Sustainable Urban Mobility: Simulation and Optimization Workshop

Controllable Physics-Aware Generative Model for Urban Travel Demand Calibration

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Urban Travel Demand Calibration

- Transportation agencies and stakeholders worldwide commonly develop traffic simulation models of their road networks and use them to inform a variety of planning and operational decisions.

- Calibrating the input parameters of these simulators is an important offline optimization problem:
  - High simulation costs;
  - Specific sample from limited observed traffic information;
  - Evaluate counterfactual (what-if) scenarios
  - …

Motivation - Origin-Destination (OD) Calibration

- (Static) OD calibration aims to <u>identify an OD matrix</u> from a hypothesized distribution, resulting in simulated metrics that accurately reflect field-observed traffic conditions:
    - high-dimensionality,
    - non-convexity,
    - underdetermined,
    - simulation-based nature
    - …
- Explore the Deep Generative Models.

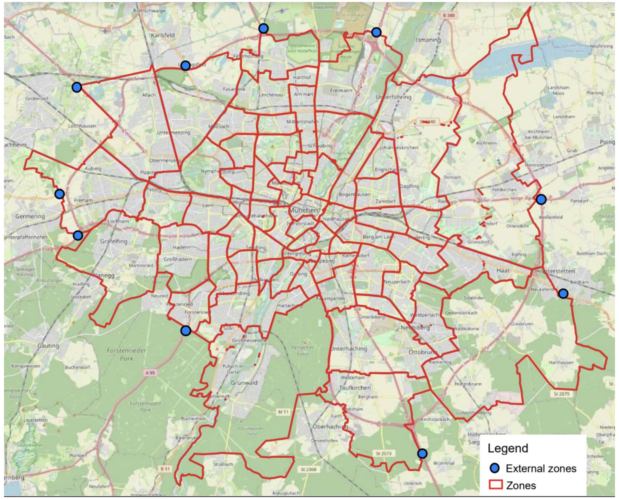

Figure 1. Topology of Munich network with major region Traffic zones

Transportation Science (Parameter tuning process) → Machine Learning (Model fitting process)

Motivation - Gray-box / Hybrid modeling

- ➢ Gray-box: data-driven + theory-driven

- ➢ Deep Generative Models:
  - E.g., Variational Autoencoders (VAEs); Generative Adversarial Networks (GANs); Diffusion Models…
  - Extracting complex relationships via data-driven method;
  - Generating samples from the learned latent distribution.

- ➢ Physics knowledge:
  - Contributing to data efficiency;
  - Constraining the generative model's latent space;
  - Carrying out counterfactually robust transportation analysis.
  - Transportation domain: analytic equations[1] such as the continuity equations.

[1] Osorio, Carolina. "Dynamic origin-destination matrix calibration for large-scale network simulators." *Transportation Research Part C: Emerging Technologies* 98 (2019): 186-206.

Outline

- **Motivation**
  - Urban Travel Demand Calibration (Black box)
  - Gray-box / Hybrid modeling
- **Problem Setting**
  - Bayesian Perspective
- **Controllable Physics-Aware Variational Autoencoders**
  - Physics analytical model
  - Controllable Physics Information
  - Conditional variational autoencoder (CVAE)
  - Training Objective

- **Results**
  - Experiments Settings
  - Comparison to SOTA Methods
  - Comparison to Neural Baselines
  - Qualitative Evaluations
    - Convergence speed
    - OD Distribution
    - Traffic Flow Calibration

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OD Calibration Problem Formulation from Bayesian Perspective

- Instead of obtaining a single calibrated point estimate d for an observed traffic flow y, we now seek a posterior $p(d|y)$.

- Samples $d \sim p(d|y)$ are OD matrices likely to have yielded the observed traffic flow under the likelihood $p_S(y|d)$ defined by the traffic simulator S.

OD Calibration Problem Formulation from Bayesian Perspective

- The posterior can be given in the standard setup for Bayesian inference:

$$p(d|y, d^{\text{prior}}) = \frac{p(y|d)p(d|d^{\text{prior}})}{p(y|d^{\text{prior}})} = \frac{p(y|d)p(d|d^{\text{prior}})}{\int p(y|d)p(d|d^{\text{prior}})dd}$$

$p(d|d^{prior})$ defines the prior distribution, conditional on the provided noisy OD d^{prior}.

- For the likelihood, we view the traffic simulator S as implicitly defining $p(y|d)$:

$$p(y|d) = \int p_S(y, z|d)dz = \int p_S(y, u_1, u_2|d)du_1 du_2,$$

i.e. marginalizing over the possible trajectories z in the simulator's latent space, where u_1, u_2 are vectors of simulators.

→ Conditional VAE

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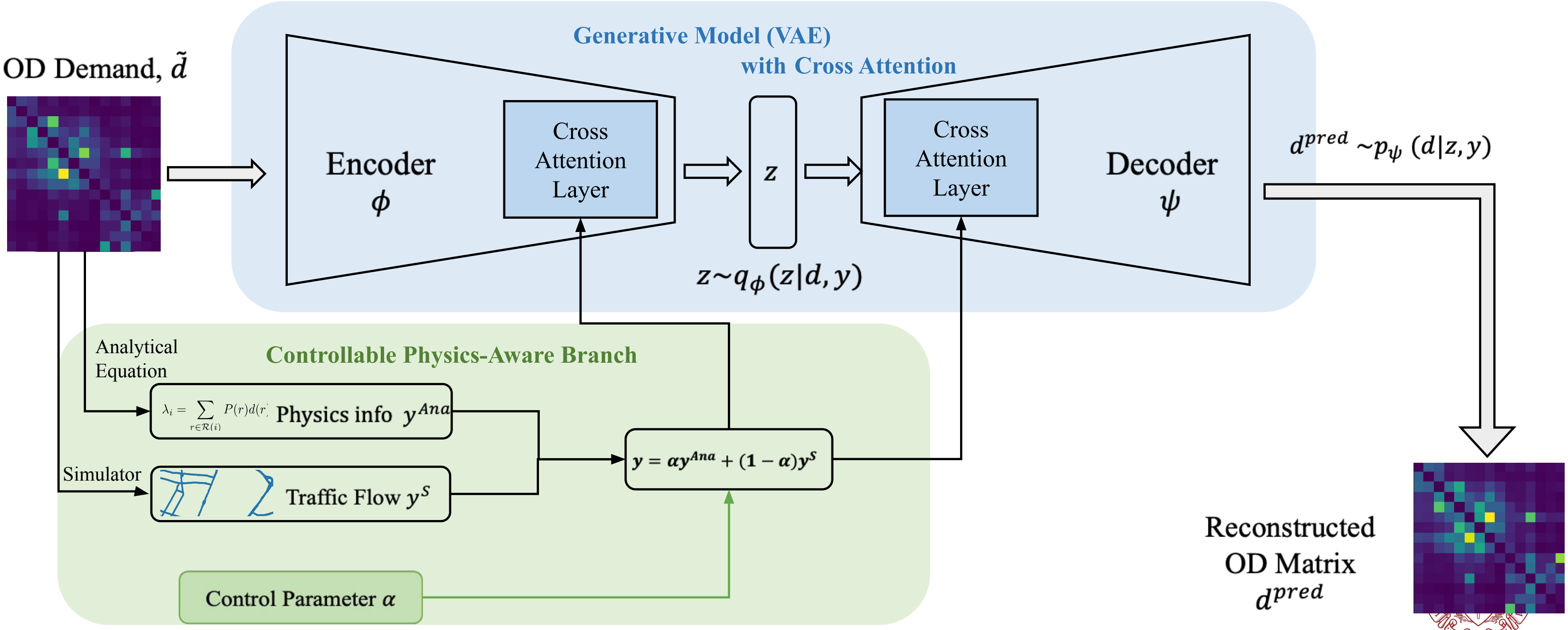
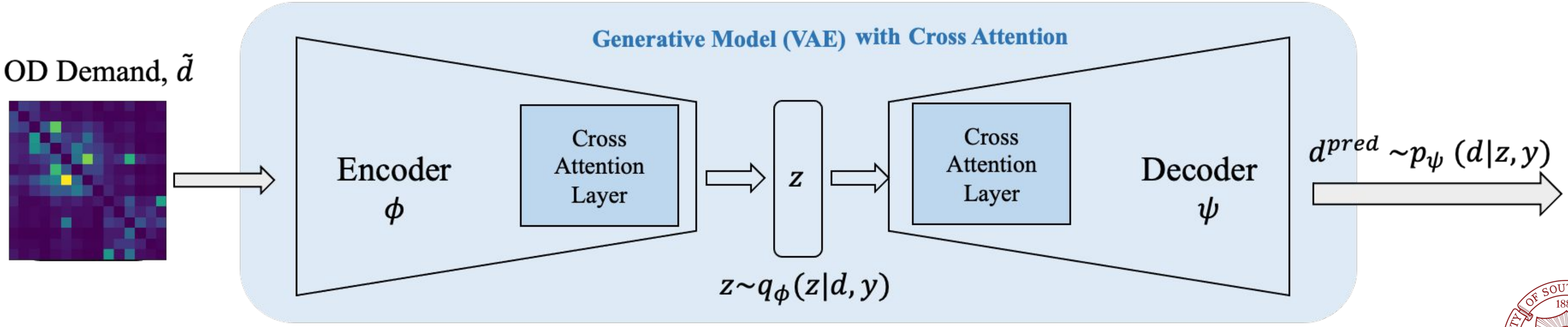
Controllable Physics-Aware Variational Autoencoders



Conditional variational autoencoder (CVAE)

- ➢ Encoder: learn the hidden representation of given data and the distribution of $q_\phi(z|d,y)$.
- ➢ Decoder: decode the hidden representation to input space and captures the distribution $p_\psi(d|z,y)$;

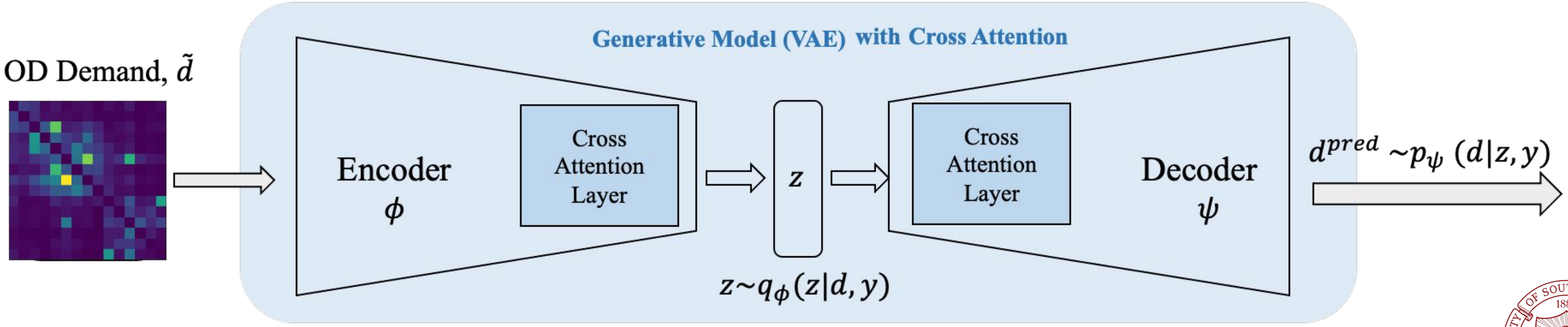


Control-VAE

- ➢ Traffic flows and OD pairs are under the same physics mechanisms but have different modalities
- ➢ Cross-attention Fusion: traffic flows as keys and values in a cross-attention mechanism

$$\mathrm{Att}_h\left(Q_h, K_h, V_h\right) = \mathrm{Softmax}\left(\frac{Q_h {K_h}^T}{\sqrt{d_k}}\right) V_h,$$

$$\text{where } Q_h = W_h^Q f(d); K_h = W_h^K g(y); V_h = W_h^V g(y).$$



Physics analytical model

➢ Linear approximation of a simulator on link i [1] based on the travel behavior:

$$\lambda_i = \sum_{r \in \mathcal{R}(i)} P(r) d(r)$$

$R(i)$ denotes the set of routes that travel through link i. $d(r)$ denotes the OD pair of route r and $P(r)$ denotes the probability of choosing route r.

➢ $P(r)$ is a multinomial logit model with a utility function that depends on the route's travel time t_r[1]:

$$P(r) = \frac{\exp(\theta t_r)}{\sum_{j \in \mathcal{R}(r)} \exp(\theta t_j)},$$

t_j denotes the travel time of route j, θ is a travel time scalar parameter.

[1] Arora, Neha, et al. "An efficient simulation-based travel demand calibration algorithm for large-scale metropolitan traffic models."
[2] Osorio, Carolina. "High-dimensional offline origin-destination (OD) demand calibration for stochastic traffic simulators of large-scale road networks." Transportation Research Part B: Methodological 124 (2019): 18-43.

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➢ Controllable Physics Information:

- balance between physics-knowledge and simulation information:

$$y = \alpha y^{Ana} + (1 - \alpha) y^s.$$

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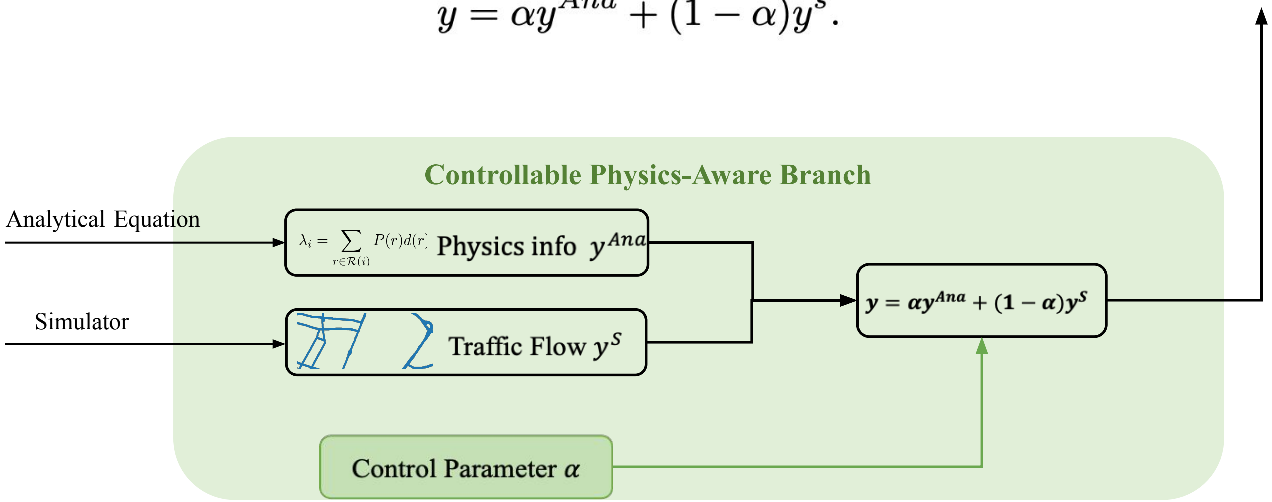

Training Objective of Control-VAE

➢ Conventional CVAE variational lower bound[1]:

$$L_{\text{CVAE}} = -\mathbb{E}_{\boldsymbol{z} \sim q_{\psi}(\boldsymbol{z}|d,y)}[\log p_{\psi}(d|y, \boldsymbol{z})] + D_{KL}(q_{\phi}(\boldsymbol{z}|d, y)||p_{\psi}(\boldsymbol{z}|y))$$

➢ Regularizer aligning the physics information with simulator's behavior:

$$L_{\text{MSE}} = ||y^{Ana} - \tilde{y}||_2^2$$

➢ Total loss:

$$L = L_{\text{CVAE}} + \gamma L_{\text{MSE}}$$

[1] Sohn, Kihyuk, Honglak Lee, and Xinchen Yan. "Learning structured output representation using deep conditional generative models." *Advances in neural information processing systems* 28 (2015).

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Experiments Setting

- High dimensional Munich network[1]:
  - 5329 origin-destination (OD) pairs;
  - 507 detector locations;
  - 5:00 am -10:00 am;
  - $x_c = (p + q \times \delta) \times \hat{d}$, p: reduction; q: randomization
    - Set I: p=0.7, q=0.15;
    - Set II: p=0.7, q=0.3.

Figure 5: Overview of Munich Traffic Network

- Simulator:
  - Simulation of Urban MObility (SUMO);
  - Other traffic simulators …

[1] Qurashi, Moeid, et al. "Dynamic demand estimation on large scale networks using Principal Component Analysis: The case of non-existent or irrelevant historical estimates." *Transportation Research Part C: Emerging Technologies* 136 (2022): 103504

Experiments Results - Comparison to SOTA Methods

Table 1: Comparison to the SOTAs on the Munich Network (RMSN (%)).

		Munich 5-6	Munich 6-7	Munich 7-8	Munich 8-9	Munich 9-10
Set I	SPSA	24.67±1.81	24.59±2.41	21.24±1.33	47.06±0.64	18.40±0.44
	PC-SPSA	**15.40**±2.71	35.05±0.44	22.64±2.61	28.36±4.66	21.94±0.51
	ControlVAE	17.40±0.87	**22.02**±1.45	**17.55**±1.29	**19.89**±1.84	**16.28**±1.22
Set II	SPSA	18.00±1.12	43.10±0.24	55.89±2.31	50.04± 0.61	36.13±0.43
	PC-SPSA	15.03±0.71	35.66±0.42	23.46±3.23	28.79±0.51	22.31±0.51
	ControlVAE	**14.89**±0.56	**21.74**±1.59	**18.32**±1.83	**21.02**±1.84	**16.38**±1.02

➢ The higher calibration quality of the data-driven approach for high-dimensional problems than traditional state-of-the-art methods (SPSA, PC-SPSA) .

Experiments Results - Comparison to Neural Baselines

Table 2: Comparison to Neural Baselines on the Munich Network (RMSN (%)).

		Munich 5-6	Munich 6-7	Munich 7-8	Munich 8-9	Munich 9-10
Set I	Original	97.08±1.23	52.20±0.72	36.40±1.63	49.76±0.80	43.92±0.56
	CVAE	22.00±1.59	22.98±2.15	19.28±2.81	23.31±2.81	30.56±1.09
	CVAE-catt	18.45±0.61	22.41±2.00	19.33±1.70	20.96±0.82	16.34±1.17
	CVAE-phy	21.43±2.85	22.04±2.48	20.78±1.35	23.92±2.37	17.48±1.30
	ControlVAE	**17.40**±0.87	**22.02**±1.45	**17.55**±1.29	**19.89**±1.84	**16.28**±1.22
Set II	Original	97.20±1.62	87.52±1.62	101.3±3.15	70.21±0.64	80.70±0.58
	CVAE	46.23±0.91	24.57±1.90	26.28±1.60	27.09±1.69	18.25±0.67
	CVAE-catt	16.43±0.79	30.72±1.76	18.47±1.75	21.60±1.55	19.42±1.15
	CVAE-phy	15.73±1.00	22.75±1.71	21.76±3.08	28.63±1.86	17.93±1.04
	ControlVAE	**14.89**±0.56	**21.74**±1.59	**18.32**±1.83	**21.02**±1.84	**16.38**±1.02

➢ Original: RMSE between the traffic flow generated by the noised OD demand and the real traffic flow.

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➢ Control VAE vs. others: demonstrate it can control the interaction of assistance between physics-informed and data-driven machine learning.

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- CVAE-catt: Cross-attention using simulation information;
- **CVAE-phy**: Cross-attention using analytic information.
  - Further improvement for efficiency.

Qualitative Evaluations - Convergence speed

- SPSA and PC-SPSA can only be serially iterated, while generative neural network-based methods can collect data **parallelly**.

- The generative neural network-based approach uses **fewer samples** to achieve the desired performance, than both SPSA and PC-SPSA, where people generally care about the best result across all current iterations.

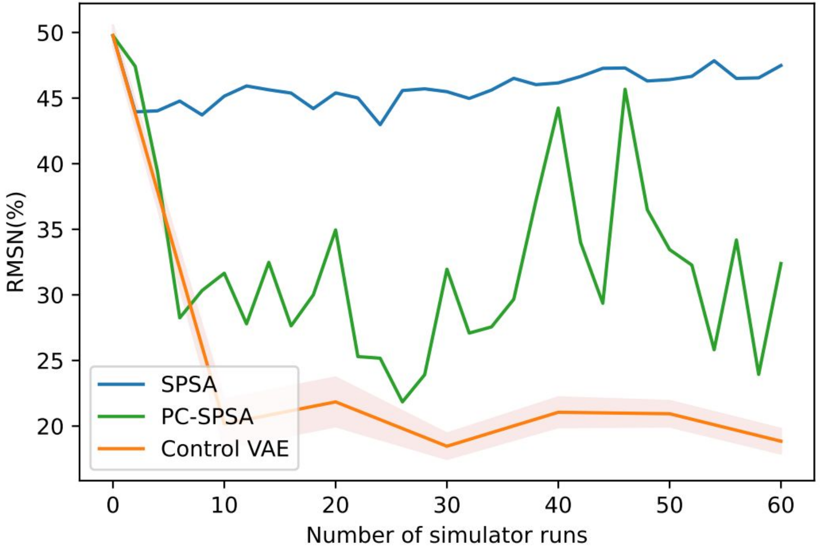


Figure 6: The converge curve based on the count of simulator running on M89, Set I.

Qualitative Evaluations - OD Distribution

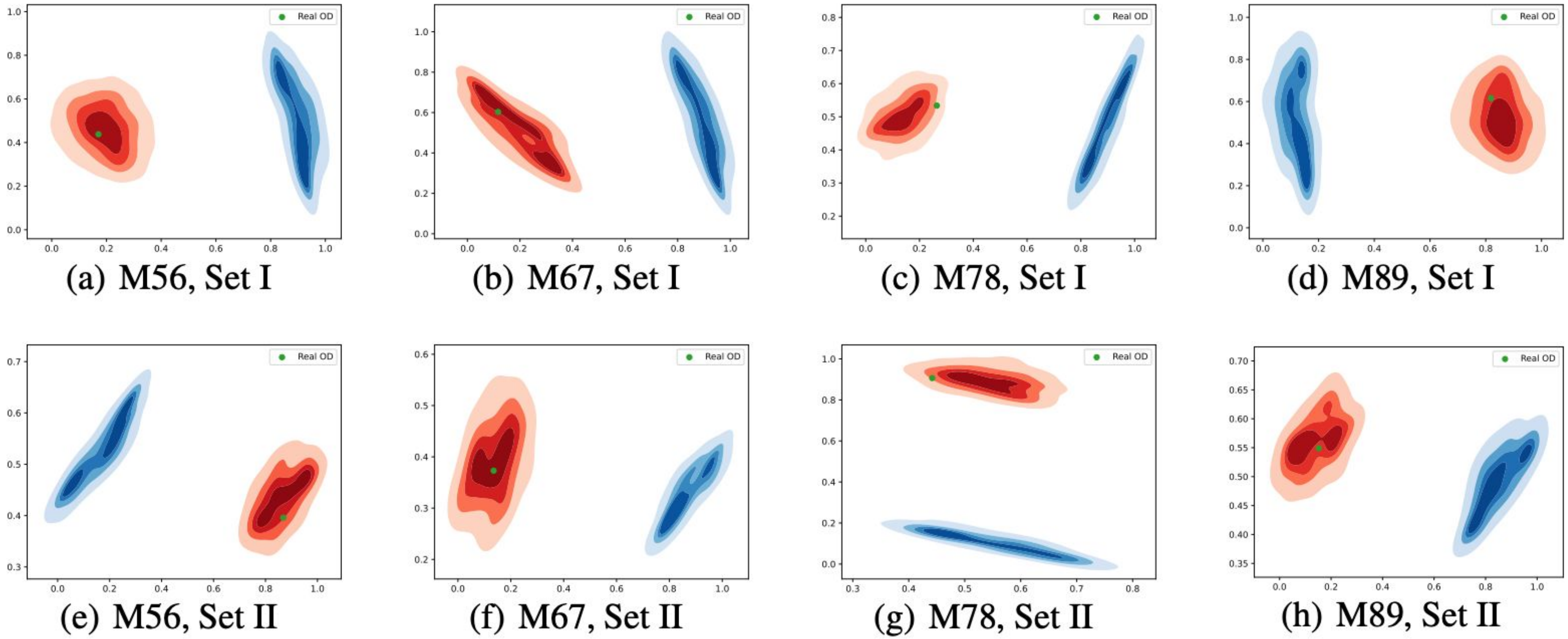
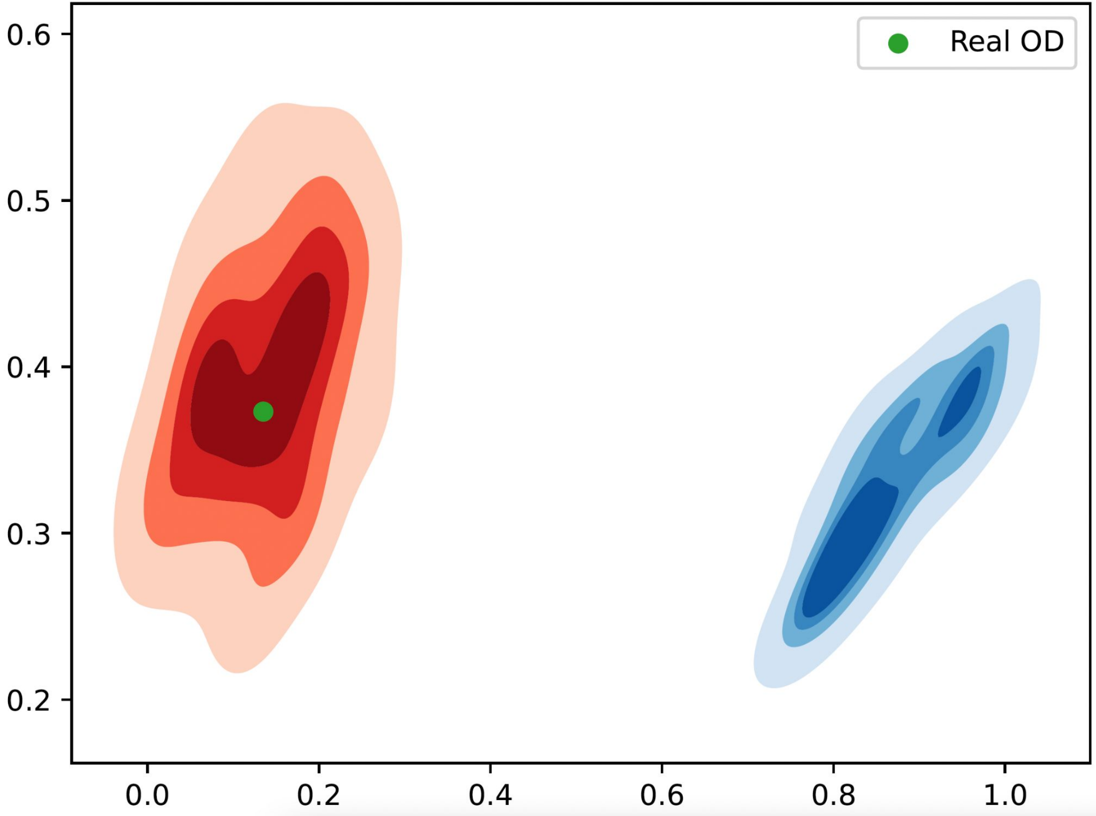


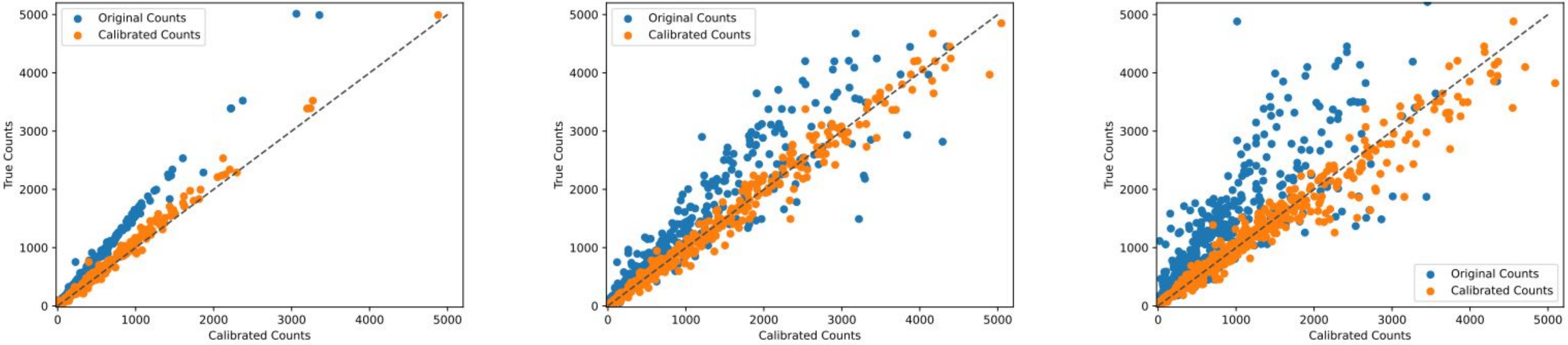
Figure 7: Calibration Distribution Results on OD demand. The blue cluster is the prior distribution of input OD and the red cluster is the calibrated OD distribution condition on observed traffic counts. The green dot refers to the real OD that we aim to identify.

Qualitative Evaluations - OD Distribution



- ➢ The effectiveness of our model on large-scale datasets to assign high probability to the true OD solution;
- ➢ Our proposed model assigns some probability to other possible solutions, not just the single most likely one.

Qualitative Evaluations - Traffic Flow Calibration



(a) M56, Set I (b) M67, Set I (c) M89, Set I

Figure 8: Calibration Results on Traffic Counts.

- ➢ The proposed method identifies ODs that yield an excellent fit to the real data (even for the morning peak period of 8:00 am-9:00 am).
- ➢ This excellent fit holds for all detector locations.

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Thank you!

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