Combining physics-informed machine learning with transportation science methods to tackle large-scale urban mobility problems

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Big Data, AI and Transportation Planning Applications
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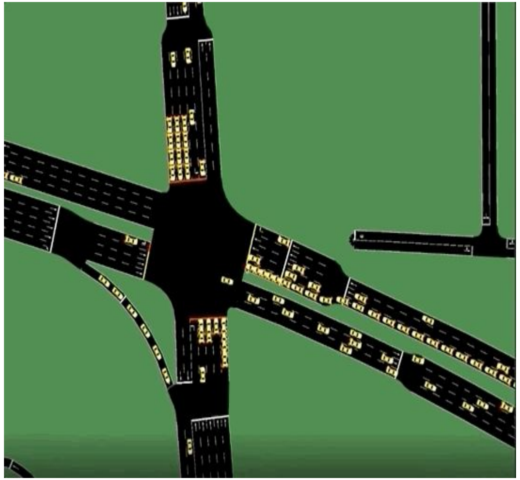
Physics-informed Traffic Optimization

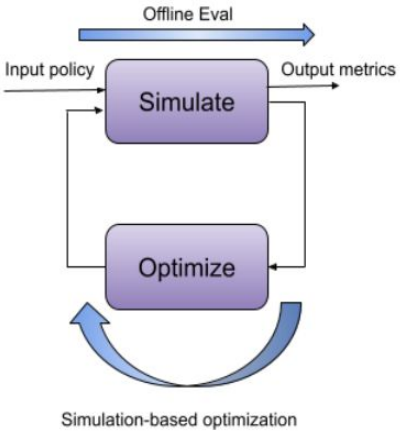
- Digital twins of mobility systems
- Physics-informed algorithms:
  - Sample efficiency
  - Dimensionality reduction
  - Variance reduction
- Future research opportunities

Simulation-based optimization for traffic operations and planning

Building high quality traffic simulations to evaluate traffic management policies and use simulation-based optimization to suggest interventions to optimize transportation networks for sustainability, safety and reduction of congestion.



Simulation of car traffic near an intersection in Salt Lake City



Urban mobility simulation + optimization finds best configurations for infrastructure and policy

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Simulation Platform

Google Maps
Routing Algorithms

Mobility Demand
(from Census, city
DOTs, 3P data
providers)

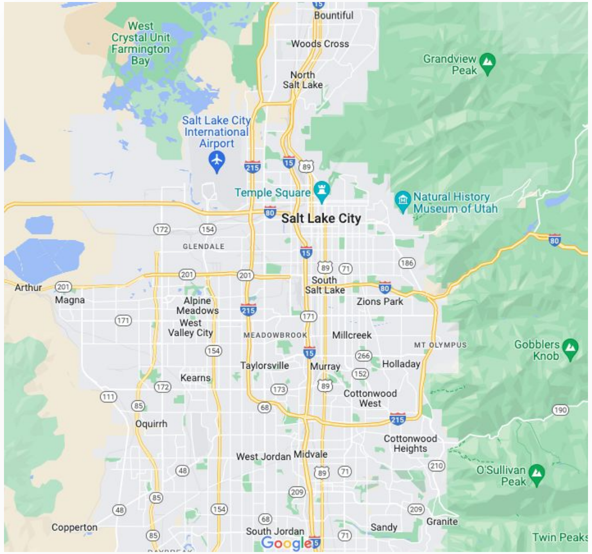
Google Maps
Network Data

Road sensor data
(from city DOTs)

SUMO
[Simulation of
Urban MObility]
based traffic
simulator

Traffic
outputs
(travel time,
speed,
volume,
emissions)

Calibration /
Optimization
Algorithms



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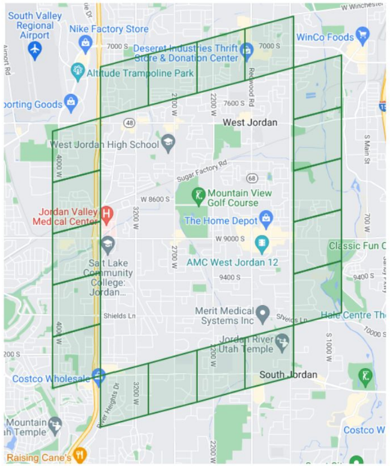
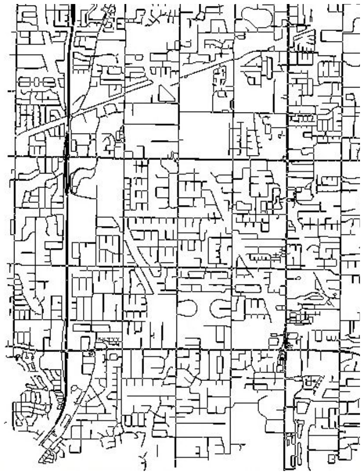
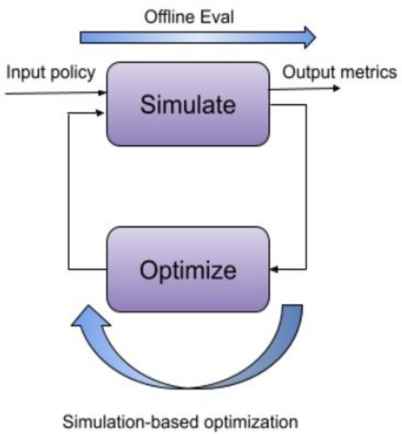
OD demand calibration







$$\min_{x} \quad f(x) = \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} w_i \left(v_i^{\mathrm{GT}} - E[v_i(x, u_1; u_2)]\right)^2$$
$$\text{s.t.} \quad 0 \le x \le x_U$$

- Goal: find a travel demand input that, once simulated, yields simulated traffic statistics that match ground truth field data.
- Traffic statistics: segment counts, segment speeds.
- Regularization
- Inverse problem
- Challenges: dimensionality, stochasticity, compute-time, non-differentiability

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(1) Achieving sample efficiency through metamodeling

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Sample efficiency: metamodeling

$$\min_{x} \quad f(x) = \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} w_i \left(v_i^{\mathrm{GT}} - E[v_i(x, u_1; u_2)]\right)^2$$
$$\text{s.t.} \quad 0 \le x \le x_U$$

$\longleftrightarrow$

$$\min_{x} \quad m_k(x; \beta_k) = \beta_{k,0} f_A(x) + \phi(x; \beta_k)$$
$$\text{s.t.} \quad f_A(x) = \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} w_i \left(v_i^{\mathrm{GT}} - v_i^{\mathrm{a}}\right)^2$$
$$\phi(x; \beta_k) = \beta_{k,1} + \sum_{z \in \mathcal{Z}} \beta_{k,z+1} x_z$$
$$\boxed{\begin{aligned} & v_i^{\mathrm{a}} = v_i^{\min} + (v_i^{\max} - v_i^{\min}) \left(1 - \left(\frac{q_i}{q_i^{\max}}\right)^{\alpha_i^1}\right)^{\alpha_i^2} \quad \forall i \in \mathcal{I} \\ & q = Ax \end{aligned}}$$
$$0 \le x \le x_U$$

- Combining macroscopic + microscopic models
- Macro: differentiable and compute-efficient
- Micro: high-resolution

Calibration on:

Path travel times:	Zhang et al. (2024) IEEE ITSC
Segment speeds:	Vishnoi et al. (2023) ACM SIGSPATIAL
Probe segment counts:	Alanqary et al. (2025) TRISTAN

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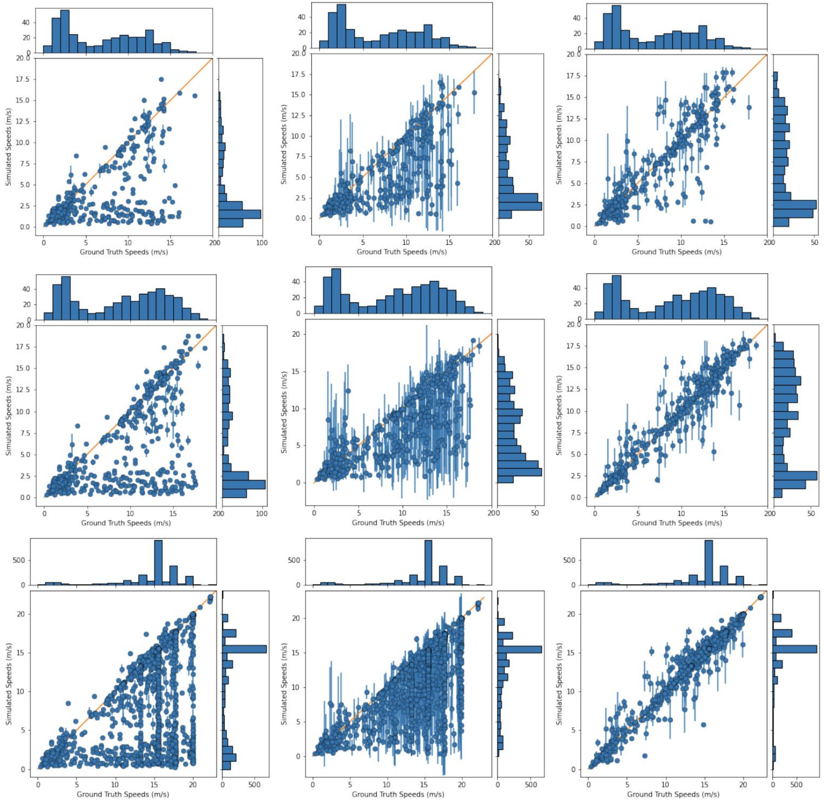
Sample efficiency: metamodeling

- Salt Lake City
- Segment speeds calibration
- 62-dimensional instance
- 100 sequential simulations



Vishnoi, S., Tsogsuren, I., Arora, N., Osorio, C. (2023) ACM SIGSPATIAL

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(2) Achieving scalability through dimensionality reduction

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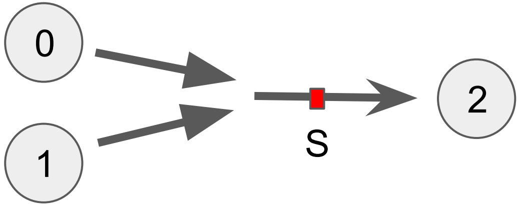
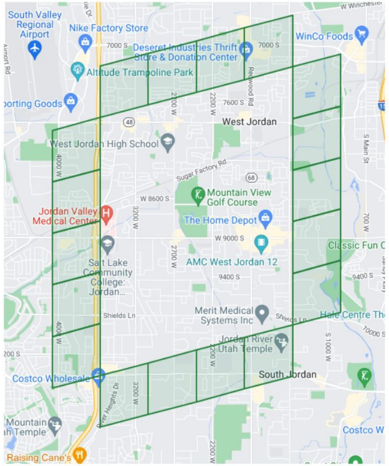
OD demand calibration

$$
\begin{aligned}
\min_{x} \quad & f(x) = \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} w_i \left(v_i^{\mathrm{GT}} - E[v_i(x, u_1; u_2)]\right)^2 \\
\text{s.t.} \quad & 0 \leq x \leq x_U
\end{aligned}
$$



- Traditional modeling approach:
  - Discretize space into disjoint zones, traffic analysis zones (TAZes)
  - Consider the set of plausible pairs of zones. High dimensional set !
- OD calibration problem is underdetermined
  - Level of underdetermination typically increases with road network size
- **Should we be solving the problem in this high-dimensional space ?**

- Find lower dimensional spaces to:
  - Enhance computational efficiency of existing calibration algorithms
  - Reduce underdetermination



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Scalability: dimensionality reduction

- Can we develop sample-efficient transportation-relevant dimensionality reduction techniques ?

- A: **assignment matrix**, network loading map
- Use a low-rank approximation of the assignment matrix A
- Singular value decomposition of A
- Select a submatrix of V of column-dimension k that captures the most information in A
- This low-rank approximation of A minimizes the L2 norm and the Frobenius norm of the difference from A
- Maps from the high d-dimensional OD space to the low k-dimensional space, designed to
    - **Preserve traffic-specific information from the assignment matrix A**
    - **Is sample-efficient: approach does not require any simulation data**
- We theoretically prove that this method reduces the underdetermination of the problem

$$A\,\theta = s$$

$$A = U\,\Sigma\,V^\top$$

$$\hat{V} \in R^{d\times k}$$

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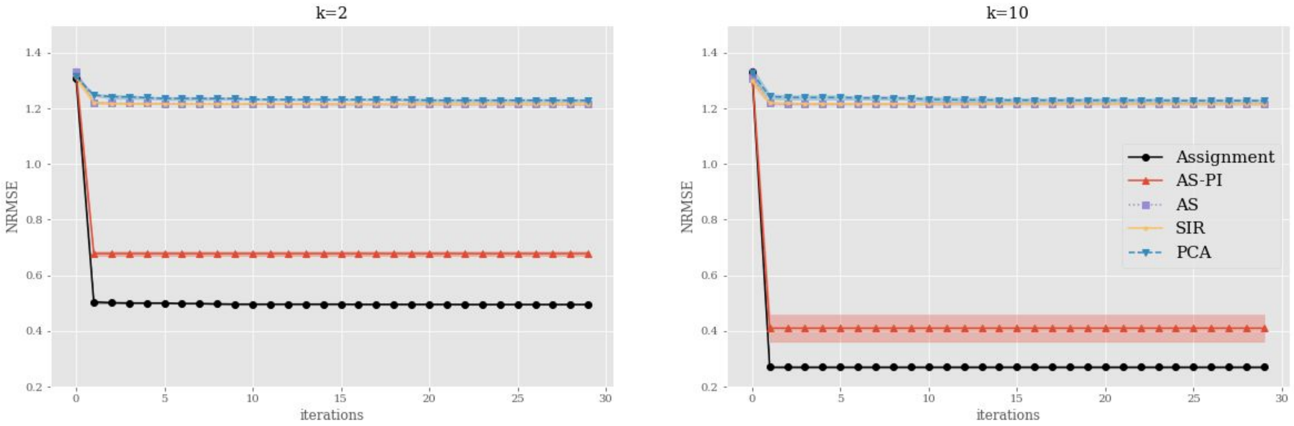
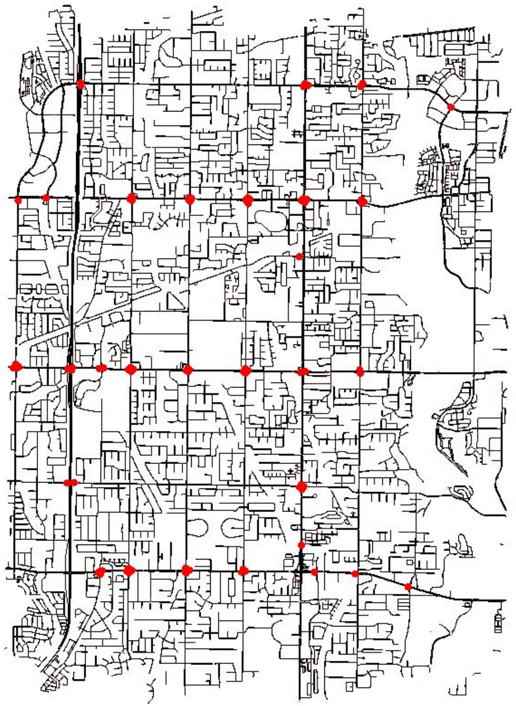
Scalability: dimensionality reduction

- 62-dimensional instance
- 79 count sensors
- Optimizer: metamodel, Osorio (2019)

- Dimensionality reduction (DR)
  - PCA principal component analysis, Pearson (1901)
  - SIR: sliced inverse regression, Li et al. (1991)
  - Active subspace, Constantine et al. (2014)
  - Physics-informed active subspace, Nguyen and Osorio (2023)
  - Assignment: Physics-informed metamodel DR, Nguyen and Osorio (2023)





Salt Lake City

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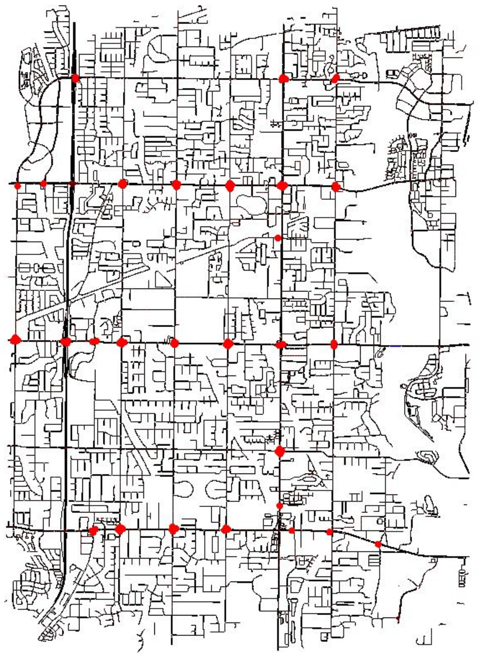
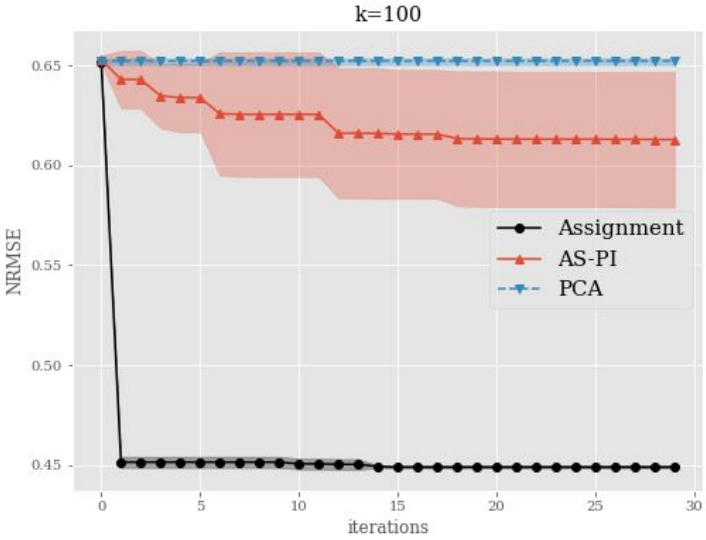
Scalability: dimensionality reduction

- 2449-dimensional instance
- 76 sensors
- Count data from Utah DOT





- Lack of sample efficiency
  - SIR: sliced inverse regression: requires initial sample of size at least d (OD dimension)
  - Active subspace: requires derivatives (simulation-based or surrogate-based)

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(3) Achieving scalability through variance reduction

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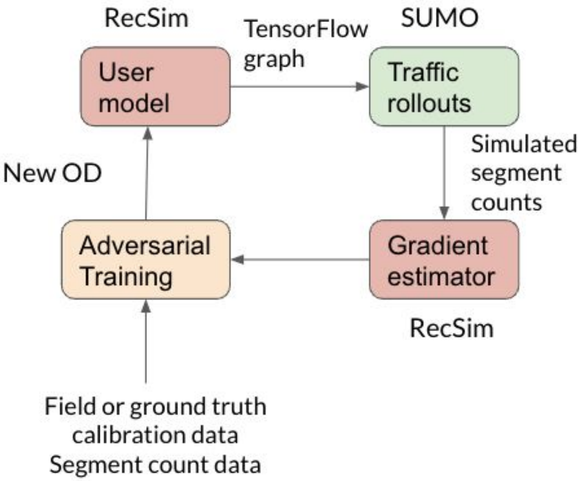
Scalability challenges: gradient estimation

- Adversarial formulation
  - Mladenov et al. (2022) ACM SIGSPATIAL
- Gradients can be estimated by a scoring function estimator:

$$\nabla_\omega \mathbb{E}_{\theta\sim\pi_\omega, o\sim s(\theta)}\left[\mathrm{loss}(o)\right] = \mathbb{E}_{\theta\sim\pi_\omega, o\sim s(\theta)}\left[\mathrm{loss}(o)\frac{\nabla_\theta \pi_\omega(\theta)}{\pi_\omega(\theta)}\right]$$

$$\approx \frac{1}{n}\sum_i \mathrm{loss}(o_i)\frac{\nabla \pi_\omega(\theta_i)}{\pi_\omega(\theta_i)} = \frac{1}{n}\sum_i \mathrm{loss}(o_i)\nabla \log \pi_\omega(\theta_i)$$



- The variance of the estimator may grow exponentially with the number of ODs (dimensi
- Mitigation:
  - variance reduction technique
  - metamodel-based control variates

Field data	$o \in O$
Parameter space:	$\theta \in \Theta$
Simulator:	$s_\theta \in \Delta(O)$

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Variance reduction techniques

- In Monte Carlo simulation the error goes as: $\sigma / \sqrt{n}$
- Reduce variance by:
  - Increasing n
  - <u>Decreasing σ</u>

- Control variates
  - Goal: estimate $E[X] = \nu$

  - Consider a r.v. Y with known mean μ
  - Choose Y such that:
    - $E[X - (Y-\mu)] = \nu$
    - $Var(X - (Y-\mu)) < Var(X)$

  - Simulate: $X - \lambda(Y-\mu)$
  - With an optimal choice of λ: $Var(X - \lambda(Y-\mu)) = Var(X) (1 - \rho^2)$
    ρ : correlation of X and Y
  - Amount of variance reduction depends on how well the two correlate.

- Define metamodel-based control variates

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Metamodel-based variance reduction

$$\nabla_\omega \mathbb{E}_{\theta\sim\pi_\omega, o\sim s(\theta)}[\text{loss}(o)] \approx \frac{1}{n}\sum_i \text{loss}(o_i)\nabla \log \pi_\omega(\theta_i)$$

$$\nabla_\omega \mathbb{E}_{\theta\sim\pi_\omega, o\sim s(\theta)}[\text{loss}(o)] = \frac{1}{n}\sum_i (\text{loss}(o_i) - \lambda \text{loss}(\mathrm{s_i}))\, \nabla \log \pi_\omega(\theta_i) + \lambda\mu$$

1. Sample ODs θ_i from π_ω
2. Simulate θ_i to obtain counts o_i
3. Compute metamodel counts s_i : $A\,\theta = s$

4. New gradient estimator based on metamodel error

$$\nabla_\omega \mathbb{E}_{\theta\sim\pi_\omega, o\sim s(\theta)}[\text{loss}(o)] = \frac{1}{n}\sum_i (\text{loss}(o_i) - \lambda \text{loss}(\mathrm{s_i}))\, \nabla \log \pi_\omega(\theta_i) + \lambda\mu$$

- μ : mean of the metamodel gradient estimator (can be computed on a much larger sample)
- λ : scaling parameter

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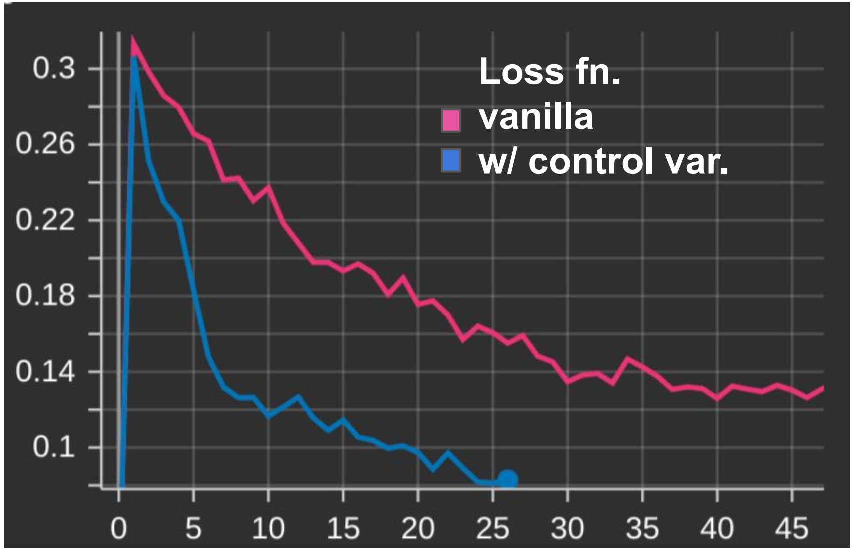
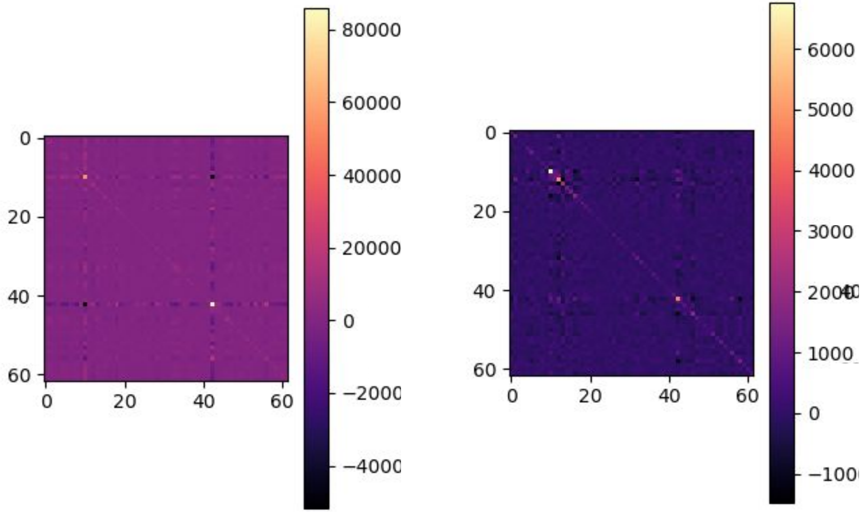
Metamodel-based variance reduction

62-dimensional Salt Lake City case study





- 2x faster convergence
- Variance reduction on the order of 10x is often observed.

Gradient covariance matrix: vanilla vs. control variate

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Opportunities

- Travel demand calibration: Traffic physics + metamodeling enables scalability through:
  - Enhanced sample efficiency
  - Dimensionality reduction
  - Variance reduction
- Treating the transportation system and data as a gray-box rather than a black-box

- Big-data + deep learning models are not plug-and-play
  - Lack sample efficiency, lack scalability
  - There is great potential to enhance them for transportation applications through the use of simple transportation science ideas

- Most transportation stakeholders live in a data sparse, and/or often compute sparse, environment: Importance of designing data-efficient and sample-efficient methods relevant for transportation

- Data-efficiency
  - How can we make the most out of our existing field data?
    - Use of higher-order statistics from, spatially or temporally, sparse field data
  - How can we use it to:
    - Quantify uncertainty, and derive more resilient and robust mobility solutions ?
      - Quantification of model parameter uncertainty: Greisemer et al. (2024) NeurIPS
    - Reduce the level undetermination or ill-posedness of fundamental transportation problems?

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Thank You

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