

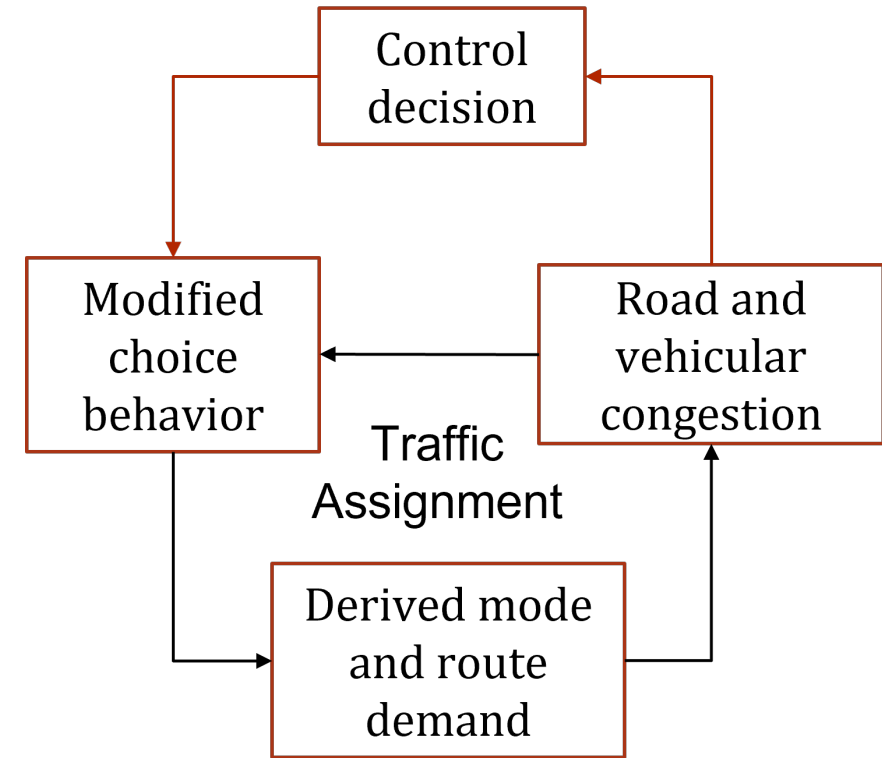
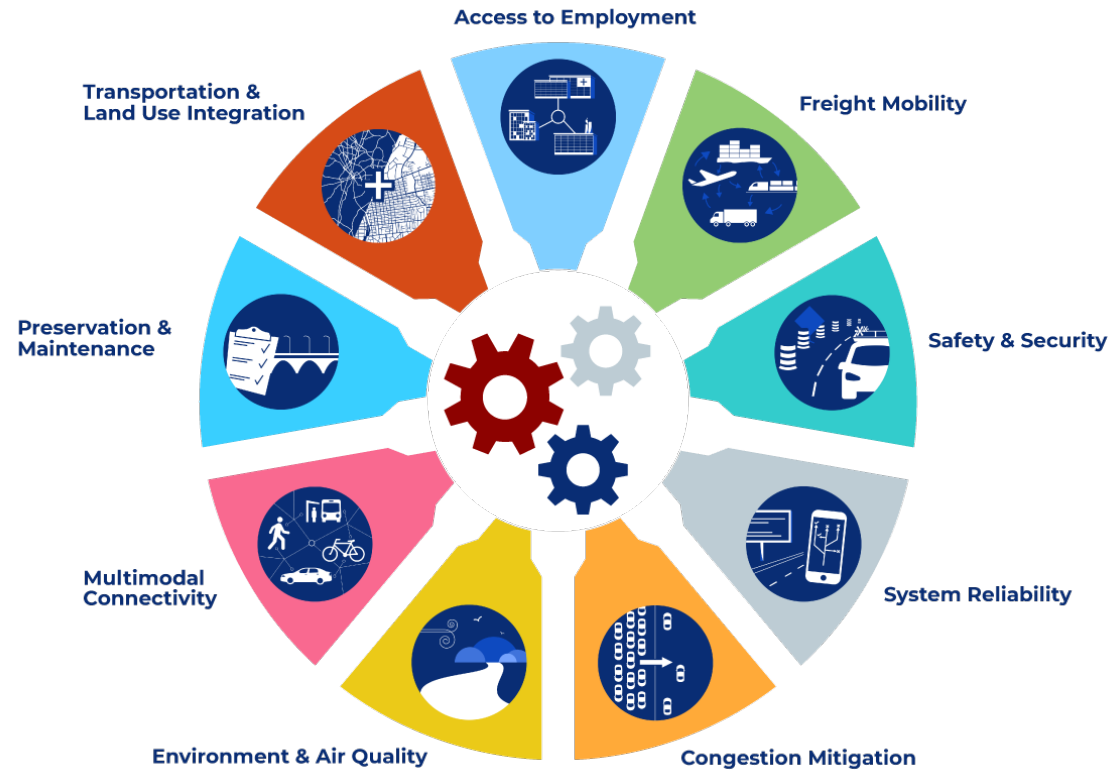
Gradient Based Optimization of MATSim Using Iterative Backpropagation

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Introduction



Challenges

- **Mathematical Complexity**
 - No closed-form formulation
 - No analytical gradient
- **Computation Time**
 - 25 days for 100% HK scenario
 - 2 days for 10% Montreal scenario
 - Tight simulation budget (maximum 20)
- **High dimension problems**
 - OD estimation (49,000 variables for HK network)
 - Pricing optimization
 - Toll Optimization etc.

Solution Algorithms

- **Heuristics:**

- **Genetic Algorithm** (Amirjamshidi and Roorda,2019; Chiappone et al., 2016; Spiliopoulou et al., 2015;Yu and Fan, 2017)
- **Monte Carlo Sampling** (de Oliveira and Cunha, 2019;Henclewood et al., 2017)
- **Artificial Bee Colony** (D. Huang et al., 2016b; Szeto and Jiang, 2012)
- **SPSA** (Lee and Ozbay, 2009; Ma et al., 2007; Lu et al., 2015 and Oh et al.,2019)

- **Response surface:**

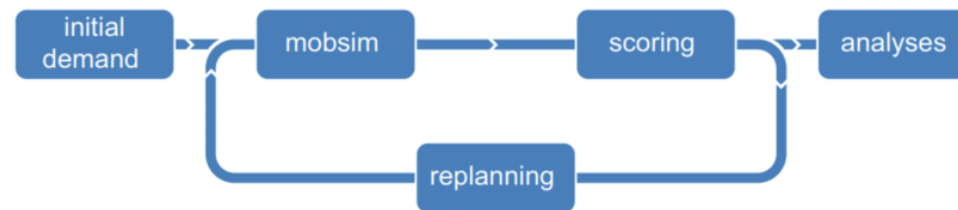
- **Generic** (Polynomial, interpolation, etc.)
- **Hybrid** (Generic + Traffic Model) (Osorio and Chong 2015, Zhang 2016, Osori 2019, Patwary et al. 2021)

Gradient Based TA Optimization

Beneficial for **high dimensional** optimization. **Moving towards negative gradient** direction is **sufficient for minimization**.

Numerical (finite difference) gradient is **too costly to evaluate**.
(2d+1) function evaluation.

Cyclic dependencies (iterative loop) **prevents closed form gradient** formulation.

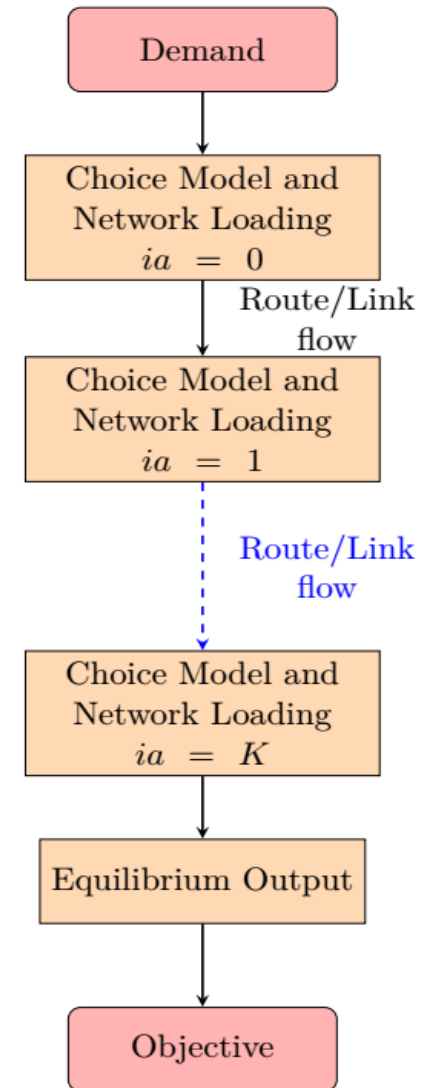


IB Gradient Estimation

TA solution procedures operates in **two steps**:

Auxiliary Flow Computation: Calculates the **choice model (scoring and choice strategy)** and **network loading model (Mobsim)**, generating subsequent flow as a function of the flow and cost of previous iteration.

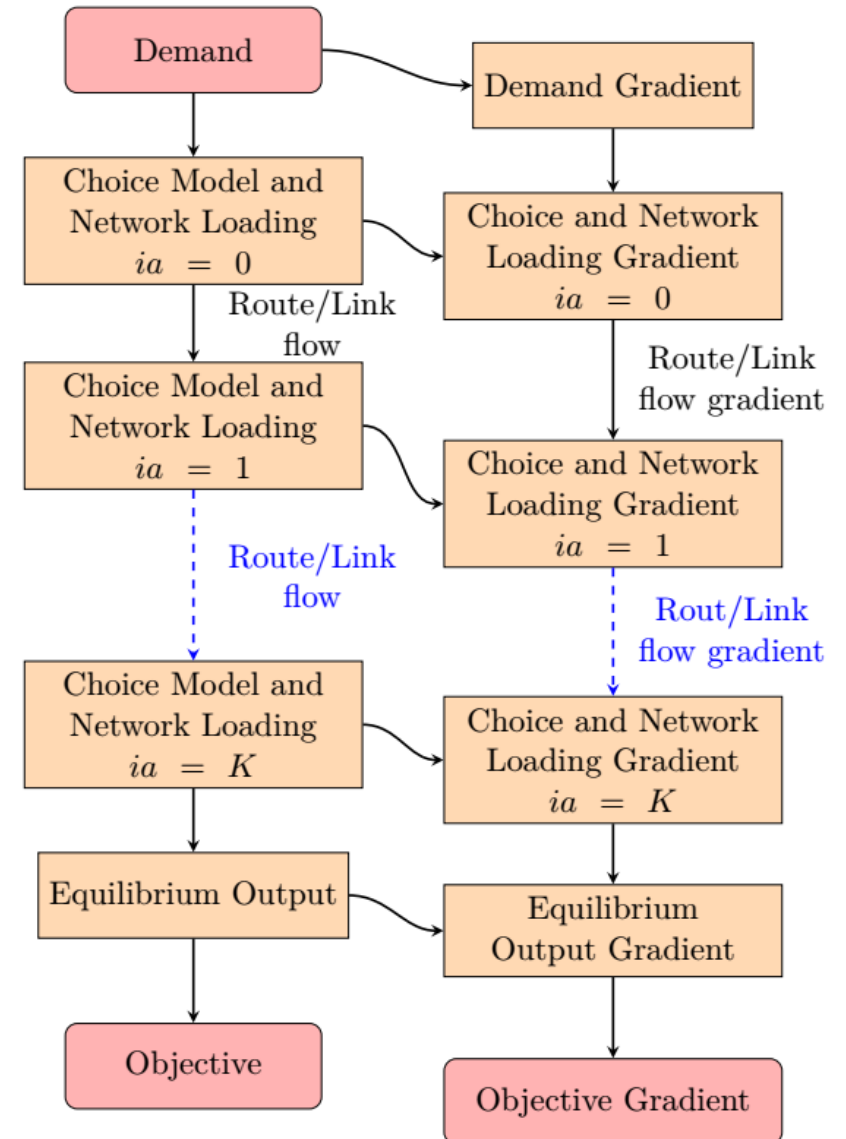
Flow Update: Updates the flow by merging previous iteration's flow and newly calculated flow with a decaying merge rule. **(MSA in MATSim)**



IB Gradient Estimation

IB introduces a '**gradient backpropagation**' step along with the network loading step.

Gradient Backpropagation: It uses information from the network loading step to **calculate the flow gradient of the current iteration as a function of the flow gradient of the previous iteration.**



Pros and Cons of IB

Pros:

- Requires **one function evaluation** to obtain **high-dimensional, accurate analytical gradient**.
- **Efficient** in computation, **can run parallelly on GPU**.
- Works well with **large-scale, multi-modal** network.

Cons:

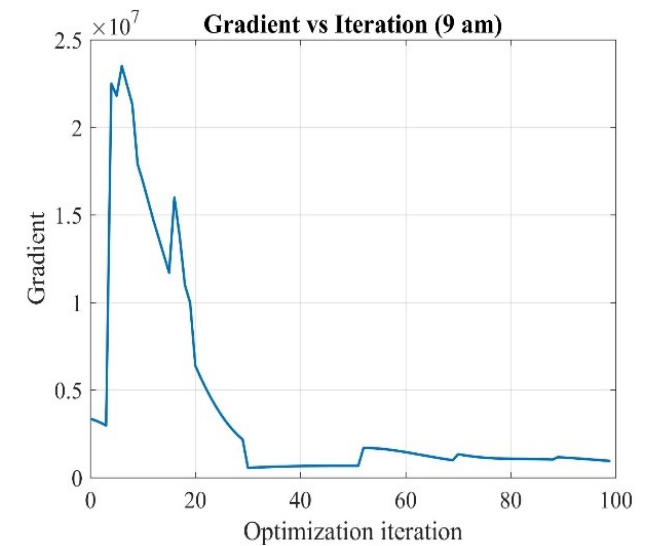
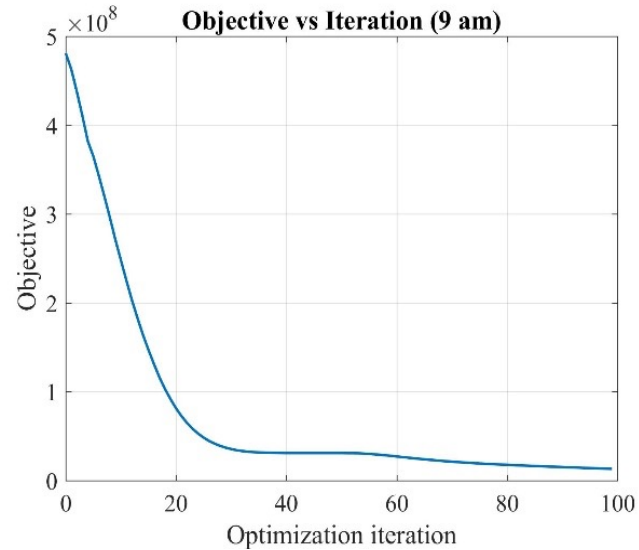
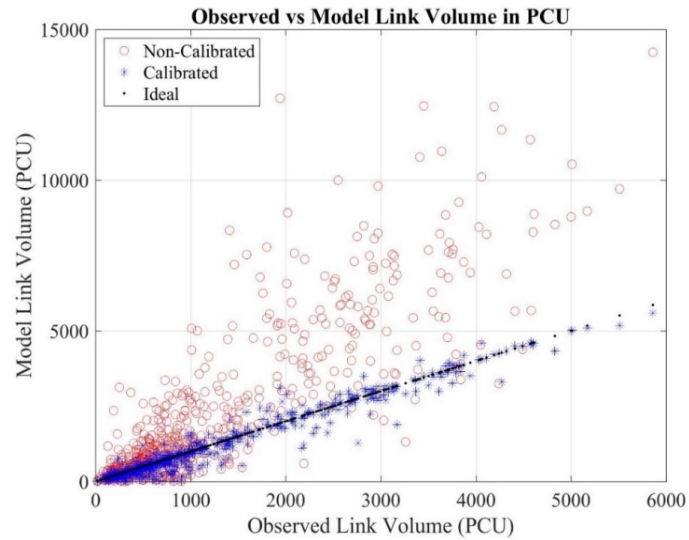
- Requires **formulation** through the **choice and network loading model**.
- Only **implemented in static setting** for now.

Application of IB in static HK Network

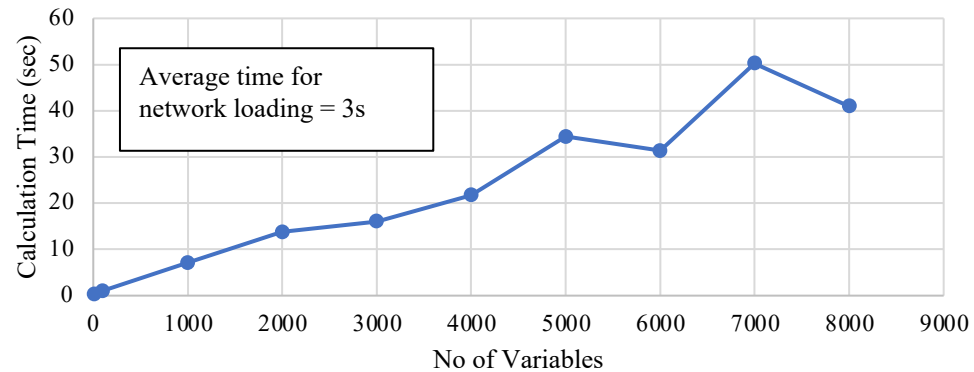


- The network contains **8,797 nodes**, **18,207 physical links**, **1,446 transit lines**, and **2,684 transit routes** with **9,222 stops** or stations.
- The number of time-specific **transit** direct and transfer **links is 433,812**.
- Transit hyper path is extracted from MATSim. The total number of **transit hyper paths** are **603,628** and **auto routes** are **56,676**.
- **591 peak hour** measurements from ATC 2016 are used for calibration.
- The total number of **origin-destination pairs** in the model is **165,509**.
- The model is **static**, and the calibration is performed **per time step** for origin and destination multiplier, i.e., $\theta \in \{\theta_{O,t}, \theta_{D,t}\}$ to save memory.
- **Variable size is 8,301**. Max memory consumption is **130 GB**.

HK OD Multiplier Calibration Result

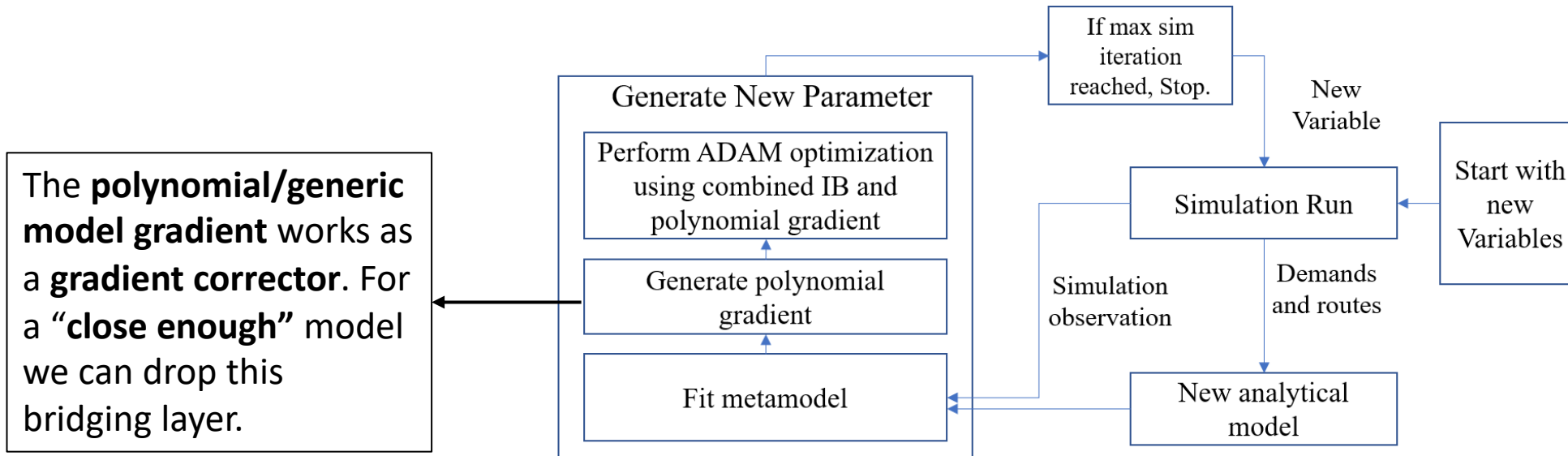


Gradient Backpropagation Calculation Time

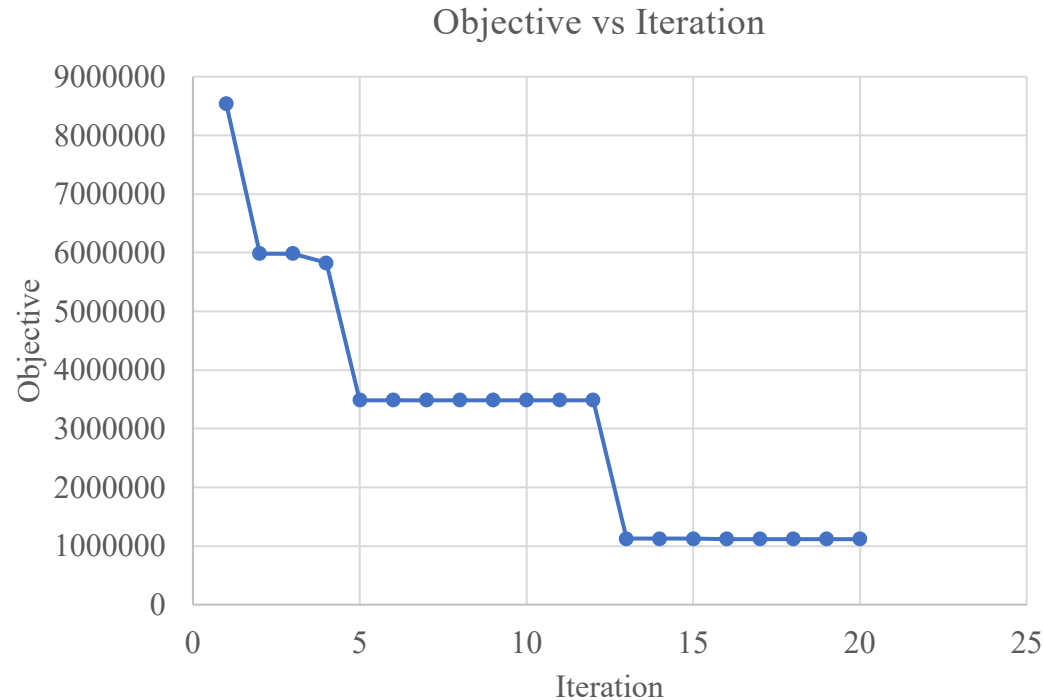


- Objective Reduction: 98.27%
- Initial vs Final MAPE: 95.29 vs 21.23%
- Initial vs Calibrated Mean GEH: 24.18 vs 6.09
- We have used ADAM (King Ma and Ba 2015) as gradient based optimizer.

Using static IB for MATSim optimization



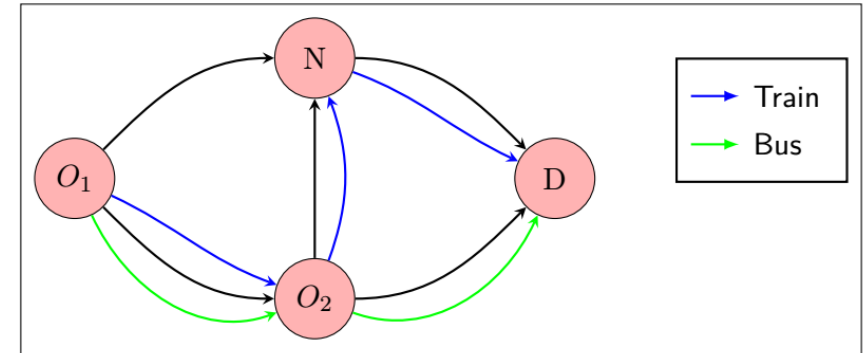
Results from a Toy Network (MATSim)



Insight:

Gradient of the fitted underdetermined polynomial worsen the convergence. Alternative metamodel should be used.

(Suggestions?)



No Polynomial Function Used

Variables: origin destination demand multipliers (O1,O2,D)

OD: O1-D, O2-D

Known: Link Counts, Train and bus passenger counts.

Dynamic Extension of IB

Key insight:

The **travel time gradient** of a route in dynamic setting is **inverse to the route output flow rate**.

Can be calculated in two ways:

- 1. Finite difference on a fixed time step DNL model.**
- 2. Flow the gradients through the network.**

We have picked Link transmission model (LTM) for its simple link and node model formulation. The insight from LTM will help push the algorithm towards event-based algorithms, i.e., Mobsim in MATSim.

Conclusion

- A metamodel corrected gradient based optimization of MATSim is explored.
- As future work, **IB** is extended for Link Transmission Model (LTM) and preferably to MATSim directly.

Thanks for your attention.

Questions?

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