



SPATIO-TEMPORAL FORECASTING

Deterministic Graph Neural Networks for Carbon Emissions and Generative
Probabilistic Stochastic Differential Equation-based Diffusion for Traffic Flow

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RESEARCH OVERVIEW

Investigations on Deterministic and Probabilistic Forecasting

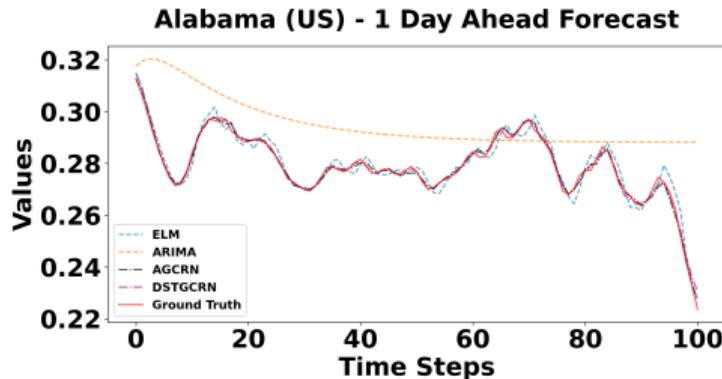


Figure 1: A glimpse of forecasts comparison for deterministic carbon emissions forecasting

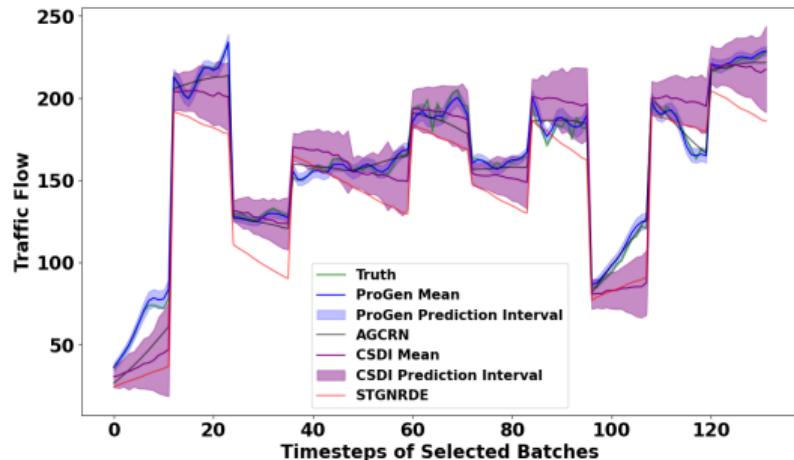


Figure 2: A glimpse of forecasts comparison for probabilistic traffic flow forecasting

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INTRODUCTION

DSTGCRN: Background and Motivation

Background:

- » Increase in carbon emissions due to fossil fuels and land degradation.
- » Accurate forecasting is vital to:
 - Inform sustainable policies.
 - Meet reduction targets:
 - China: Peak by 2030.
 - US: Reduce 50-52
 - EU: Cut 55

Challenges:

- » Models often overlook non-linear trends and regional dependencies.
- » Forecasting difficulties:
 - Variability within regions impacts total emissions.
 - Dynamics between regions significantly influence local emissions.

INTRODUCTION

DSTGCRN: Motivations and Contributions

Motivations:

- » Overcome limitations of traditional methods in handling complex, dynamic environmental data.
- » Leverage insights from the success of Graph Neural Networks (GNNs) in sectors such as traffic and energy to enhance spatial-temporal analysis.

Contributions:

- » Combines Graph Convolutional Networks (GCN) and Recurrent Neural Networks (RNN) to model evolving inter-regional relationships and spatial-temporal dynamics.
- » Boosts predictive accuracy and offers comprehensive insights to guide environmental policy.
- » Facilitates informed, real-time policy decisions adapted to specific regional contexts.

LITERATURE REVIEW

Statistical and Machine Learning Approaches

» Statistical Methods:

- **ARIMA Models:** Employed for time series forecasting; adjusts for trends and seasonality.
- **Grey Forecasting Models (GM):** Effective under conditions of limited or incomplete data, applicable in emerging markets.
- **Hybrid Models:** Combining GM and ARIMA to address non-linear and non-stationary data, enhancing forecast accuracy.

» Machine Learning Methods:

- **Deep Learning:** Excels in learning complex data patterns, significantly improving prediction capabilities.
- **Hybrid Approaches:** Integration of neural networks with statistical methods boosts accuracy and reliability.
- **Regional Variability:** Challenges include accommodating diverse environmental conditions, impacting scalability and model performance.

LITERATURE REVIEW

Advancements in Spatial-Temporal Predictions

» **Spatial-Temporal Graph Neural Networks (STGNNs):**

- At the cutting edge for modeling dynamic interdependencies across locations and times, crucial for precise environmental forecasts.
- Adaptive graph structures in these models allow responsiveness to temporal changes, enhancing long-term prediction reliability.

» **Attention Mechanisms:**

- Prioritize crucial features and time steps, improving focus on significant data and reducing irrelevant noise.
- Demonstrates enhanced detail and accuracy in environmental data analysis, effectively managing spatial and temporal dimensions.

METHODOLOGY

Problem Definitions and Setup

- » **Multisource Time Series Forecasting:** Forecast future values using data from multiple regions on features like temperature and AQI.

Forecast $\mathbf{Y}_{t+1}, \dots, \mathbf{Y}_{t+Q}$ using $f : \mathbb{R}^{N \times P \times C} \rightarrow \mathbb{R}^{N \times Q}$

Here, $\mathbf{Y}_t \in \mathbb{R}^N$ denotes the output vector at time t , P is the number of past time steps considered, and C represents the number of features per step.

- » **Regional Carbon Emission Network:** Models interdependencies among regions through a graph structure to enhance predictive accuracy by integrating spatial dynamics.

$$\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{A}), \quad \mathbf{A}_{ij} = \begin{cases} 1 & \text{if there is a direct connection between regions } i \text{ and } j, \\ 0 & \text{otherwise.} \end{cases}$$

Here, \mathcal{V} are nodes (regions), \mathcal{E} are edges (connections), and \mathbf{A} is the adjacency matrix showing regional connections.

METHODOLOGY

AGCRN-Core Modeling Approach

» Node Embedding and Graph Convolution:

$$\mathbf{X}'_t = \left(\mathbf{I}_N + \text{softmax} \left(\text{ReLU} \left(\mathbf{E} \cdot \mathbf{E}^\top \right) \right) \right) \mathbf{X}_t \Theta$$

where \mathbf{I}_N is the identity matrix, Θ is the weight matrix.

» Integration with GRU:

$$\tilde{\mathbf{A}} = \text{softmax}(\text{ReLU}(\mathbf{E} \cdot \mathbf{E}^T))$$

$$\mathbf{R}_t = \sigma \left(\tilde{\mathbf{A}}[\mathbf{X}_t, \mathbf{H}_{t-1}] \mathbf{E} \mathbf{W}_r + \mathbf{E} \cdot \mathbf{b}_r \right)$$

$$\mathbf{U}_t = \sigma \left(\tilde{\mathbf{A}}[\mathbf{X}_t, \mathbf{H}_{t-1}] \mathbf{E} \mathbf{W}_u + \mathbf{E} \cdot \mathbf{b}_u \right)$$

$$\hat{\mathbf{H}}_t = \tanh \left(\tilde{\mathbf{A}}[\mathbf{X}_t, \mathbf{U}_t \odot \mathbf{H}_{t-1}] \mathbf{E} \mathbf{W}_h + \mathbf{E} \cdot \mathbf{b}_h \right)$$

$$\mathbf{H}_t = \mathbf{R}_t \odot \mathbf{H}_{t-1} + (1 - \mathbf{R}_t) \odot \hat{\mathbf{H}}_t$$

METHODOLOGY

Dynamic Spatial-Temporal Modeling

- » **Dynamic Embeddings:** Generate node embeddings that evolve over time, reflecting changing regional interdependencies. The update mechanism for these embeddings is given by:

$$\mathbf{E}_t = \text{DynamicEmbedding}(\mathbf{x}_t), \quad \mathbf{x}_t \in \mathbb{R}^{P \times N \times C}$$

where \mathbf{x}_t represents the input features across P past time steps, N regions, and C features.

- » **Multihead Attention:** Applies multihead attention to capture distinct temporal patterns, enhancing the model's predictive accuracy. The mechanism is defined as:

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax} \left(\frac{(\mathbf{x}_t'' \mathbf{W}_Q)(\mathbf{x}_t'' \mathbf{W}_K)^\top}{\sqrt{d_e}} \right) \mathbf{x}_t'' \mathbf{W}_V$$

where \mathbf{Q} , \mathbf{K} , \mathbf{V} are the queries, keys, and values, respectively, transformed by the weight matrices \mathbf{W}_Q , \mathbf{W}_K , \mathbf{W}_V , \mathbf{x}_t'' is the processed input, and d_e denotes the embedding dimension.

METHODOLOGY

Framework Visualization

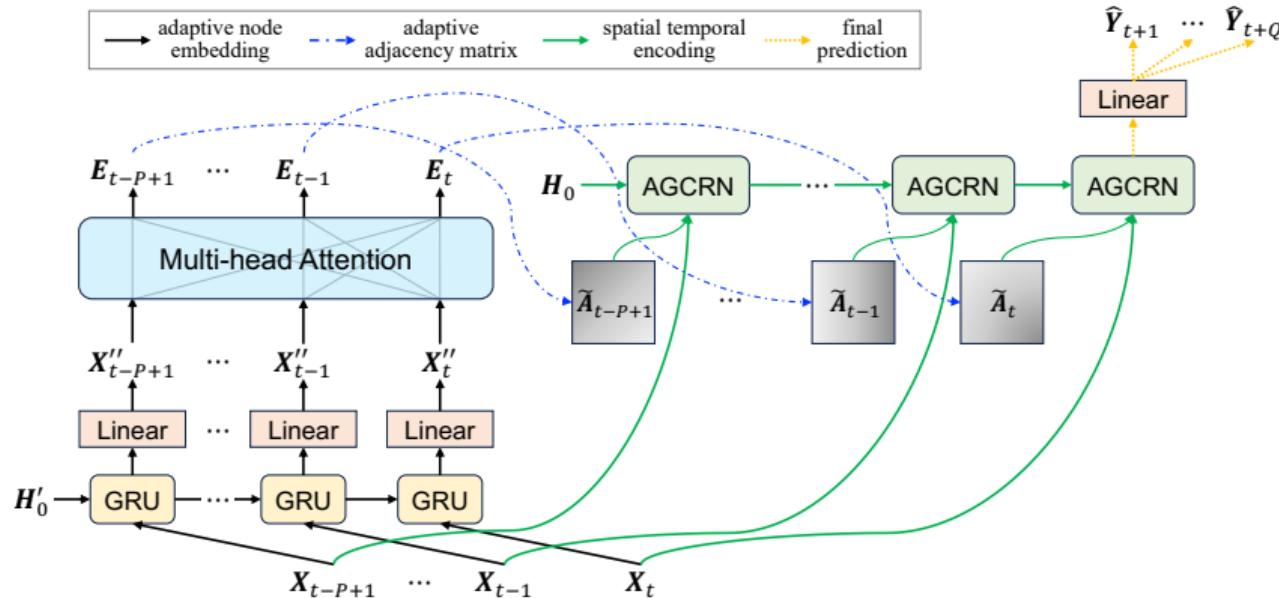


Figure 3: The architecture of the Dynamic Spatial-Temporal Graph Convolutional Recurrent Network (DSTGCRN).

RESULTS

Performance Across Datasets

Horizon	Model	MAE			MAPE			RMSE			RMSPE			R^2		
		China	US	EU	China	US	EU	China	US	EU	China	US	EU	China	US	EU
Q=1	AR/VAR*	.113	.038	.049	12.80%	16.02%	23.71%	.133	.045	.061	15.17%	18.90%	31.63%	-2.434	-3.123	-0.725
	SVR	.036	.011	.021	4.57%	5.22%	5.89%	.044	.013	.028	5.53%	6.22%	7.40%	0.363	0.313	0.743
	ARIMA	.083	.027	.059	9.83%	11.34%	15.29%	.101	.032	.076	11.63%	13.35%	18.68%	-1.656	-1.434	-0.908
	MLP	.045	.018	.032	5.80%	7.02%	11.11%	.070	.030	.069	8.33%	9.41%	15.93%	0.715	0.535	0.453
	FC-LSTM	.075	.023	.031	9.97%	9.50%	11.99%	.112	.040	.064	13.36%	12.17%	17.08%	0.263	0.312	0.426
	ELM	.025	.005	.005	2.36%	1.71%	1.41%	.032	.006	.007	3.19%	2.19%	1.86%	0.772	0.907	0.985
	AGCRN*	.014	.003	.003	1.79%	1.10%	1.08%	.025	.005	.006	2.89%	1.49%	1.51%	0.964	0.989	0.994
	GMAN*	.069	.020	.036	9.76%	10.10%	12.97%	.094	.028	.046	14.08%	14.56%	18.90%	0.211	0.273	0.186
	MISTAGCN*	.062	.018	.027	8.28%	8.74%	9.06%	.092	.029	.058	11.21%	12.41%	13.49%	-0.958	-0.173	0.469
	MTGNN*	.016	.004	.007	4.56%	3.62%	3.71%	.027	.008	.018	16.98%	9.83%	7.16%	-0.411	0.741	0.765
Q=3	DSTGCRN*	.012	.003	.002	1.54%	1.07%	0.78%	.021	.005	.005	2.41%	1.42%	1.11%	0.975	0.991	0.997
	Improvement	16.1%	7.8%	38.6%	14.0%	3.1%	38.5%	16.7%	13.4%	38.2%	16.7%	4.9%	35.8%	1.2%	0.2%	0.3%
	STD	.001	.000	.000	.001	.001	.001	.001	.000	.001	.002	.001	.002	.004	.001	.001
	AR/VAR*	.122	.039	.051	13.82%	15.90%	23.92%	.144	.046	.064	16.40%	18.67%	32.01%	-3.035	-3.251	-0.823
	SVR	.040	.012	.025	5.01%	5.76%	6.96%	.048	.015	.032	6.08%	6.82%	8.67%	0.249	0.176	0.662
	ARIMA	.085	.026	.056	10.00%	10.68%	14.84%	.103	.030	.072	11.77%	12.57%	18.02%	-1.797	-2.119	-0.745
	MLP	.045	.017	.032	5.85%	6.99%	11.04%	.070	.030	.069	8.37%	9.37%	15.81%	0.708	0.529	0.458
	FC-LSTM	.079	.024	.032	10.39%	9.90%	12.27%	.116	.040	.068	13.99%	12.90%	17.18%	0.223	0.297	0.383
	ELM	.025	.007	.022	2.62%	2.83%	4.84%	.033	.009	.027	3.66%	3.66%	6.17%	0.770	0.794	0.844
	AGCRN*	.016	.004	.003	1.97%	1.58%	1.21%	.027	.008	.007	3.17%	2.19%	1.74%	0.956	0.975	0.992
Q=5	GMAN*	.071	.021	.033	9.84%	10.46%	12.29%	.112	.039	.076	14.55%	15.76%	19.50%	0.204	0.247	0.261
	MISTAGCN*	.065	.018	.042	8.76%	8.92%	11.53%	.095	.028	.092	11.96%	12.56%	15.53%	-1.186	-0.141	0.050
	MTGNN*	.022	.007	.011	3.76%	4.84%	8.29%	.038	.015	.023	8.14%	12.42%	17.19%	0.610	0.688	-1.087
	DSTGCRN*	.009	.004	.003	1.19%	1.48%	1.01%	.016	.006	.006	1.93%	1.98%	1.50%	0.983	0.981	0.995
Q=7	Improvement	40.6%	12.5%	21.7%	39.6%	7.0%	20.3%	40.3%	24.6%	20.8%	39.0%	11.0%	16.4%	2.8%	0.6%	0.3%
	STD	.002	.001	.000	.002	.003	.001	.003	.001	.001	.003	.003	.002	.005	.006	.001

Figure 4: Comparison of DSTGCRN with baselines after 5 runs on datasets from China, the US, and the EU.

RESULTS

Long Term Predictions

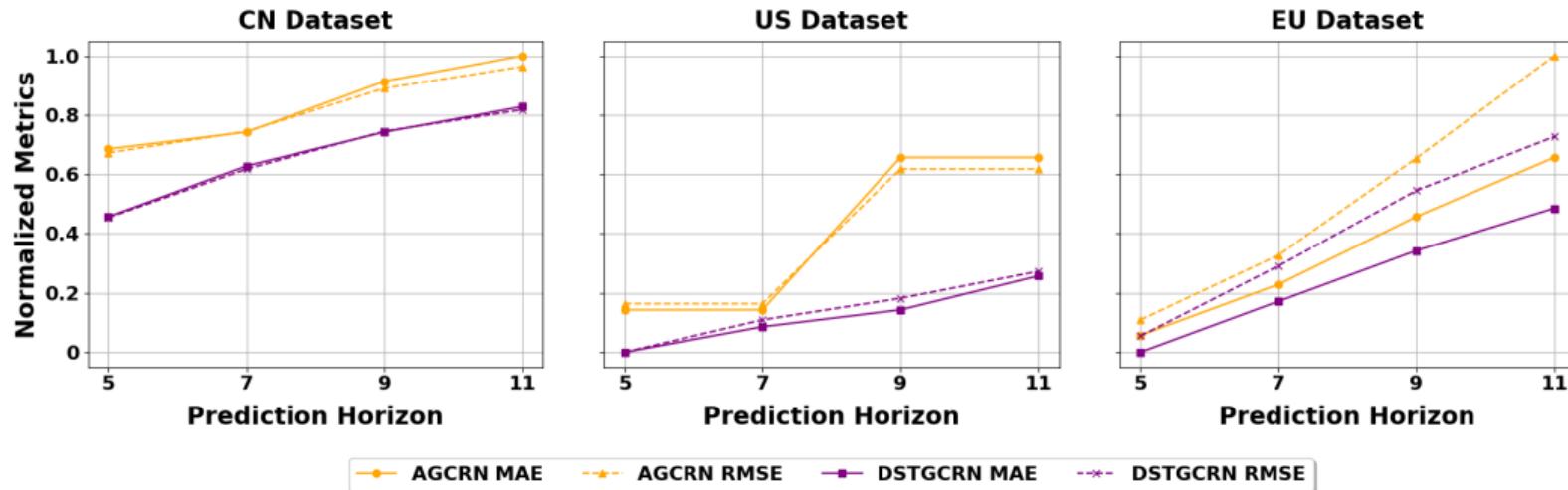


Figure 5: Performance comparison of AGCRN and DSTGCRN across geographies over longer horizons.

RESULTS

Factor Analysis

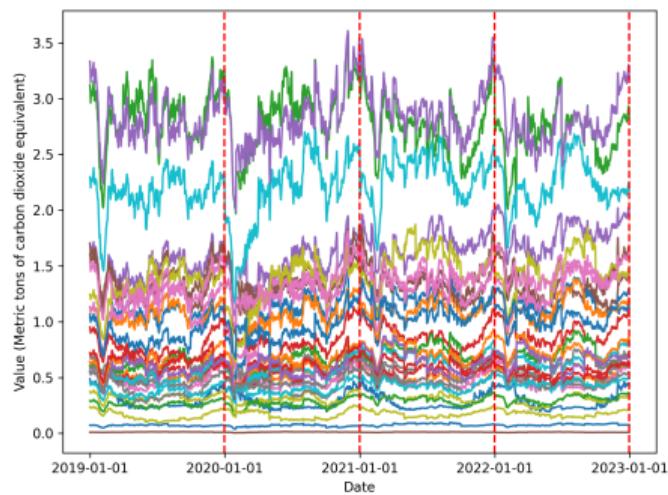


Figure 6: Carbon Emissions Trends from 2019 to 2022 in China.

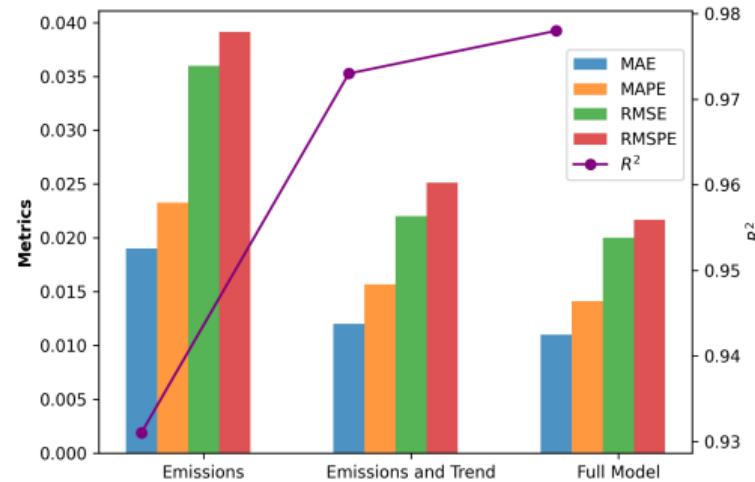


Figure 7: Performance metrics across three scenarios.

RESULTS

Relationship Evolution and Ablation Studies

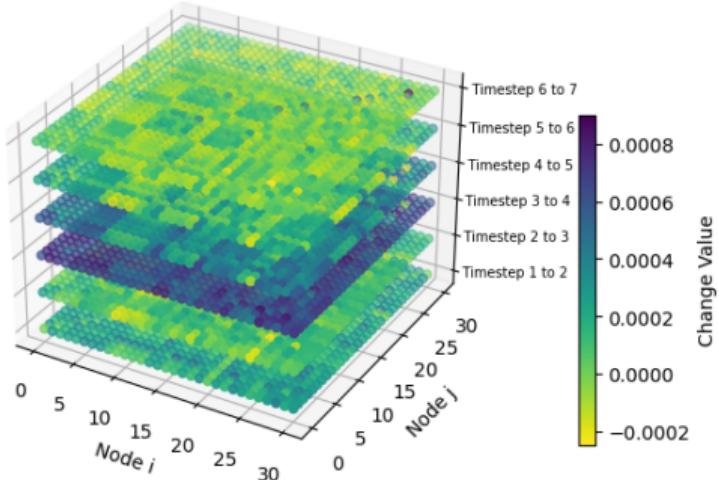


Figure 8: Differential Temporal Adjacency Matrix Evolution.

Model	MAE	MAPE	RMSE	RMSPE	R^2
Static	0.014	1.791%	0.025	2.881%	0.964
Time Specific	0.016	2.017%	0.029	3.275%	0.950
w/o GRU	0.019	2.559%	0.033	4.149%	0.930
w/o Attention	0.012	1.491%	0.021	2.467%	0.974
w/o GRU/ATT	0.017	2.230%	0.030	3.508%	0.947
DSTGCRN	0.011	1.410%	0.020	2.169%	0.978

Figure 9: Ablation experiments on DSTGCRN.

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INTRODUCTION

Background and Challenges

Background:

- » Spatial-temporal data exhibits complex spatial dependencies and dynamic temporal evolution.
- » Conventional forecasting models often provide deterministic outputs, which do not account for data uncertainties.

Challenges:

- » Modeling spatial-temporal interactions is complex due to their intricate structures.
- » Traditional deterministic approaches fail to handle the probabilistic nature of real-world data, impairing decision-making.

INTRODUCTION

Motivation and Contributions

Motivation:

- » Advances in generative AI, especially diffusion models, offer new avenues for probabilistic forecasting that embrace data uncertainty.
- » ProGen leverages stochastic differential equations to model data's continuous-time evolution, improving forecast precision.

Contributions:

- » **Conceptual:** Pioneering a generative modeling framework for continuous-time spatial-temporal forecasting.
- » **Technical:** Develops a unique denoising approach and custom SDE for improved spatiotemporal correlation handling.
- » **Empirical:** Proven enhancements over traditional models validated through rigorous real-world data testing.

INTRODUCTION

Practical Implementation and Forecasting Implications

ProGen's implementation of DSM and SDEs offers several key advantages for spatio-temporal forecasting:

- » **Improved Forecast Accuracy:** By accounting for uncertainty and enabling the model to explore a range of possible futures.
- » **Robustness to Noise:** The use of SDEs helps handle the inherent noise and variability in spatio-temporal data effectively.
- » **Flexibility in Model Application:** Suitable for various types of spatio-temporal data beyond just traffic or weather, including economic and biological datasets.

Additionally, the continuous-time approach of ProGen allows for finer temporal resolution in predictions, crucial for dynamic systems monitoring and decision-making.

LITERATURE REVIEW

Diffusion Models and Probabilistic Time Series Forecasting

Diffusion Models:

- » Originated by Ho et al. (2020) and Song et al. (2021), using discrete and continuous SDEs to generate data from noise.
- » Enhanced for conditional generation by Nichol and Dhariwal (2021), aligning outputs with specific attributes.

Probabilistic Time Series Forecasting:

- » Diffusion models adapted for time series, exemplified by TimeGrad and ScoreGrad, though challenges persist with speed and precision.
- » ProGen employs a continuous approach, enhancing the capture of spatial and temporal correlations.

LITERATURE REVIEW

Spatio-Temporal Forecasting Methods

Spatio-Temporal Forecasting:

- » Techniques such as AGCRN and DSTAGNN use dynamic graphs; STG-NRDE employs neural rough differential equations.

Continuity in Time Series:

- » Discrete diffusion models explored probabilistic forecasting but struggled with continuity; ProGen introduces a novel continuous-time method, offering a distinct solution.

METHODOLOGY

Problem Setup

Our objective is to forecast future values of a spatio-temporal series based on historical data:

- » Define $\mathcal{D} = \{\mathbf{X}_t\}_{t=1}^T$ where $\mathbf{X}_t \in \mathbb{R}^{N \times D}$ denotes observations at time t across N locations, each with D features.
- » Spatial dependencies are modeled through a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, A)$, comprising nodes \mathcal{V} , edges \mathcal{E} , and an adjacency matrix A .

Probabilistic Prediction Task

Aim to predict the distribution:

$$q_X(\mathbf{X}_{T+1:T+H} \mid \mathbf{X}_{T-L+1:T}, \mathcal{G}, \mathcal{C})$$

where L and H denote the length of the historical window and the forecasting horizon, respectively.

METHODOLOGY

Stochastic Differential Equations

SDEs provide a framework for modeling continuous-time stochastic processes:

$$d\mathbf{X} = f(\mathbf{X}, t)dt + g(\mathbf{X}, t)dW, \quad (1)$$

where:

- » $\mathbf{X} \in \mathbb{R}^d$ represents the state at time t .
- » $f(\mathbf{X}, t)$ is the drift function, dictating deterministic dynamics.
- » $g(\mathbf{X}, t)$ is the diffusion function, modeling stochastic effects.
- » dW denotes differential Brownian motion.

METHODOLOGY

Reverse Stochastic Differential Equations

Reverse SDEs describe how to denoise data back to its original distribution:

$$d\mathbf{X} = [f(\mathbf{X}, t) - g^2(\mathbf{X}, t)\nabla_{\mathbf{X}} \log p_t(\mathbf{X})] dt + g(\mathbf{X}, t)d\bar{W}, \quad (2)$$

- » The score function $\nabla_{\mathbf{X}} \log p_t(\mathbf{X})$ guides the denoising process.
- » \bar{W} is the reverse Wiener process, introducing reverse dynamics.

METHODOLOGY

Denoising Score Matching (DSM)

DSM optimizes the match between the gradients of the log probabilities (scores) of the model and data distributions through the diffusion process:

$$\mathcal{L}(\theta) = \mathbb{E}_{t \sim \text{Uniform}(0, K)} \mathbb{E}_{X \sim p_{\text{data}}} [\|\nabla_X \log q_\theta(\mathbf{X}^t | t) - \nabla_X \log p_{\text{data}}(\mathbf{X}^t | t)\|^2] \quad (3)$$

where:

- » $q_\theta(\mathbf{X}^t | t)$ and $p_{\text{data}}(\mathbf{X}^t | t)$ are the model and data distributions at diffusion timestep t , respectively.
- » $\nabla_X \log$ represents the gradient of the log probability.
- » θ denotes the model parameters optimized during training.

OVERVIEW OF PROGEN FRAMEWORK

Operational Processes

ProGen combines a forward diffusion process with a reverse prediction process:

- » **Forward Diffusion:** Transforms training data into a Gaussian state while training a score model.
- » **Reverse Prediction:** Iteratively denoises to generate predictions, guided by the score model.

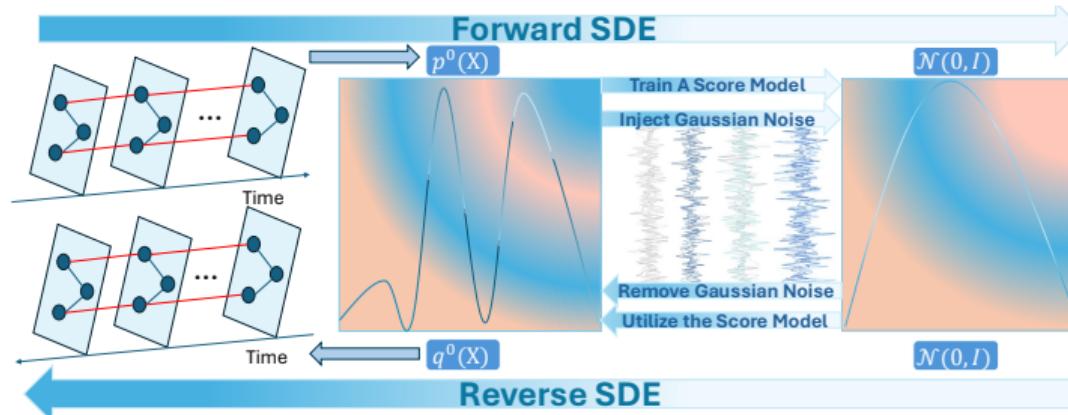


Figure 10: Overview of the two primary processes in ProGen.

FORWARD DIFFUSION PROCESS

Transforming Data into Gaussian State

The forward process perturbs the data point by point into Gaussian noise:

$$\tilde{\mathbf{X}}_{\mathbf{F}}^t = \mu(\mathbf{X}_{\mathbf{F}}, t) + \sigma(\mathbf{X}_{\mathbf{F}}, t) \times Z, \quad Z \sim \mathcal{N}(0, I) \quad (4)$$

where μ and σ control the mean and standard deviation across discretized time steps.

This process trains the model to understand and simulate the transition from real data distributions to noise.

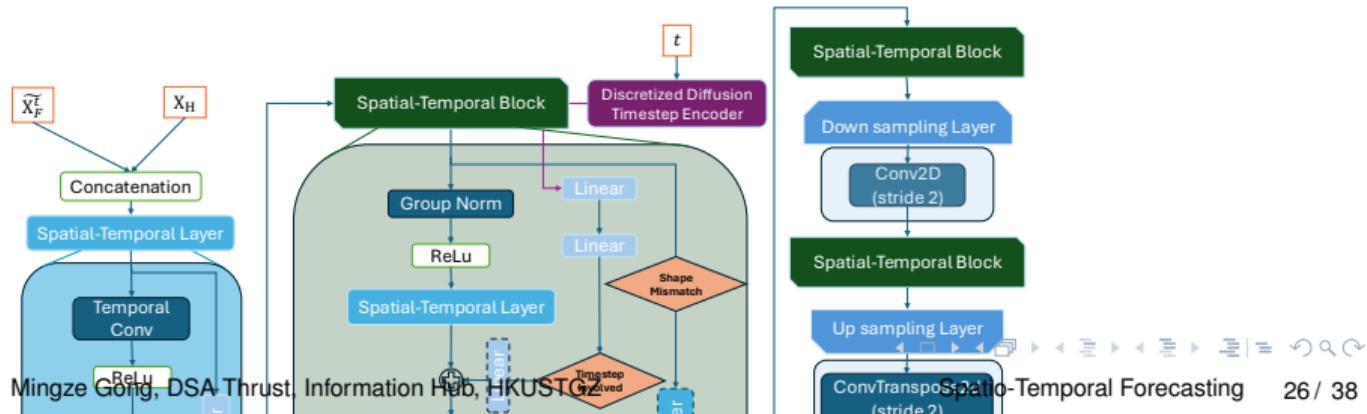
TRAINING THE DENOISING SCORE MODEL

Optimizing the Score Estimation

Training focuses on minimizing the discrepancy between the estimated and true data gradients:

$$\mathcal{L}(\theta) = \mathbb{E}_t \left\{ \mathbb{E}_{\mathbf{X}_F, \mathbf{X}_H} \left[\|\nabla \log p(\tilde{\mathbf{X}}_F^t | \mathbf{X}_F) - s_\theta(\tilde{\mathbf{X}}_F^t, \mathbf{X}_H)\|^2 \right] \right\} \quad (5)$$

This loss function aligns the model's score estimates with the true distribution changes, enhancing prediction accuracy.



ADAPTIVE REVERSE PREDICTION PROCESS

Restoring Original Data Distribution

The reverse SDE effectively restores data from its noisy state using learned scores:

$$d\mathbf{X} = (f(\mathbf{X}, t) - g(\mathbf{X}, t)^2 \nabla \log p(\mathbf{X}|t))dt + g(\mathbf{X}, t)d\bar{W} \quad (6)$$

This equation integrates insights from the score model to reverse the diffusion, guiding the data back to its original state.

ProGen's approach modifies traditional methods by adapting to data dynamics more effectively and efficiently.

OVERVIEW OF PROGEN PERFORMANCE

Full Test Run

Datasets	Metric	AGCRN	STGCN	DSTAGNN	STGNCDE	STGNRDE	ARIMA	FCLSTM	MTGNN	ASTGCN(r)	ProGen
PEMS03	MAE	15.98	17.48	15.57	15.57	15.50	35.41	21.33	16.46	17.34	15.07
	RMSE	28.25	29.21	27.21	27.09	27.06	47.59	35.11	28.56	29.56	25.09
PEMS08	MAE	15.95	17.13	15.67	15.45	15.32	31.09	23.09	15.71	18.25	14.99
	RMSE	25.22	26.80	24.77	24.81	24.72	44.32	35.17	24.62	28.06	24.00

Figure 12: Distribution and mean values of predictions vs. actual truths across initial batch iterations in PEMS04.

Method	MAE	RMSE	CRPS
Latent ODE	26.05	39.50	0.11
DeepAR	21.56	33.37	0.07
CSDI	32.11	47.40	0.11
TimeGrad	24.46	38.06	0.09
MC Dropout	19.01	29.35	0.07
DiffSTG	18.60	28.20	0.06
ProGen	14.99	24.00	0.05

Figure 13: Training loss curves for different spatiotemporal layers in PEMS08 over 100 epochs.

OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs

Datasets	Metric	AGCRN*	DSTAGNN*	STGNRDE*	DeepAR	DiffSTG	CSDI	ProGen
PEMS03	MAE	16.79	17.03	25.40	23.76	53.52	24.52	14.14
	RMSE	29.26	31.05	37.93	37.82	69.62	38.93	22.71
	CRPS	/	/	/	0.11	0.24	0.11	0.07
	MIS	/	/	/	205.78	466.97	245.86	106.50
PEMS04	MAE	21.60	21.25	30.67	29.59	32.55	27.83	18.87
	RMSE	34.32	32.82	44.29	46.01	46.89	42.71	30.01
	CRPS	/	/	/	0.10	0.11	0.10	0.07
	MIS	/	/	/	237.75	209.85	223.77	138.88
PEMS07	MAE	21.50	24.06	33.48	28.77	37.80	30.57	21.91
	RMSE	36.08	39.02	46.49	44.80	50.31	45.92	35.11
	CRPS	/	/	/	0.07	0.09	0.07	0.05
	MIS	/	/	/	242.61	293.45	262.15	186.78
PEMS08	MAE	16.90	15.78	25.10	23.15	44.47	19.00	15.46
	RMSE	26.47	24.36	36.32	35.92	60.72	28.99	24.71
	CRPS	/	/	/	0.08	0.15	0.07	0.05
	MIS	/	/	/	191.20	284.64	146.06	120.53

Figure 14: Distribution and mean values of predictions vs. actual truths across initial batch iterations in PEMS04.

OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs

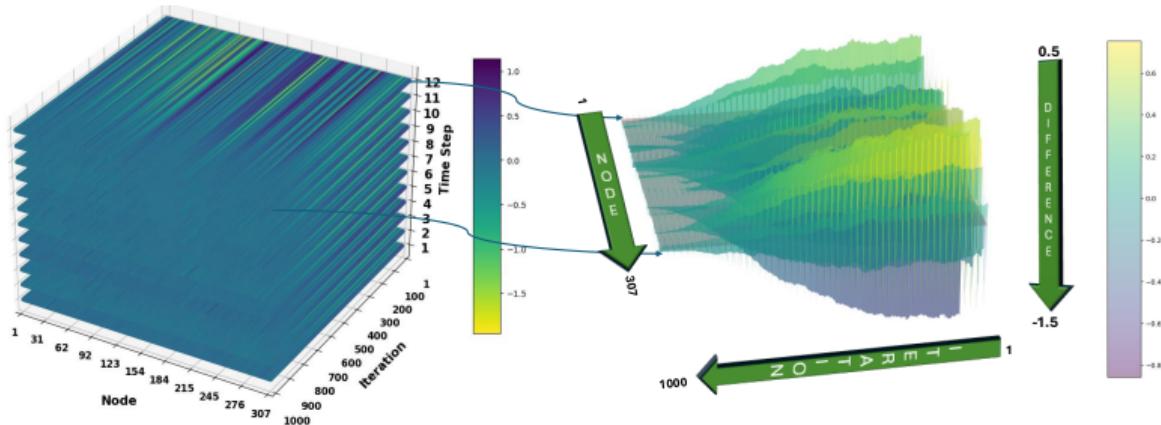
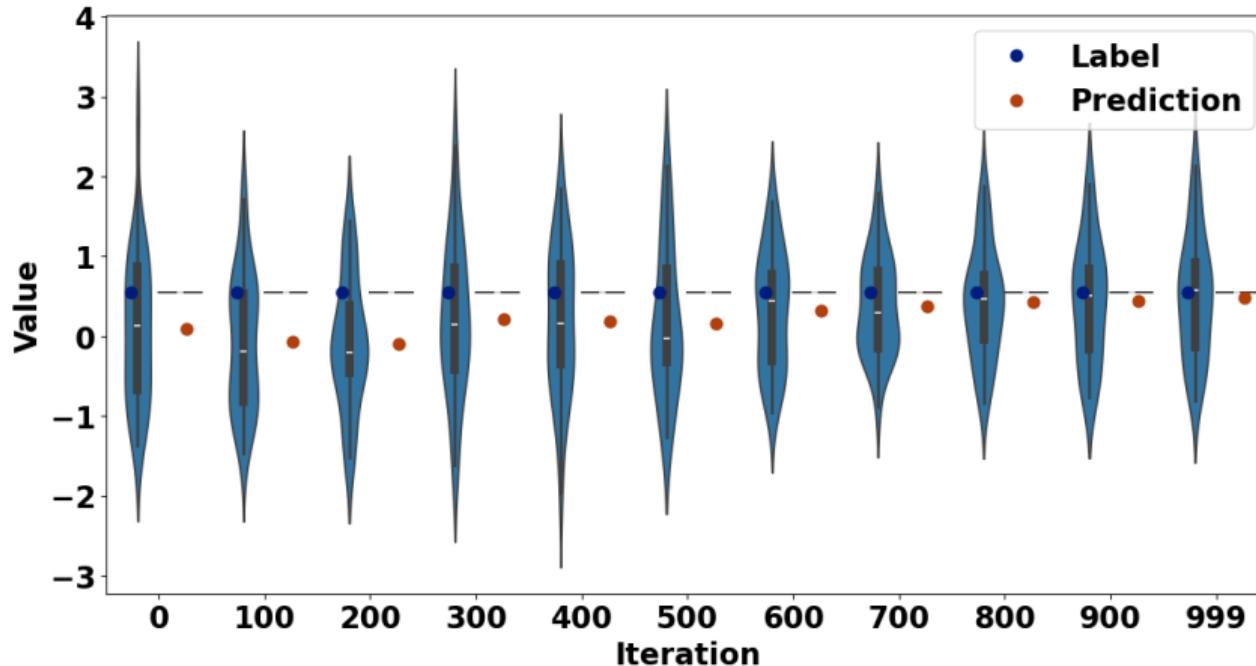


Figure 15: Distribution and mean values of predictions vs. actual truths across initial batch iterations in PEMS04.

OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs



OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs

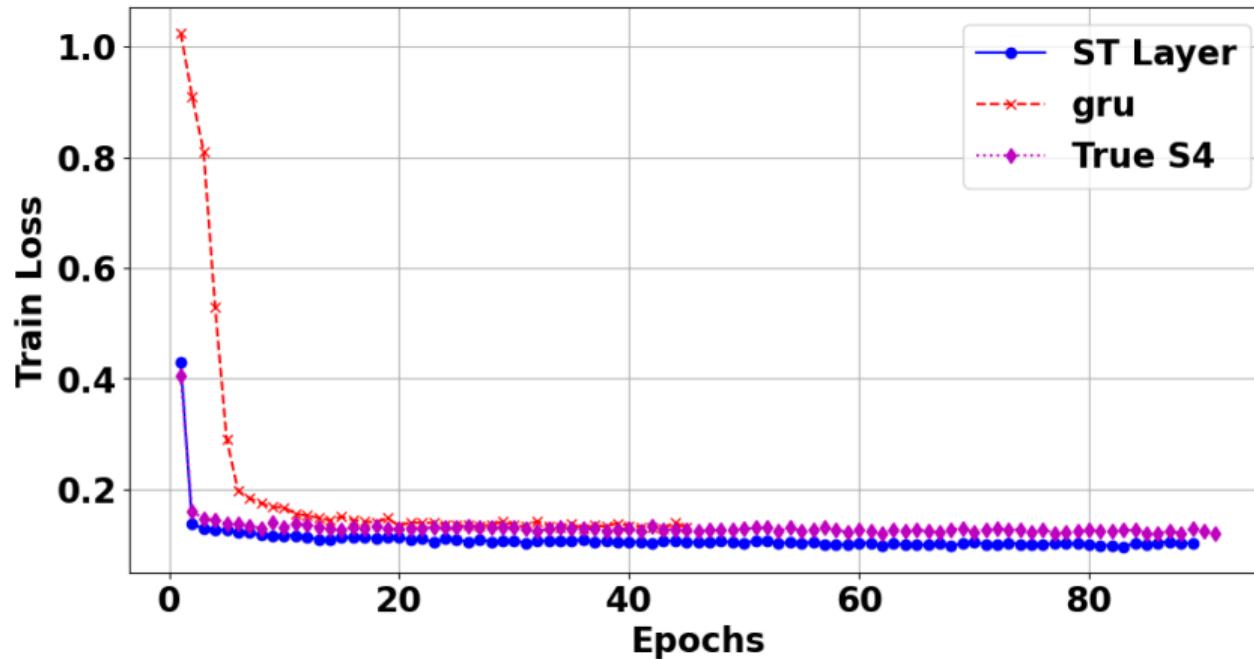
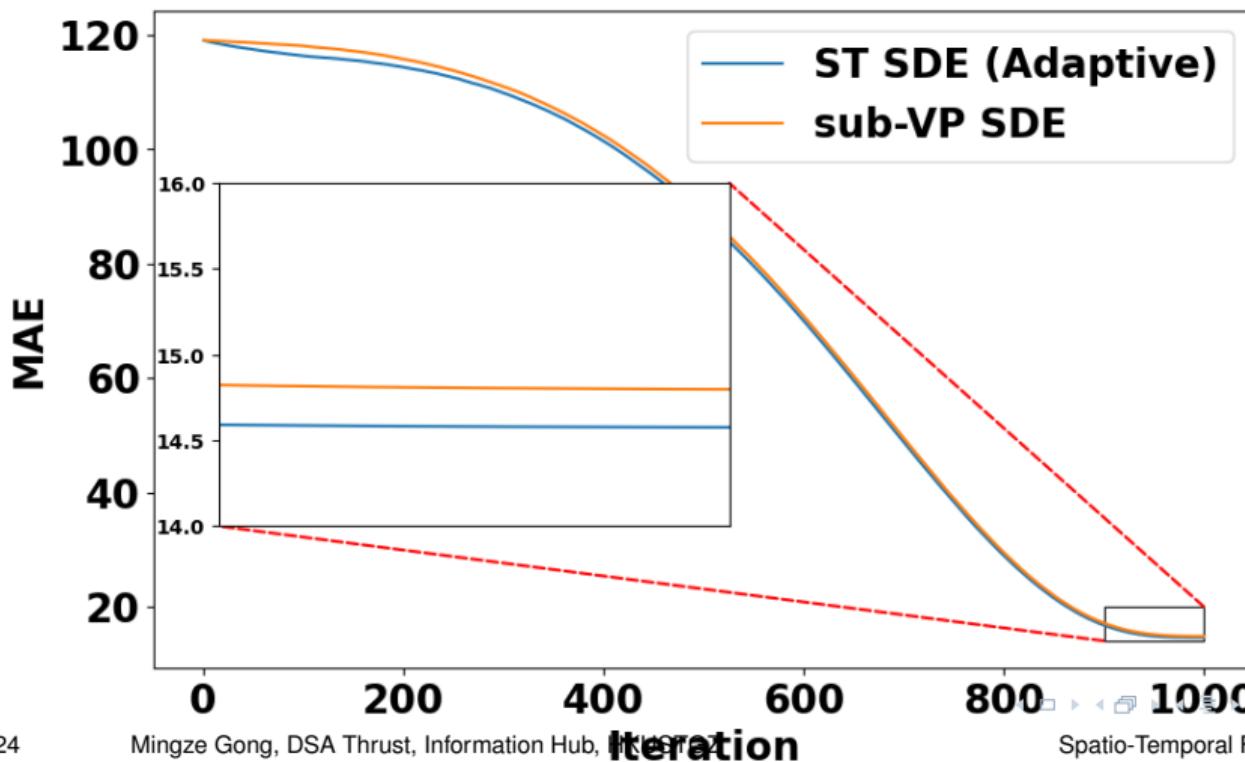


Figure 17: Distribution and mean values of predictions vs. actual truths across initial batch iterations in PEMSO4.

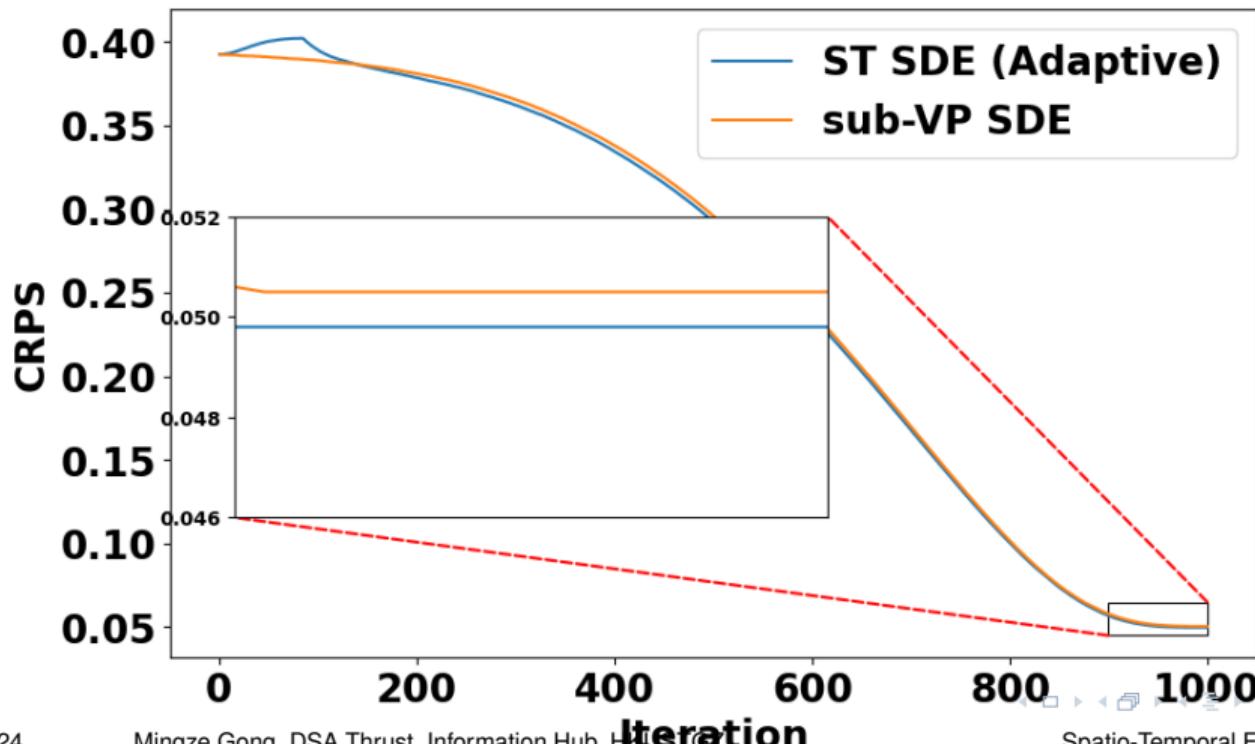
OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs



OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs



OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs

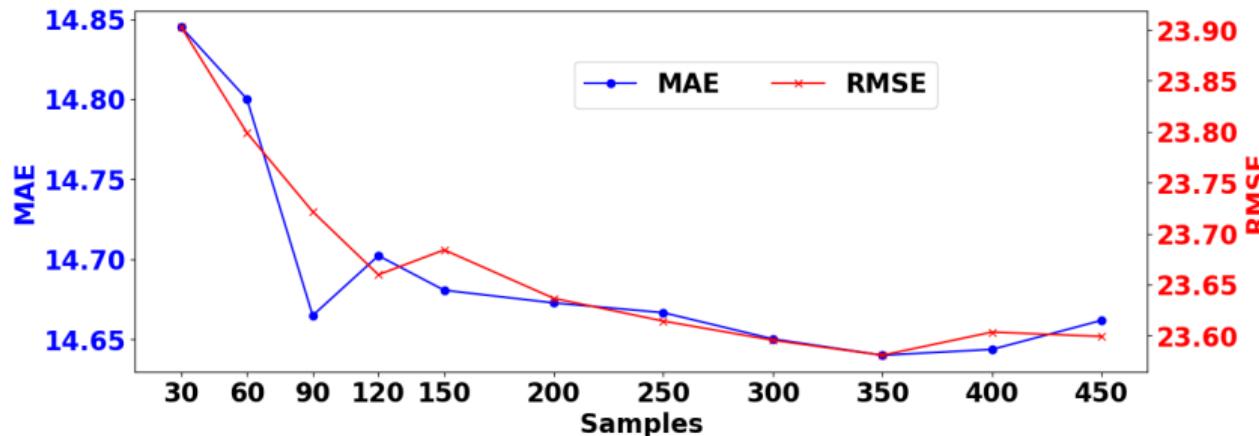


Figure 20: Distribution and mean values of predictions vs. actual truths across initial batch iterations in PEMS04.

OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs

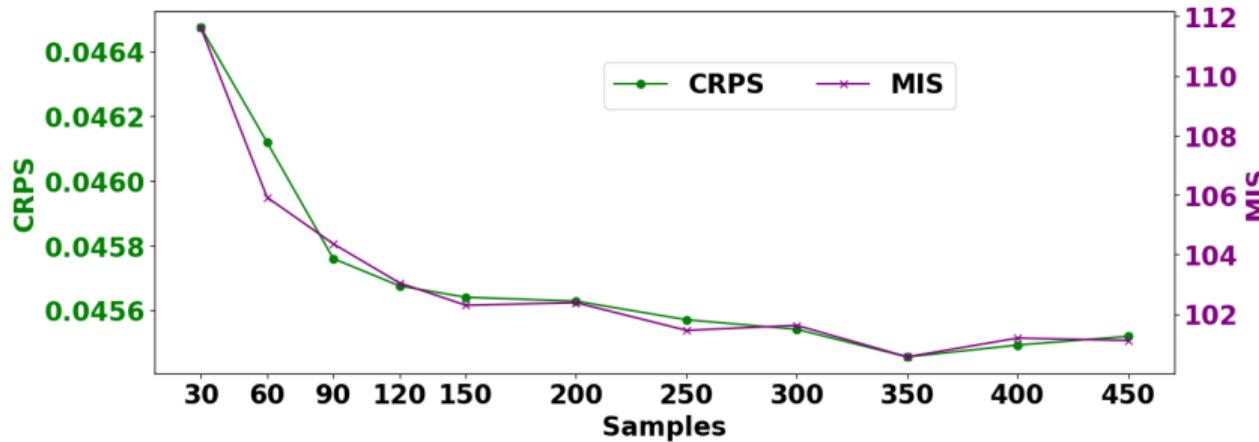


Figure 21: Distribution and mean values of predictions vs. actual truths across initial batch iterations in PEMS04.

OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs

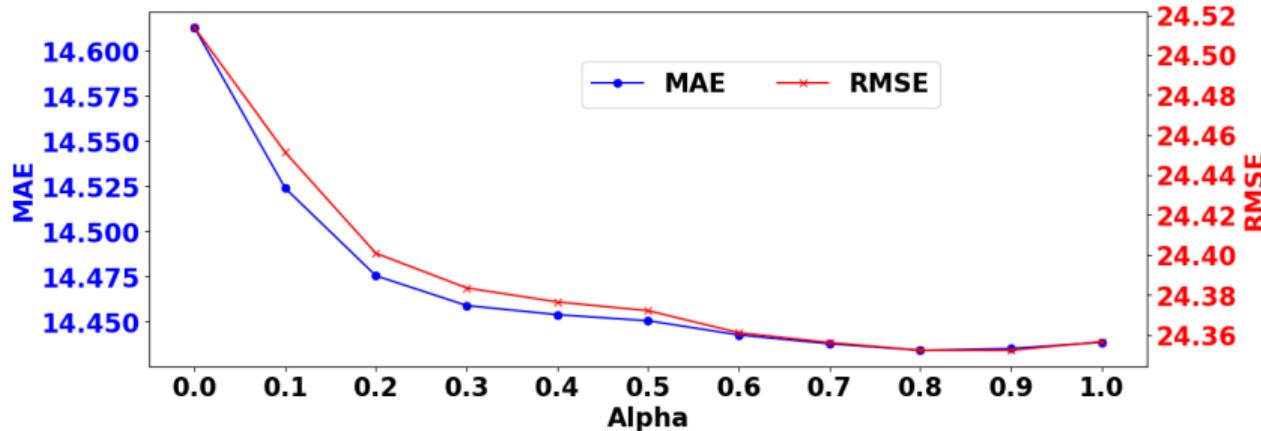


Figure 22: Distribution and mean values of predictions vs. actual truths across initial batch iterations in PEMS04.

OVERVIEW OF PROGEN PERFORMANCE

Random Test Runs

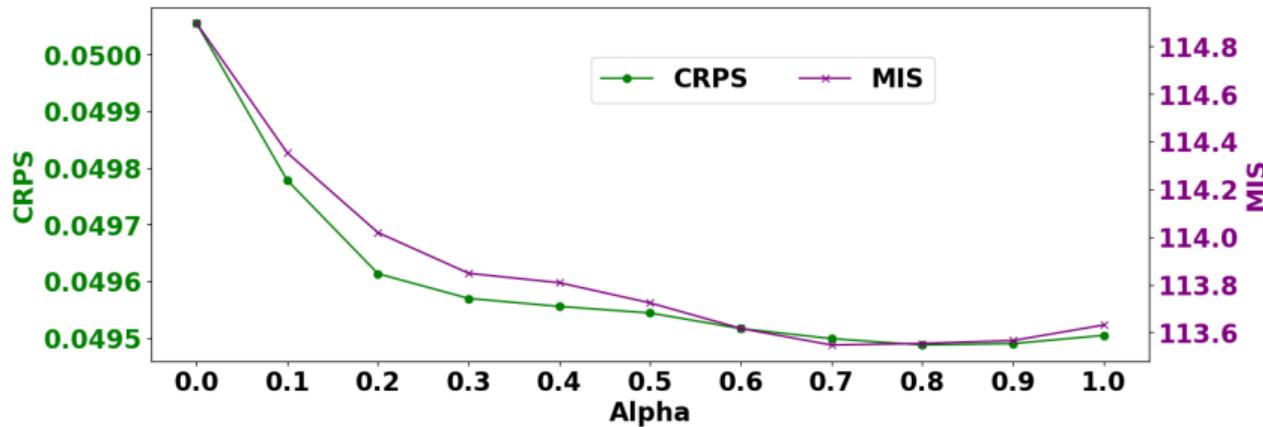


Figure 23: Distribution and mean values of predictions vs. actual truths across initial batch iterations in PEMS04.

References



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THANK YOU!