflows0, rpaths0, node_counts, arc_counts)
util.print_solution(tug, rflows0, rpaths0, sort='descending')
print(f'RSSE: {np.sqrt(sse):.2f}')
```

```
1.96: 0,0 > 1,0 > 2,0 > 3,2
1.86: 0,0 > 1,0 > 2,0 > 3,3
0.79: 0,0 > 1,0 > 2,0 > 3,0
RSSE: 25.58
```

- Since we are restricted to a subset of paths, the RSSE is no longer 0

A Look at the Residuals

Then we can extract the residuals, i.e. $Vx - \hat{v}$ and $Ex - \hat{e}$

```
In [7]: nres0, ares0 = util._get_residuals(tug, rflows0, rpaths0, node_counts, arc_counts)
        print('NODE RESIDUALS')
        print('\t'.join(f'{k}:{v:.2f}' for k, v in nres0.items()))
        print('ARC RESIDUALS')
        print('\t'.join(f'{k}:{v:.2f}' for k, v in ares0.items()))
```

```
NODE RESIDUALS
(0, 0):4.61     (0, 1):-4.89    (0, 2):-5.47    (0, 3):0.00     (1, 0):1.29     (1, 1):-4.
89      (1, 2):-5.47    (1, 3):0.00     (2, 0):-3.60    (2, 1):0.00     (2, 2):-5.47
(2, 3):-8.17    (3, 0):-4.10    (3, 1):0.00     (3, 2):-6.83    (3, 3):-10.05
ARC RESIDUALS
(1, 0, 0):4.61  (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):1.29  (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):-4.10 (3, 0, 1):0.00  (3, 1, 1):0.00  (3, 0, 2):-1.36
(3, 2, 2):-5.47 (3, 0, 3):1.86  (3, 3, 3):-8.17 (3, 1, 0):0.00  (3, 1, 2):0.00
```

- This is enough information to compute $\frac{\partial}{\partial x_j} f(x)$ for all paths
- ...Except that doing that would still not solve all our issues :-(