Deep learning and process understanding for data-driven urban prediction

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What is Urban?

城

Physical environment

市

Human activities

燕寻杭城|杭州古地图变迁
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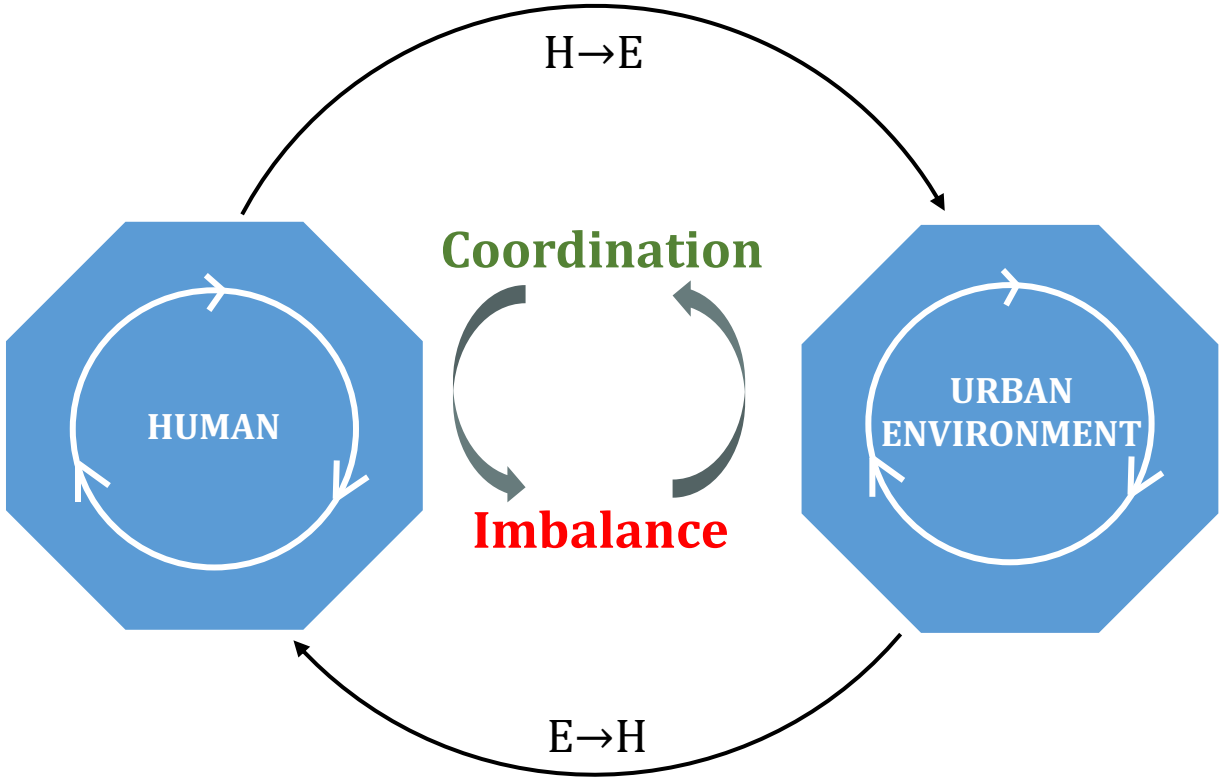
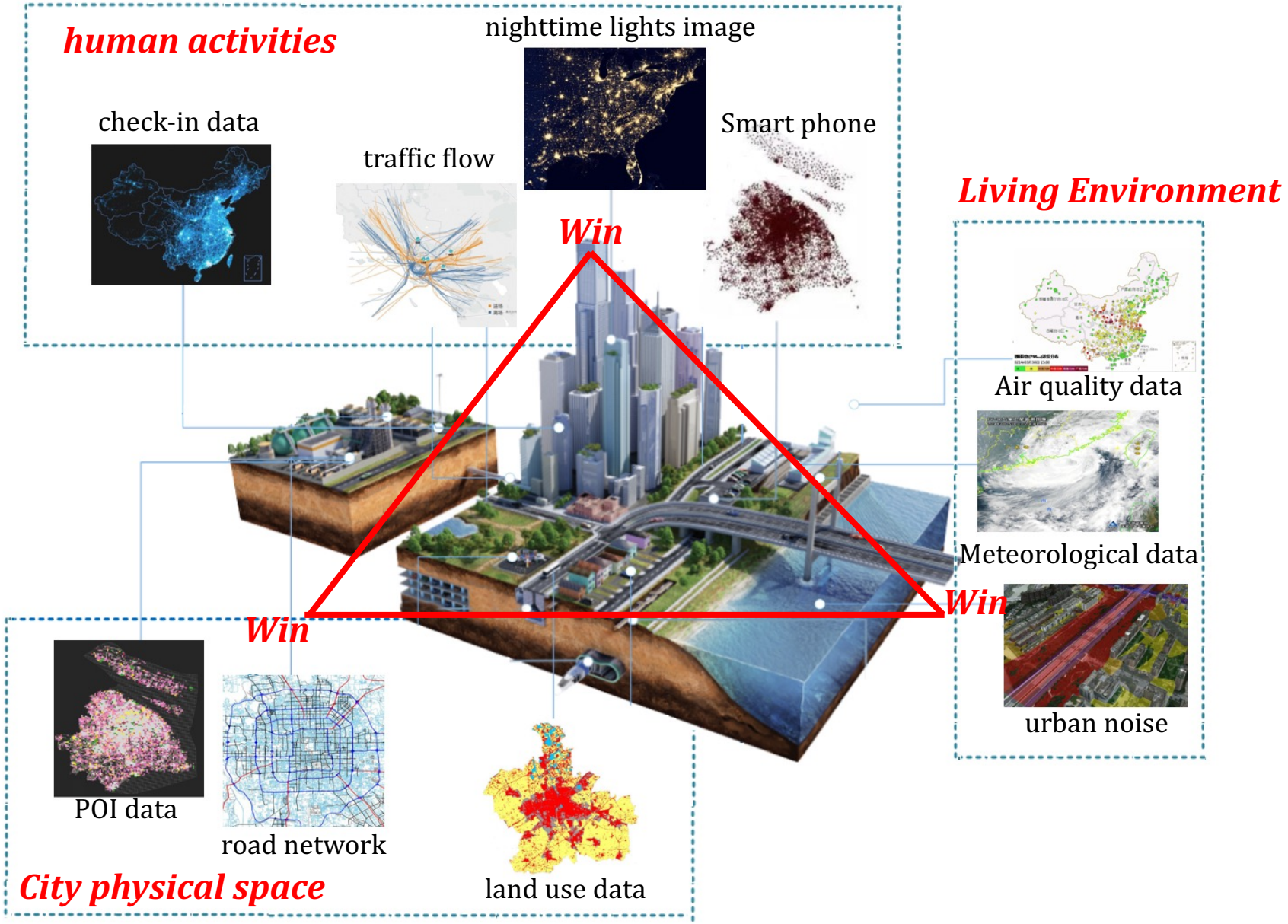
Urban Dynamic system

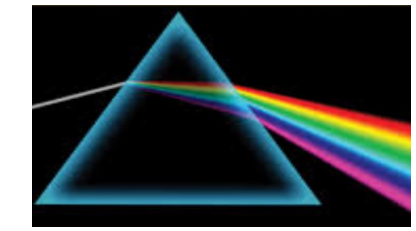


- Conditions for survival and development
- Environment control human action and activities
- Environment change human attitude and decision making

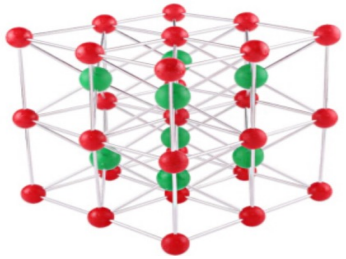
Urban Big Data

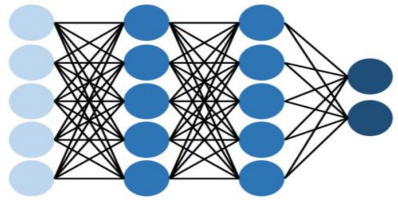


Data-driven: the fourth paradigm of scientific research



$$e^{i\pi} + 1 = 0$$
$$\mathbf{F} = m\mathbf{a}$$
$$E_0 = mc^2$$
$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \hat{H}\Psi(\mathbf{r}, t)$$





1st PARADIGM
Empirical Science

Experiments

2nd PARADIGM
Theoretical Science

Laws of classical mechanics, electrodynamics, etc.

3rd PARADIGM
Computational Science Simulations

Density-functional theory and beyond; molecular dynamics

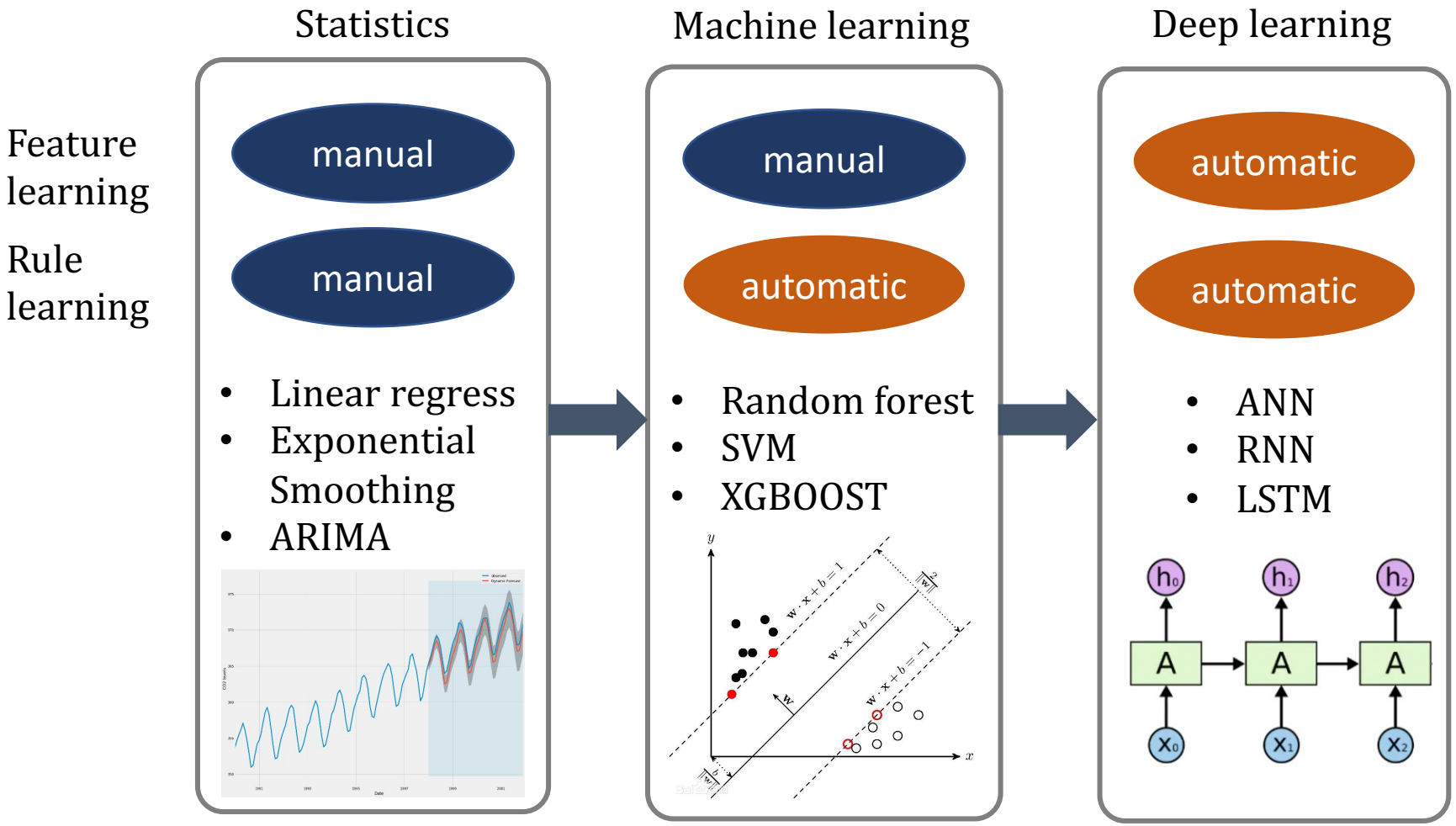
4th PARADIGM
Big-Data-Driven Science

Detection of patterns and anomalies in Big Data; artificial intelligence; etc.

1600 1950 2010

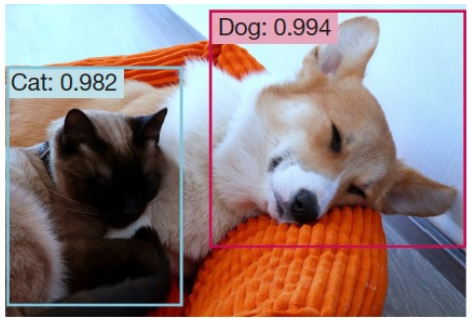
Tansley S, Tolle K M. The fourth paradigm: data-intensive scientific discovery[M]. Redmond, WA: Microsoft research, 2009.

Data-driven models for geographic research

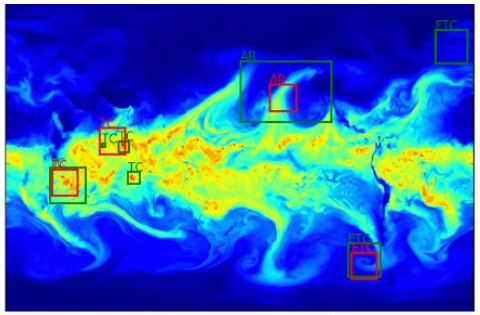


Deep learning in Geoscience

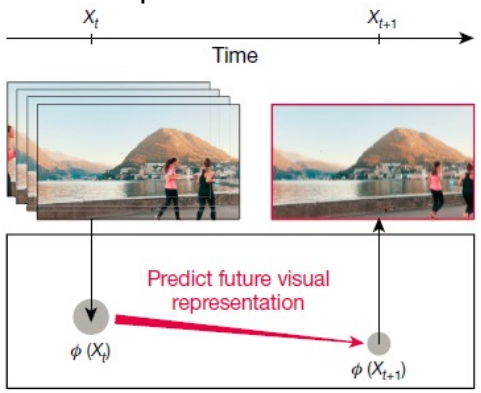
Object classification and localization



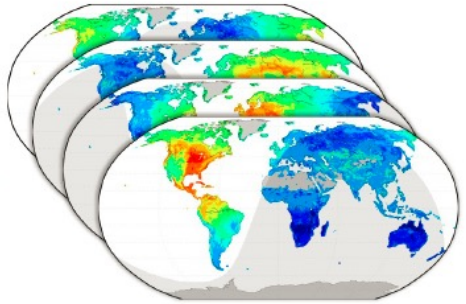
Pattern classification

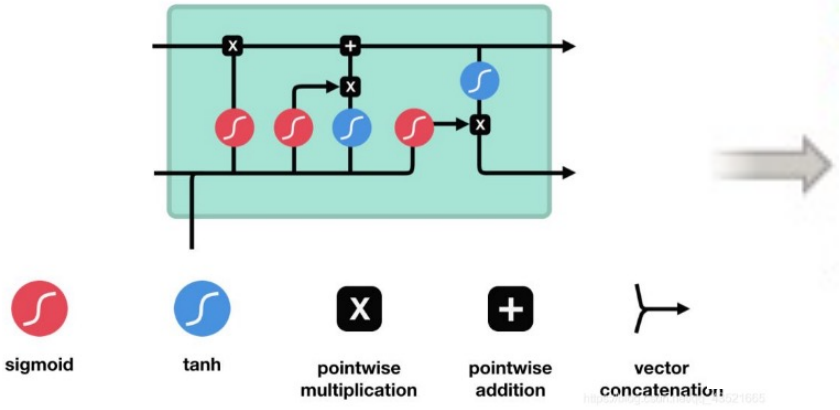


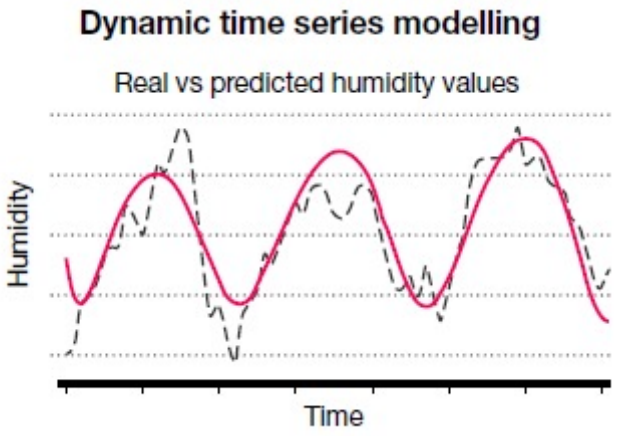
Video prediction

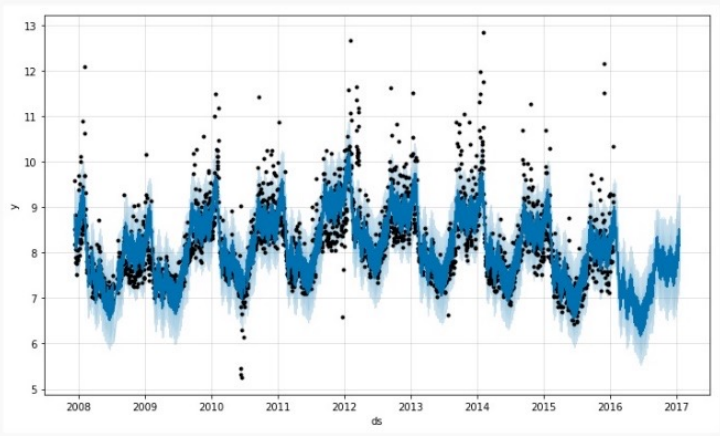


Short-term forecasting







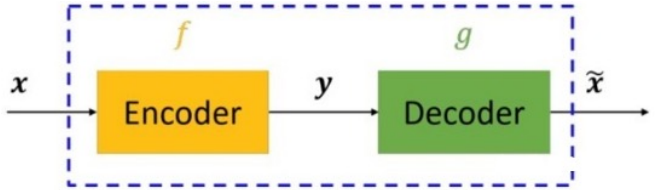


Reichstein, M., Camps-Valls, G., Stevens, B. *et al.* Deep learning and process understanding for data-driven Earth system science. *Nature* **566,** 195–204 (2019).

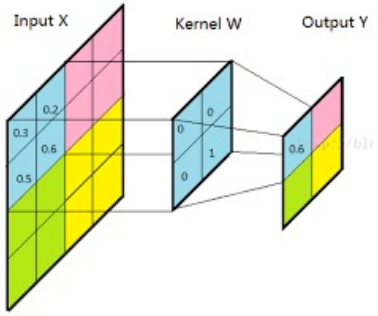
Urban prediction helps to

- improve urban planning
- easing traffic congestion
- controlling of environmental pollution
- reducing energy consumption
- …….

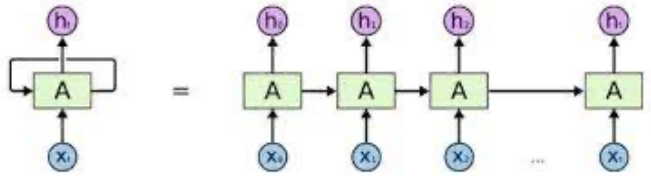
Deep learning models for prediction



Auto Encoder (AE)

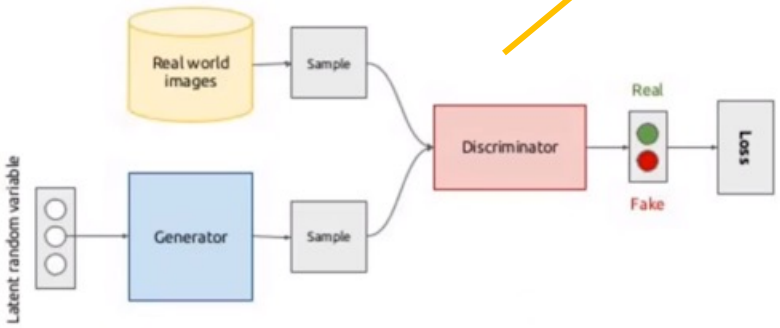


Convolutional Neural Network (CNN)

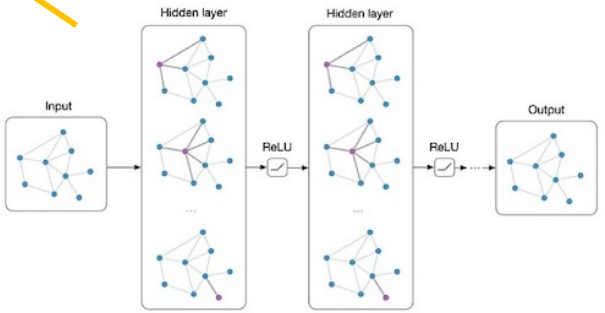


Recurrent Neural Network (RNN)

Variations & Combinations



Generative Adversarial Networks (GAN)



Graph Neural Networks (GNN)

Challenges

1. **Interpretability**

   Black-box deep learning models suffer from poor interpretability since they are not explicitly designed for representing physical relationships and providing mechanistic insights.

2. **Physical consistency**

   Deep learning models can fit observations very well, but predictions may be physically inconsistent or implausible.

3. **Accuracy dilution**

   Strongly nonlinear features tend to cause underfitting or overfitting in deep learning modeling, which makes it difficult to find the global optimal solution and accumulate significant errors.

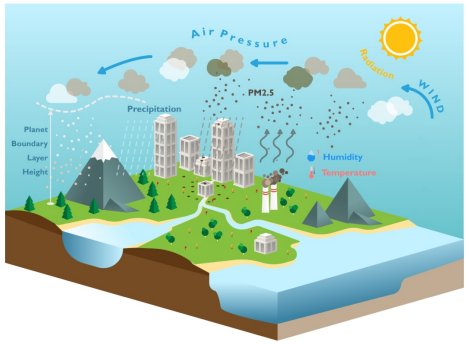
4. **Sample demand**

   The data available for several scientific problems are far smaller than what is needed to effectively train advanced data-driven models.

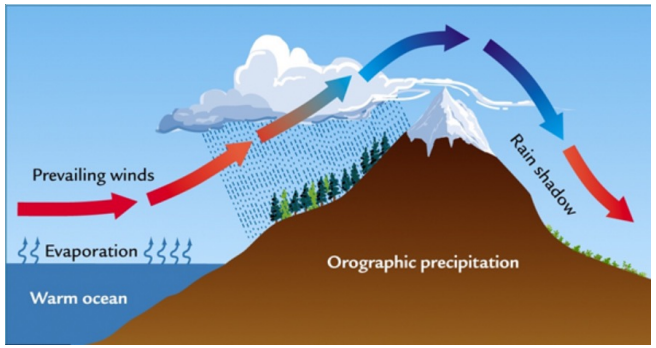
Spatio-temporal processes in the city

Theory-driven

Process understanding

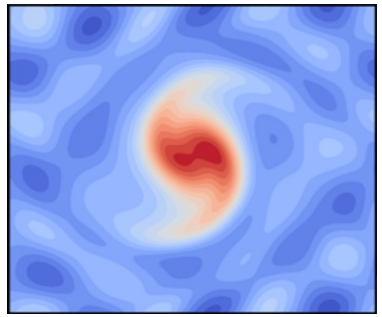


Pollution dispersion



Precipitation processes

traffic wave theory



Fluid dynamics

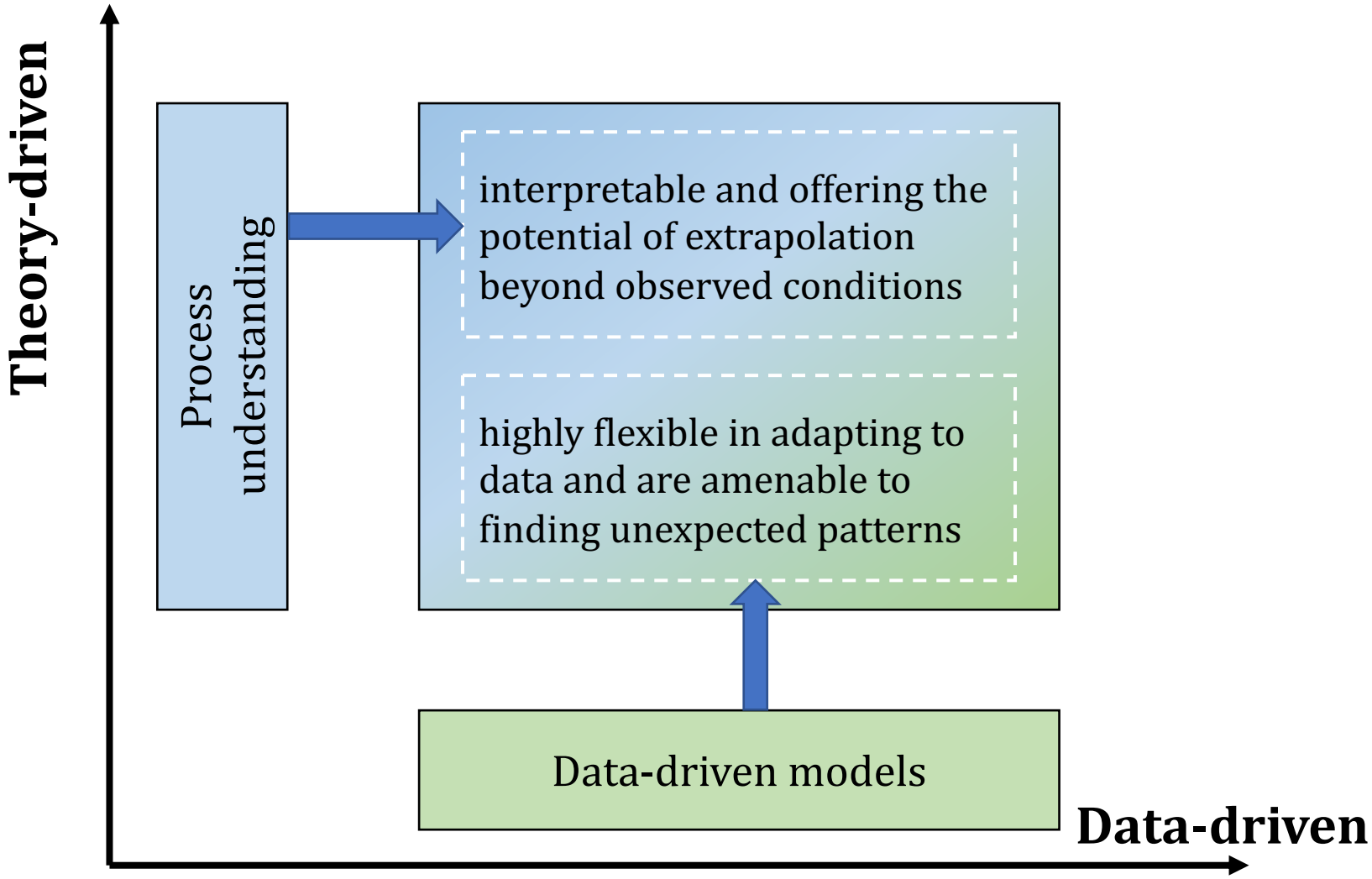
fine-grained parametric data ✓

enormous computational resources ✓

detect complex and unknown high-dimensional relationships ✗

Data-driven

Spatio-temporal processes in the city



The two research paradigms can complement each other, and hybrid models can integrate the strengths of both approaches

How to integrate theory-driven and data-driven models?

1. Optimizing theory-driven models with data-driven models

2. Theory-guided data driven models

3. Data-driven prediction that uncovers dynamic patterns

How to integrate theory-driven and data-driven models?

1. **Optimizing theory-driven models with data-driven models**
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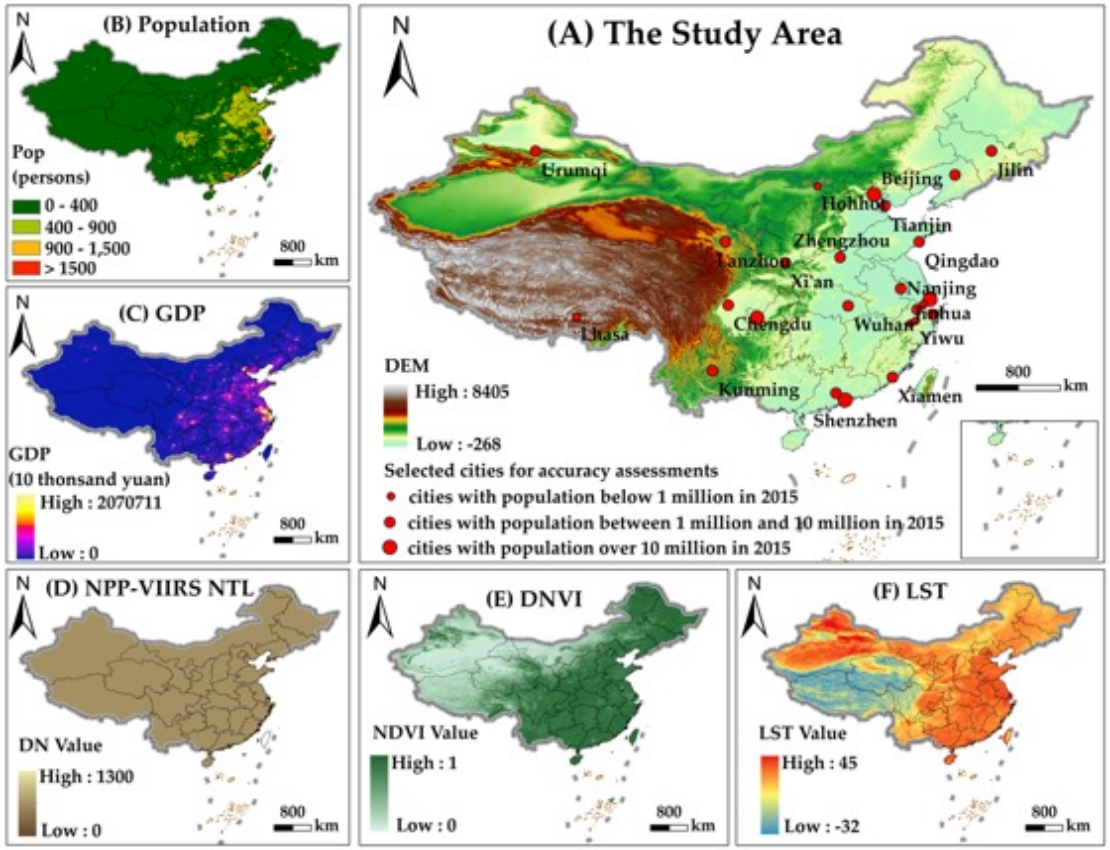
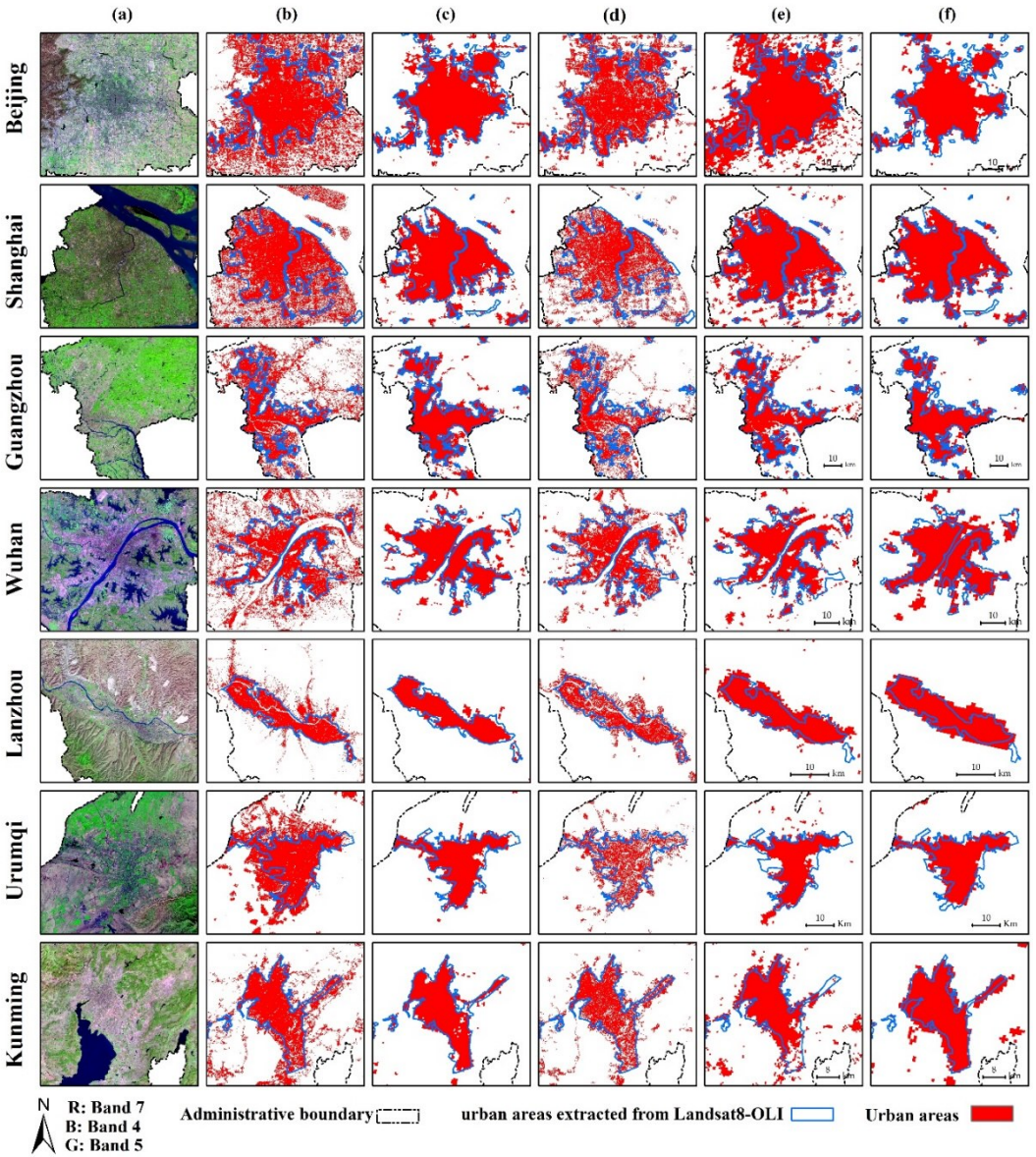
Urban Extent recognition

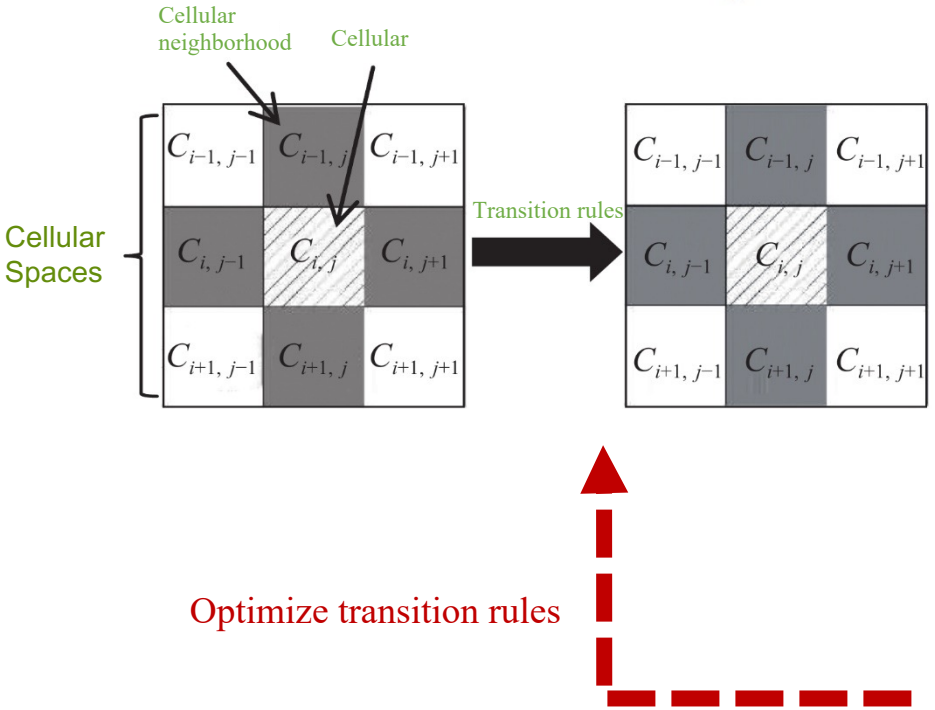


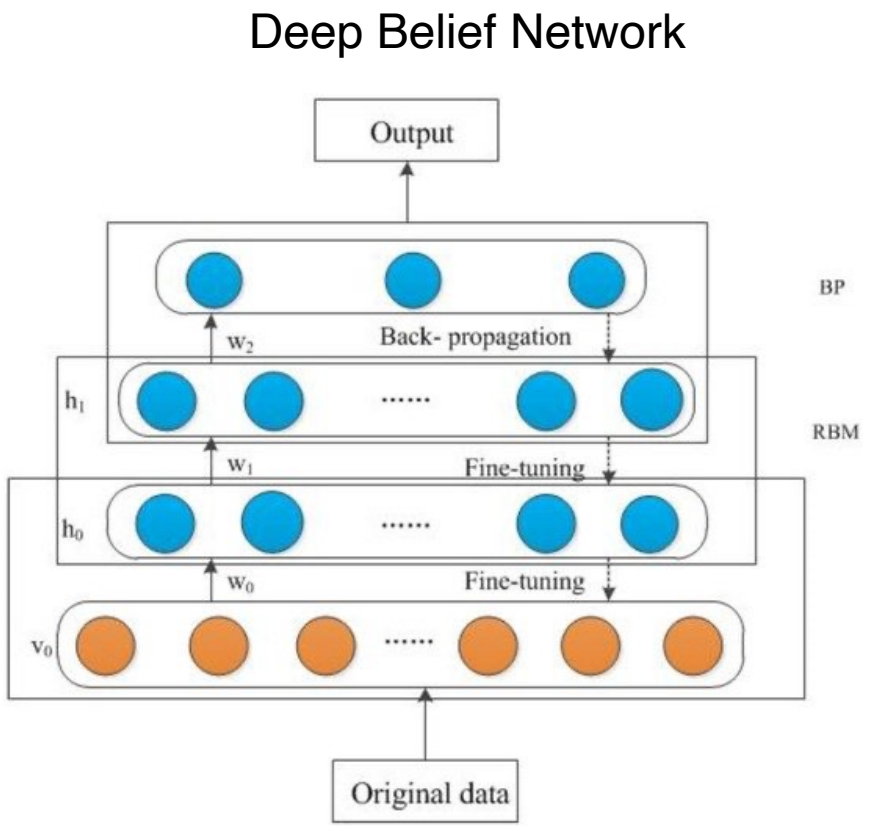


Chen X , Zhang F , Du Z , et al. An Unsupervised Urban Extent Extraction Method from NPP–VIIRS Nighttime Light Data[J]. Remote Sensing, 2020

Urban Growth Simulating (DBN-CA)

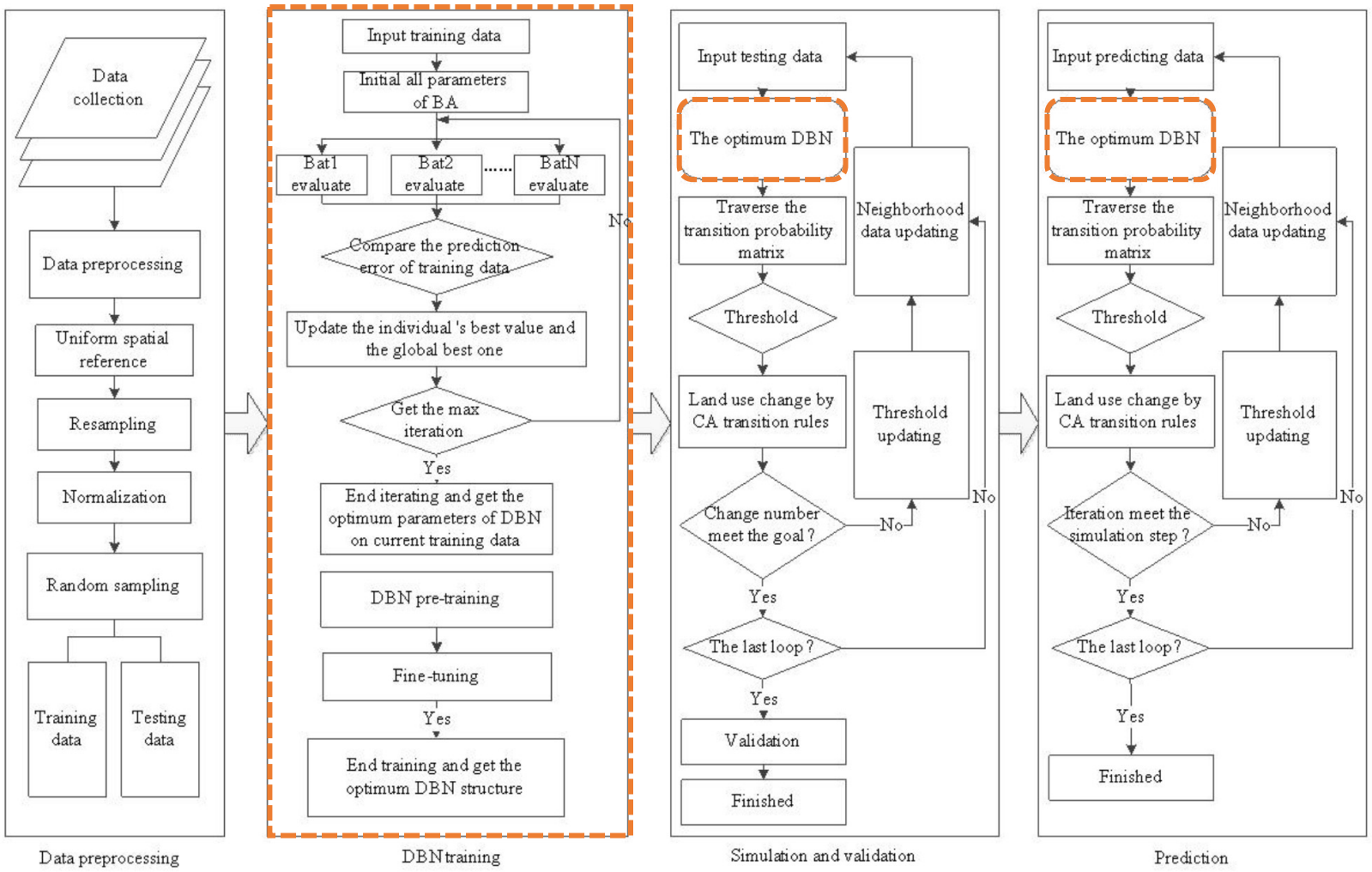
$$State_{ij}^{t+1} = f\left(Neighbour_{ij}^{t}, Global_{ij}^{t}, Constraint_{ij}^{t}\right) = \begin{cases} urban, & p_{ij}^{t} > pthreshold \\ non-urban, & p_{ij}^{t} \le pthr \end{cases}$$





Zhou, Y.; Zhang, F.; Du, Z.; Ye, X.; Liu, R. Integrating Cellular Automata with the Deep Belief Network for Simulating Urban Growth. Sustainability 2017,

Urban Growth Simulating (DBN-CA)



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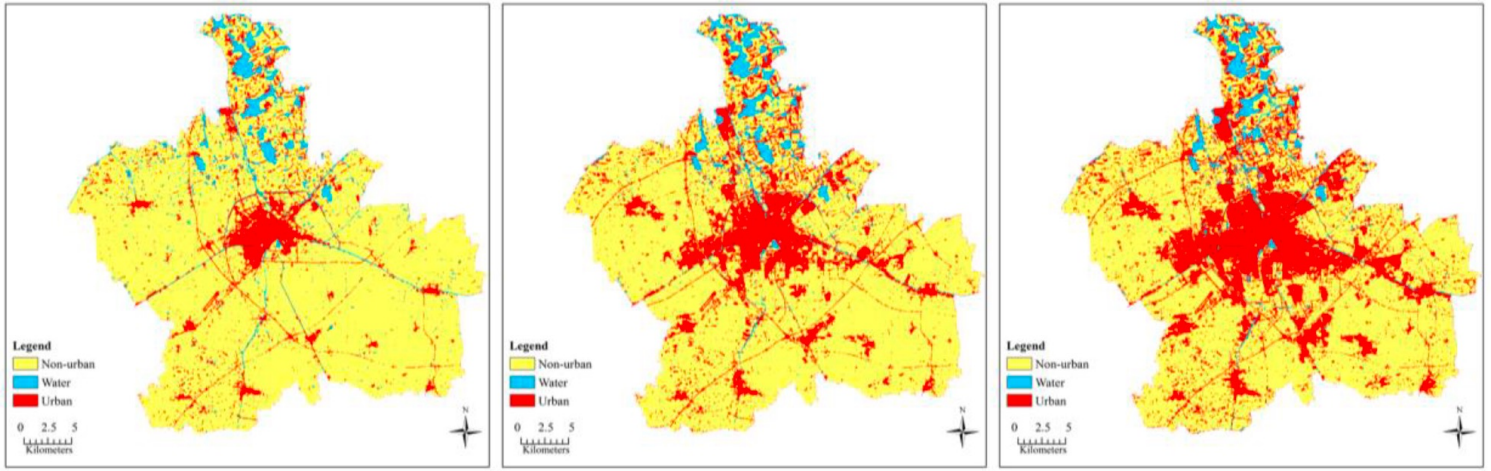
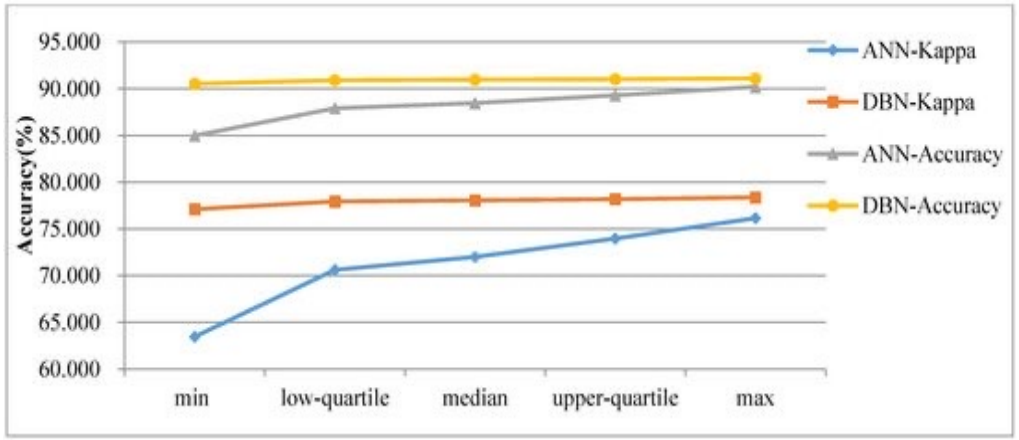
Urban Growth Simulating (DBN-CA)

Land of Jiaxing City in 2000, 2008 and 2015

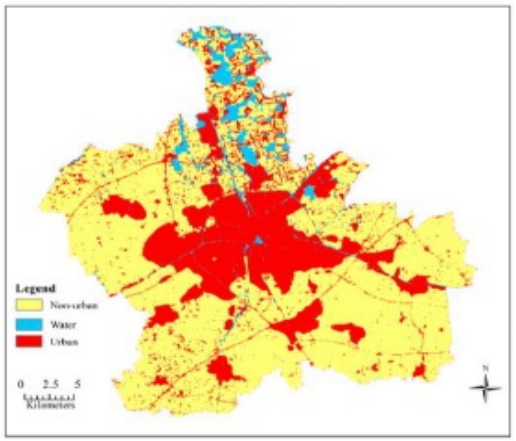




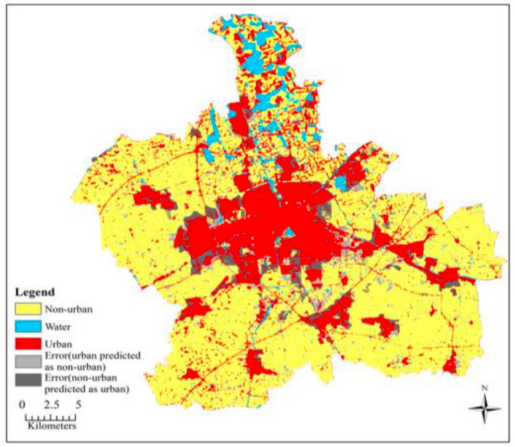
The Accuracy and the Kappa coefficient of DBN-CA and ANN-CA

Zhou, Y.; Zhang, F.; Du, Z.; Ye, X.; Liu, R. Integrating Cellular Automata with the Deep Belief Network for Simulating Urban Growth. Sustainability 2017,

Urban Growth Simulating (DBN-CA)

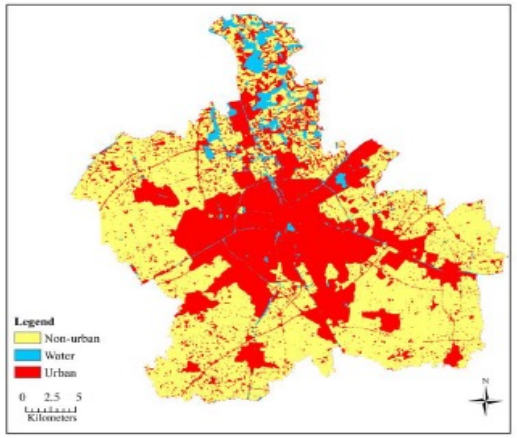


DBN-CA in 2015 (simulation)

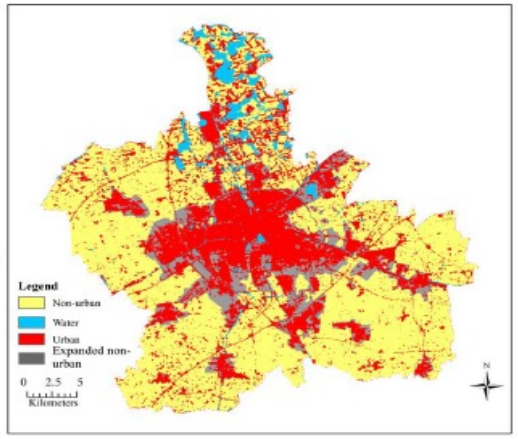


Error

The simulation and the error of DBN-CA in 2015



DBN-CA in 2024 (prediction)



Expansion area in 2024

The prediction and expansion area of DBN-CA in 2024

Zhou, Y.; Zhang, F.; Du, Z.; Ye, X.; Liu, R. Integrating Cellular Automata with the Deep Belief Network for Simulating Urban Growth. Sustainability 2017,

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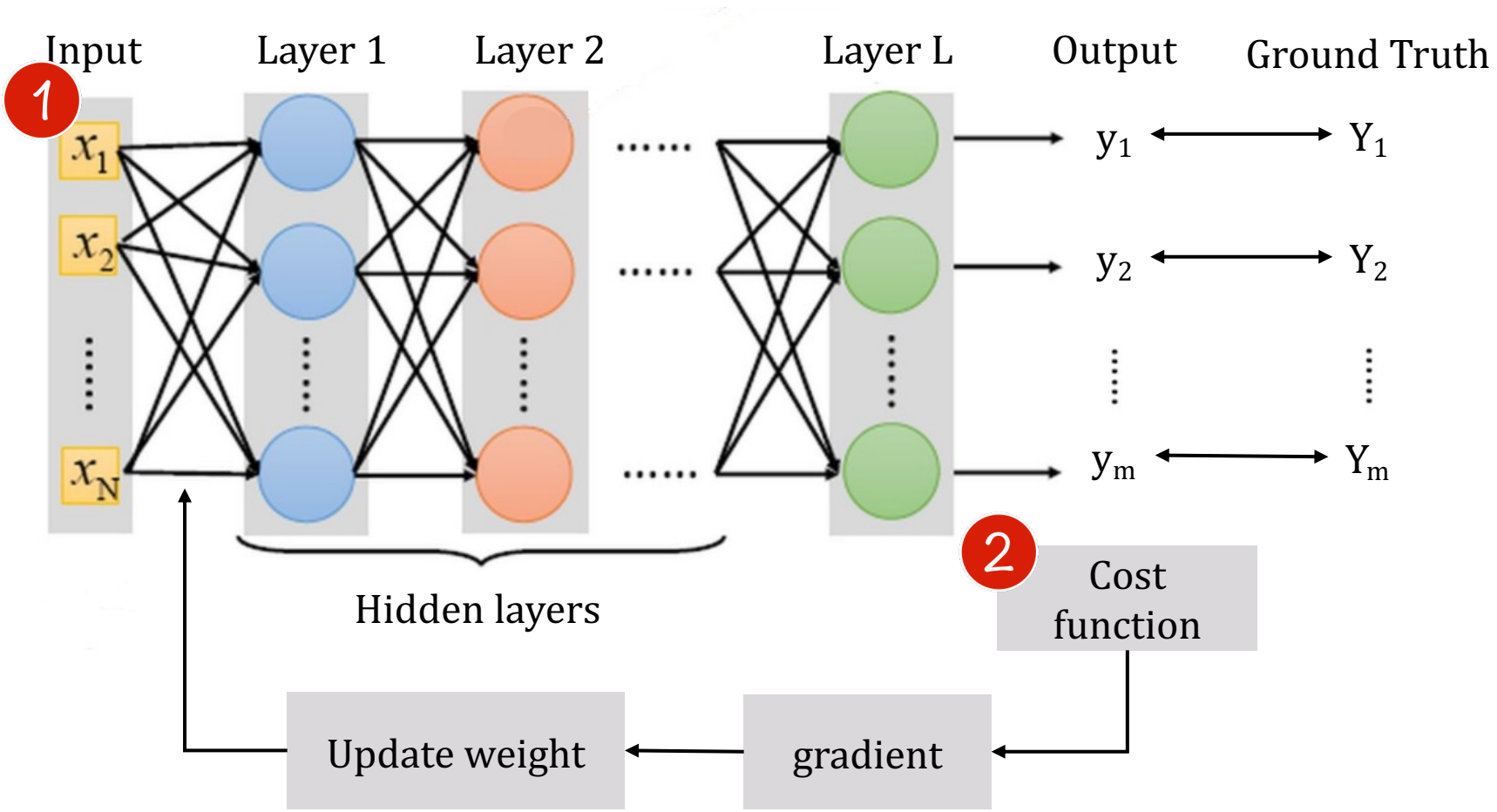
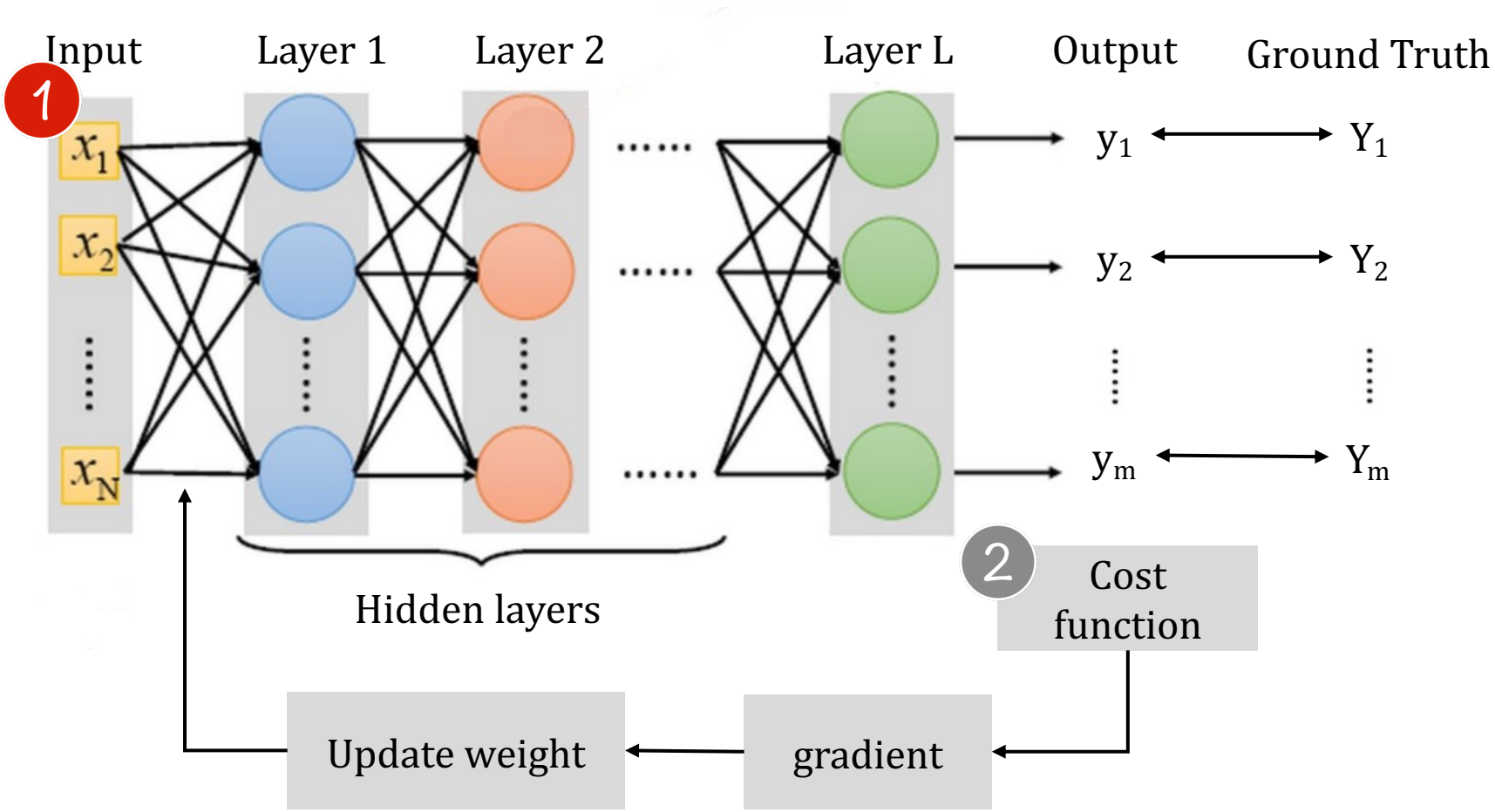
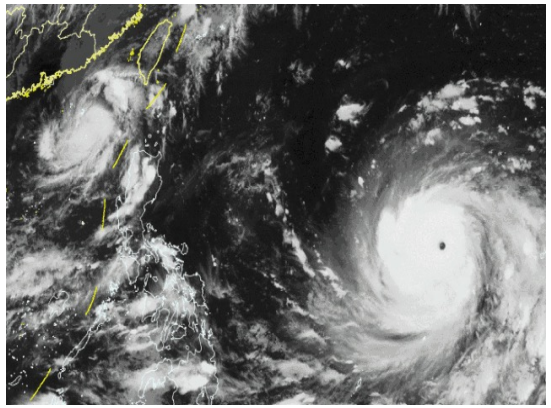
Theory-guided data driven models

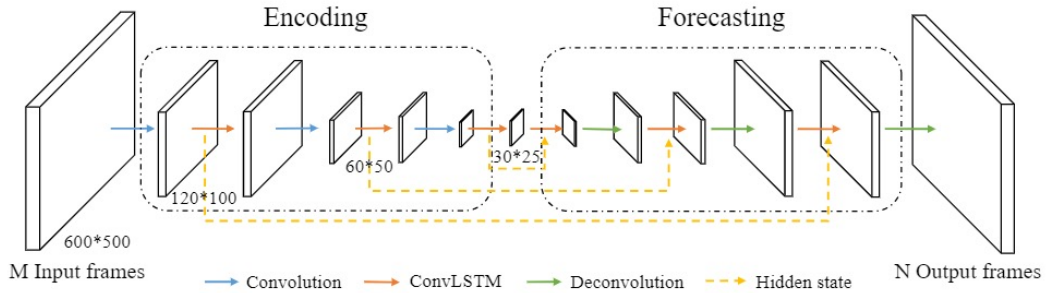


Theory-guided data driven models

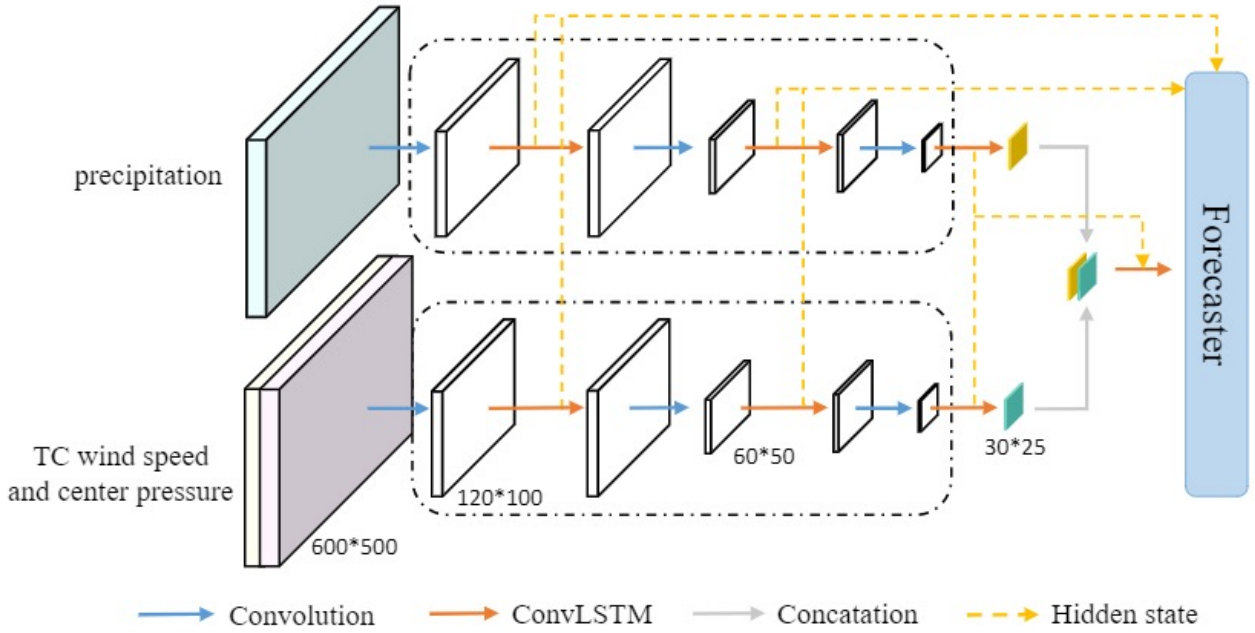


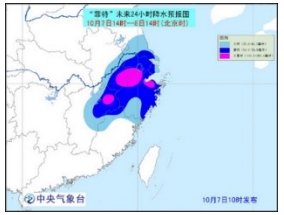
Typhoon Precipitation Nowcasting





The fusion of typhoon data

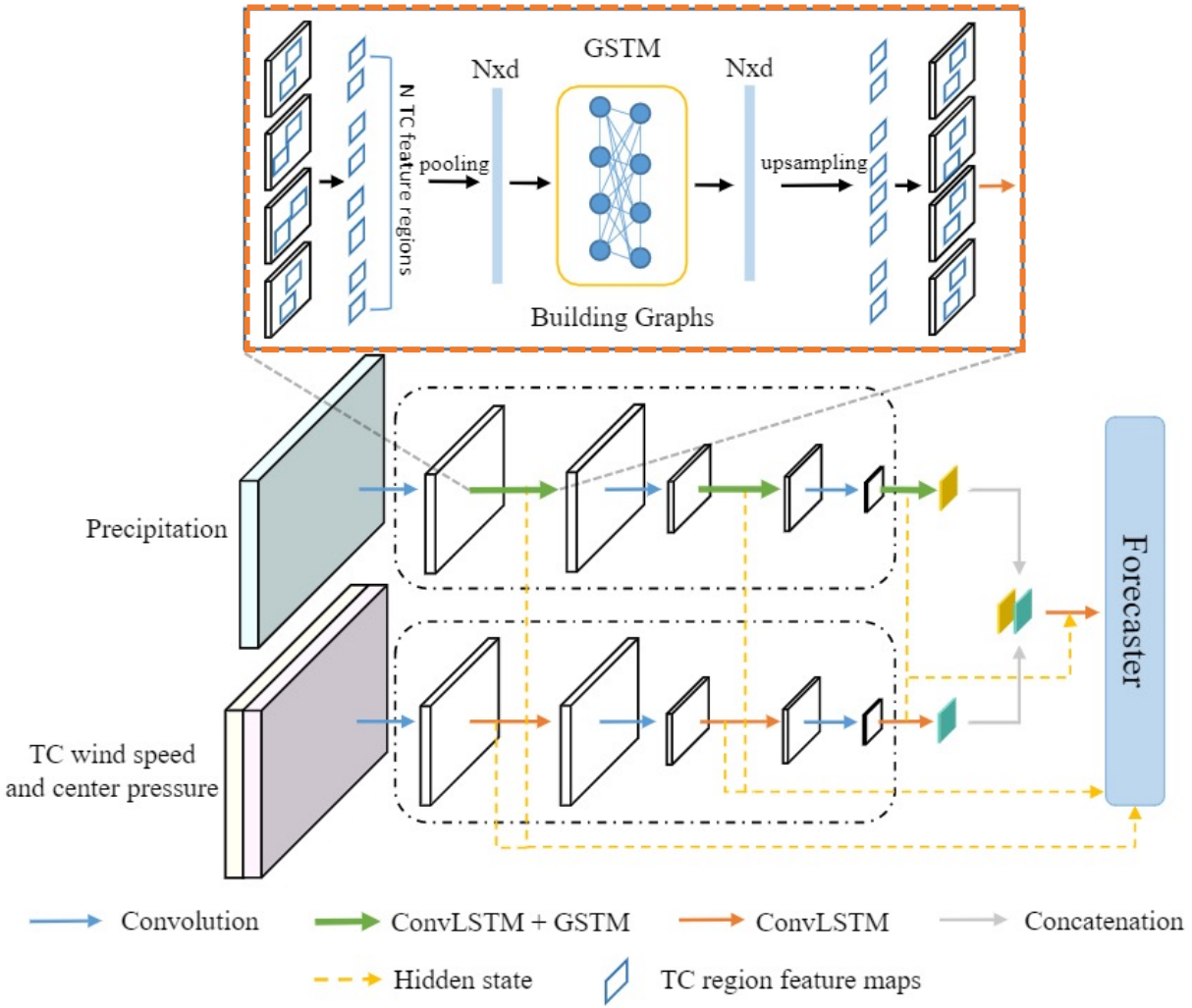




Yang X, Zhang F., et al. A Dynamic Graph-guided Network for Tropical Cyclone Precipitation Nowcasting [J]. Applied soft computing (under review)

Typhoon Precipitation Nowcasting

Graph-guided Spatio-Temporal Module （GSTM）



Extract the regional series and construct the spatio-temporal inference graph

$$NF = \text{AvgPool}(RF)$$

$$Adj = Softmax((NF)(NF^T))$$

Propagate the information on the graph

$$NF' = (Adj)(NF)W + NF$$

$$RF' = Unsampling(NF')$$

$$FRF = \lambda RF' + RF$$

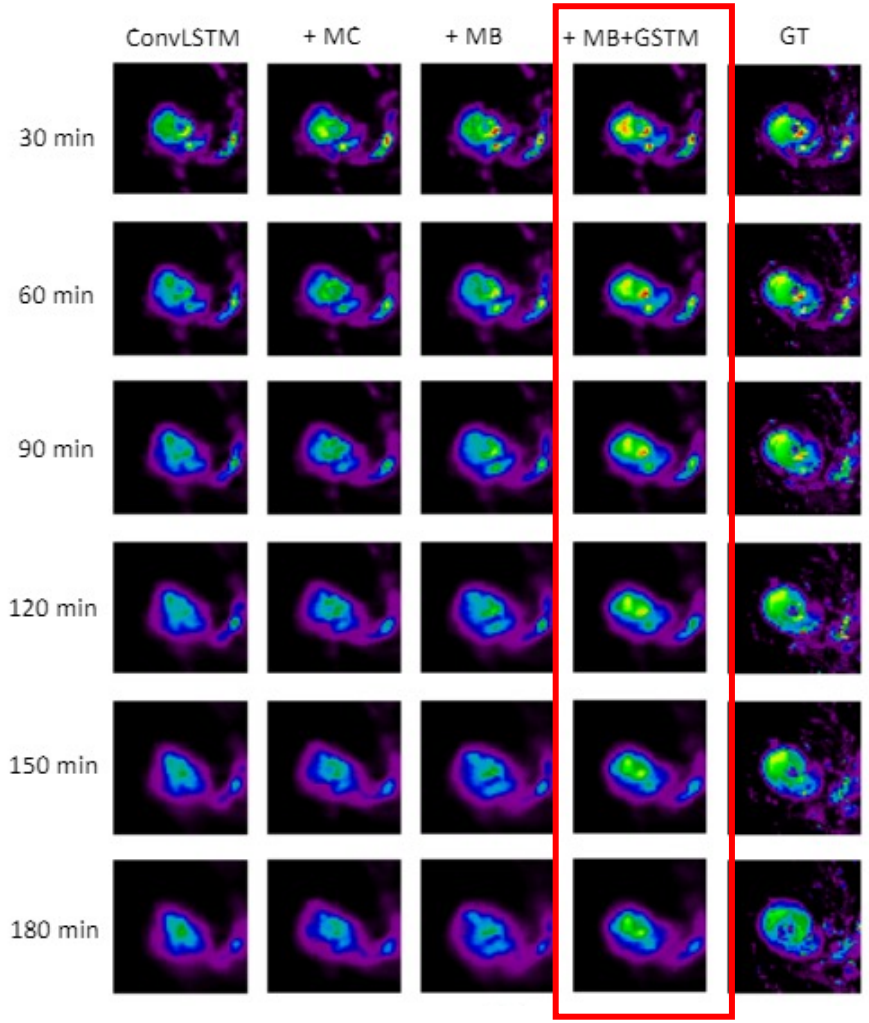
Yang X, Zhang F., et al. A Dynamic Graph-guided Network for Tropical Cyclone Precipitation Nowcasting [J]. Applied soft computing (under review)

Typhoon Precipitation Nowcasting

Algorithms	CSI ↑					
	$r \geq 0.5$	$r \geq 2$	$r \geq 5$	$r \geq 10$	$r \geq 20$	$r \geq 30$
2D CNN	0.4456	0.374	0.291	0.2194	0.138	0.082
TrajGRU	0.4650	0.3913	0.2971	0.2274	0.1620	0.1133
ConvLSTM	0.4643	0.3913	0.3003	0.2307	0.1596	0.1067
ConvLSTM+MC	0.469	0.4011	0.3092	0.2352	0.1697	0.1149
ConvLSTM+MB	**0.4728**	0.4027	0.3191	0.2553	0.1859	0.1236
ConvLSTM+MB+GSTM	0.4716	**0.4027**	**0.3246**	**0.2632**	**0.2015**	**0.149**

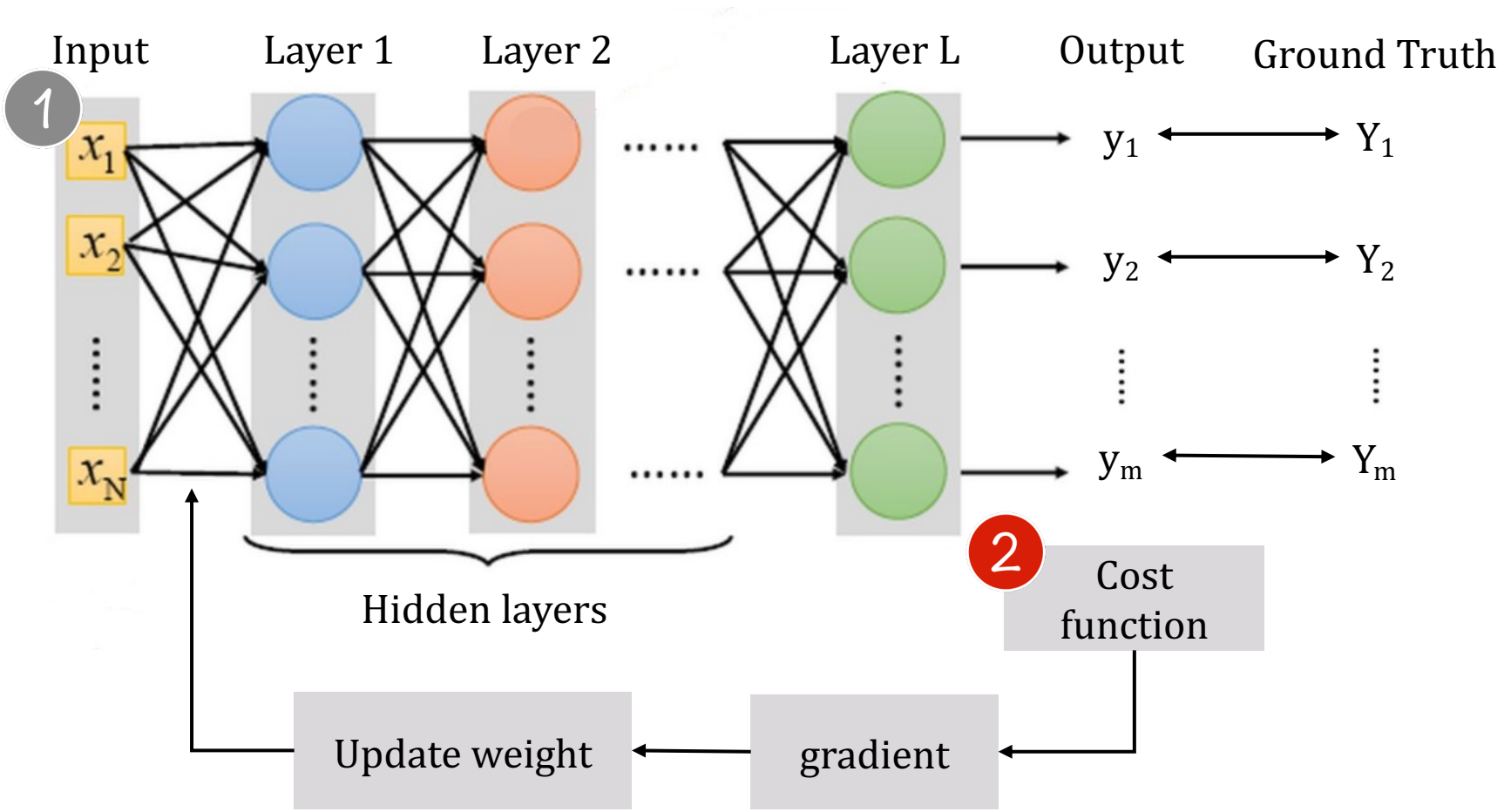
Algorithms	HSS ↑					
	$r \geq 0.5$	$r \geq 2$	$r \geq 5$	$r \geq 10$	$r \geq 20$	$r \geq 30$
2D CNN	0.58	0.5273	0.4402	0.3506	0.2328	0.1432
TrajGRU	0.6009	0.5452	0.4458	0.3597	0.2668	0.1918
ConvLSTM	0.5998	0.5452	0.4501	0.3651	0.265	0.1835
ConvLSTM+MC	0.6036	0.5555	0.4616	0.3719	0.2814	0.1985
ConvLSTM+MB	**0.6072**	0.557	0.4727	0.3982	0.305	0.2114
ConvLSTM+MB+GSTM	0.6055	**0.5581**	**0.4793**	**0.4085**	**0.328**	**0.2523**

Algorithms	F1 score ↑					
	$r \geq 0.5$	$r \geq 2$	$r \geq 5$	$r \geq 10$	$r \geq 20$	$r \geq 30$
2D CNN	0.6147	0.541	0.4454	0.3524	0.2332	0.1433
TrajGRU	0.6323	0.5579	0.4506	0.3614	0.2673	0.1920
ConvLSTM	0.6315	0.5581	0.455	0.3668	0.2655	0.1837
ConvLSTM+MC	0.6361	0.5687	0.4665	0.3736	0.2819	0.1987
ConvLSTM+MB	**0.6394**	0.5697	0.4776	0.4	0.3055	0.2116
ConvLSTM+MB+GSTM	0.6374	**0.5699**	**0.4844**	**0.4106**	**0.3286**	**0.2525**

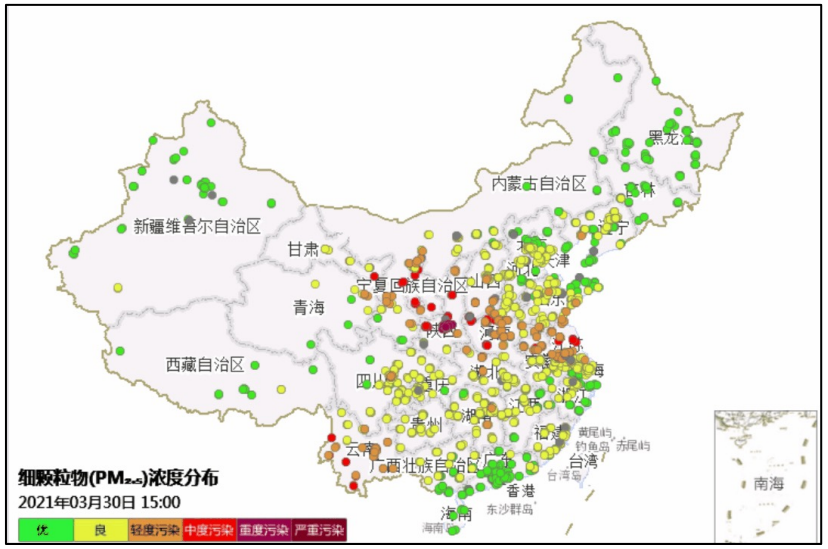


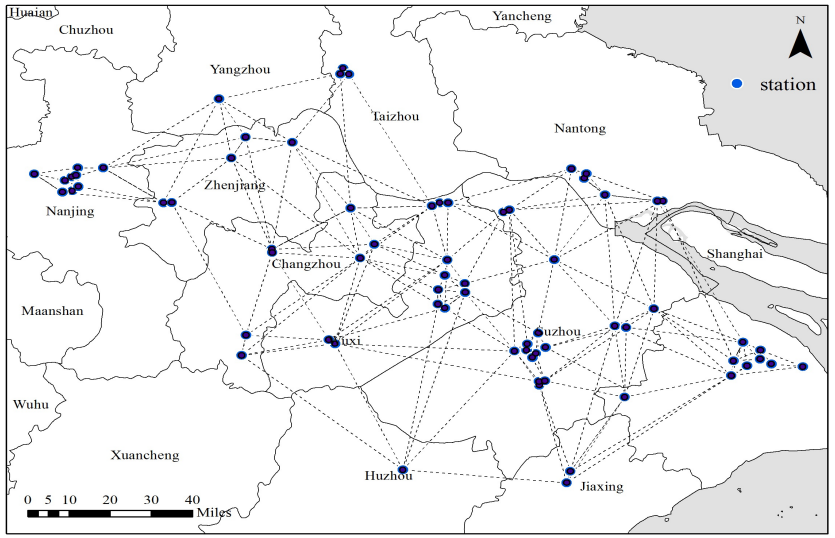
Yang X, Zhang F., et al. A Dynamic Graph-guided Network for Tropical Cyclone Precipitation Nowcasting [J]. Applied soft computing (under review)

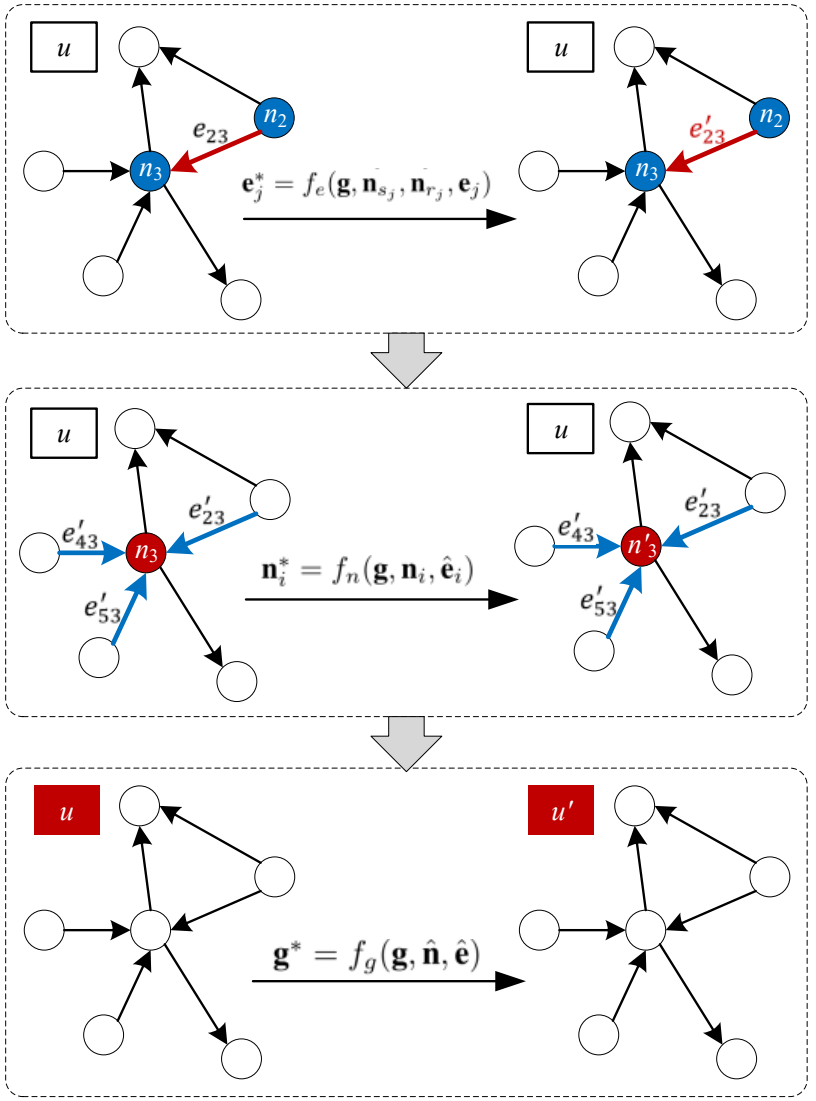
Theory-guided data driven models



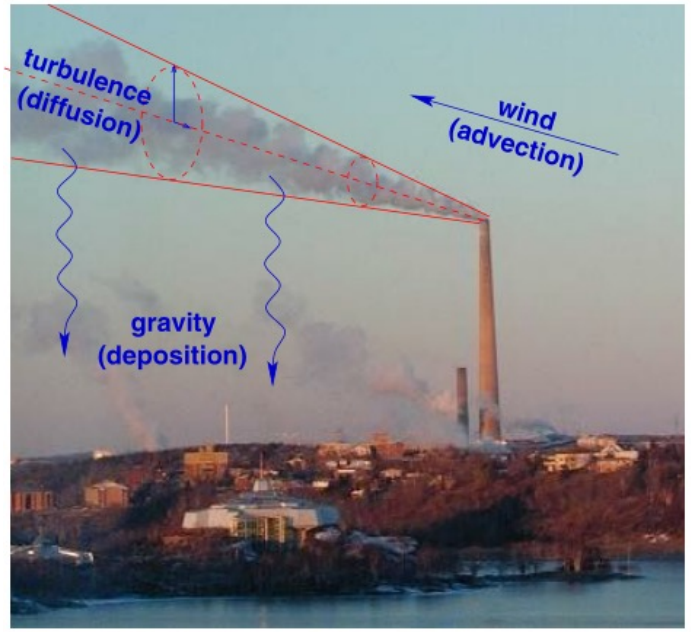
PM2.5 forecasting

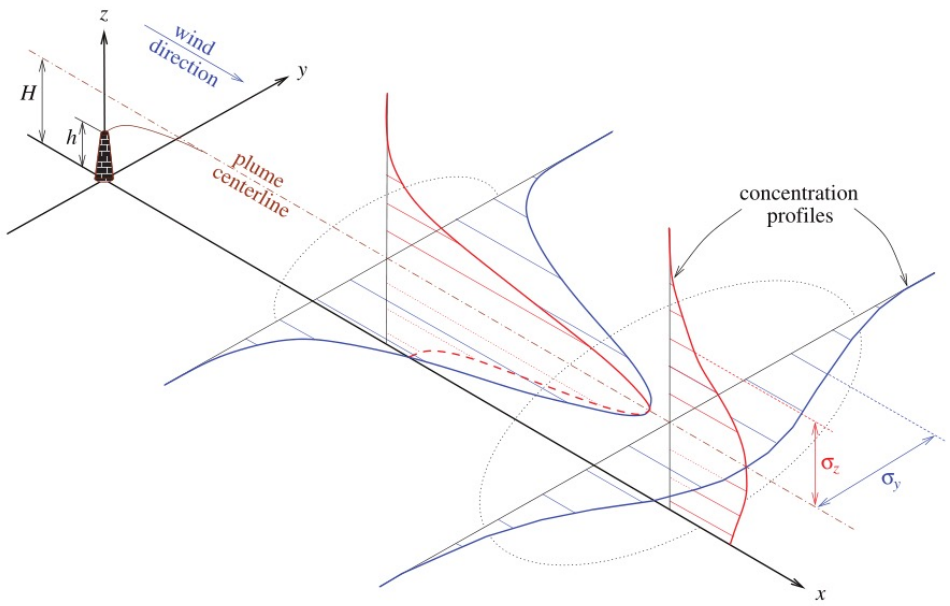






The atmospheric dispersion model

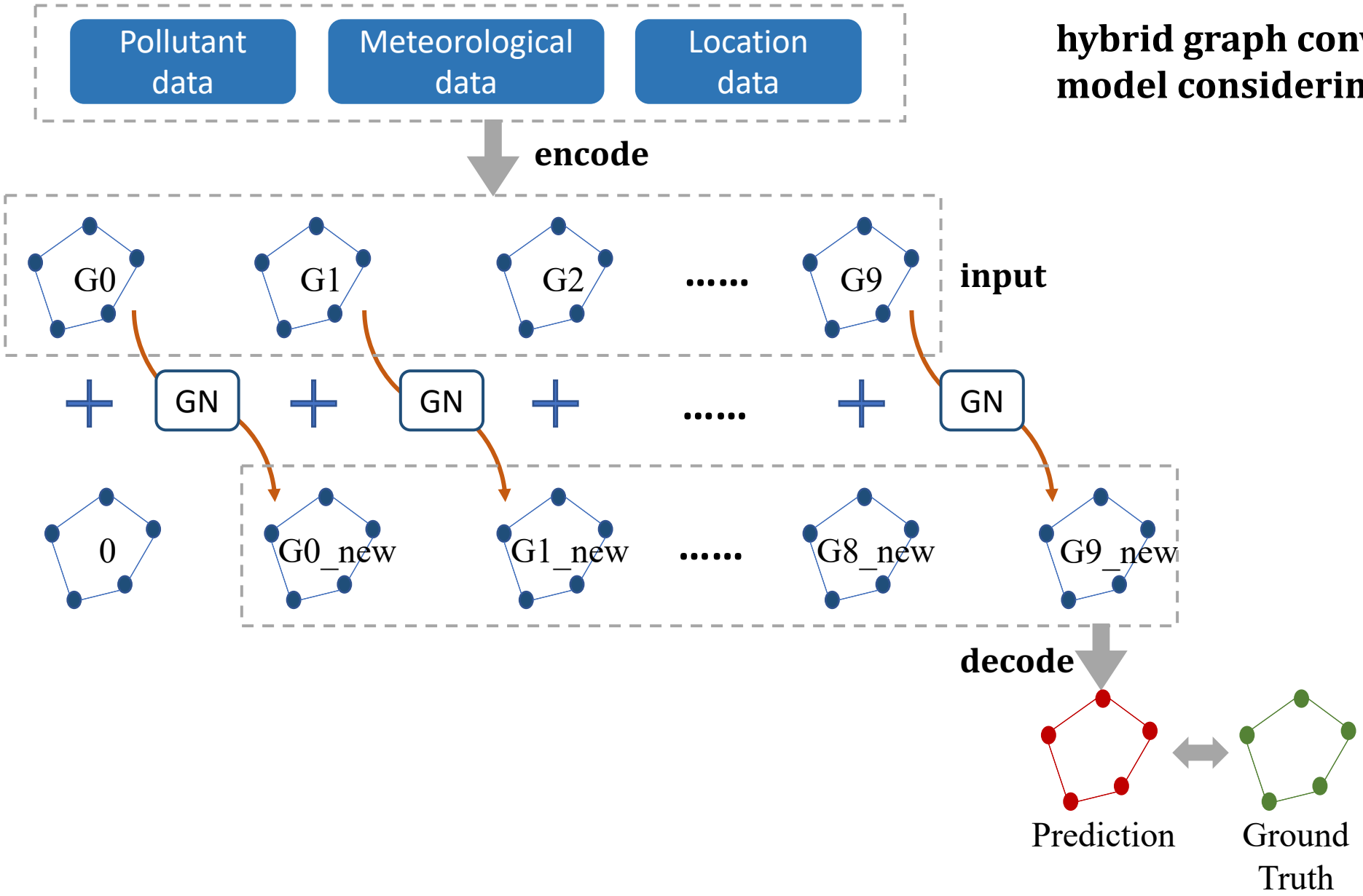




$$\frac{\partial c}{\partial t}+u_x\frac{\partial c}{\partial x}+u_y\frac{\partial c}{\partial y}+u_z\frac{\partial c}{\partial z}=\frac{\partial}{\partial x}\left(D_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial c}{\partial z}\right)+S(x,y,z,c,t)$$

advection effect **diffusion effect** **Pollution source**

Zhou H , Zhang F , et al. Forecasting PM2.5 using hybrid graph convolution–based model considering dynamic wind–field to offer the benefit of spatial interpretability[J]. Environmental Pollution, 2021



hybrid graph convolution-based model considering dynamic wind-field

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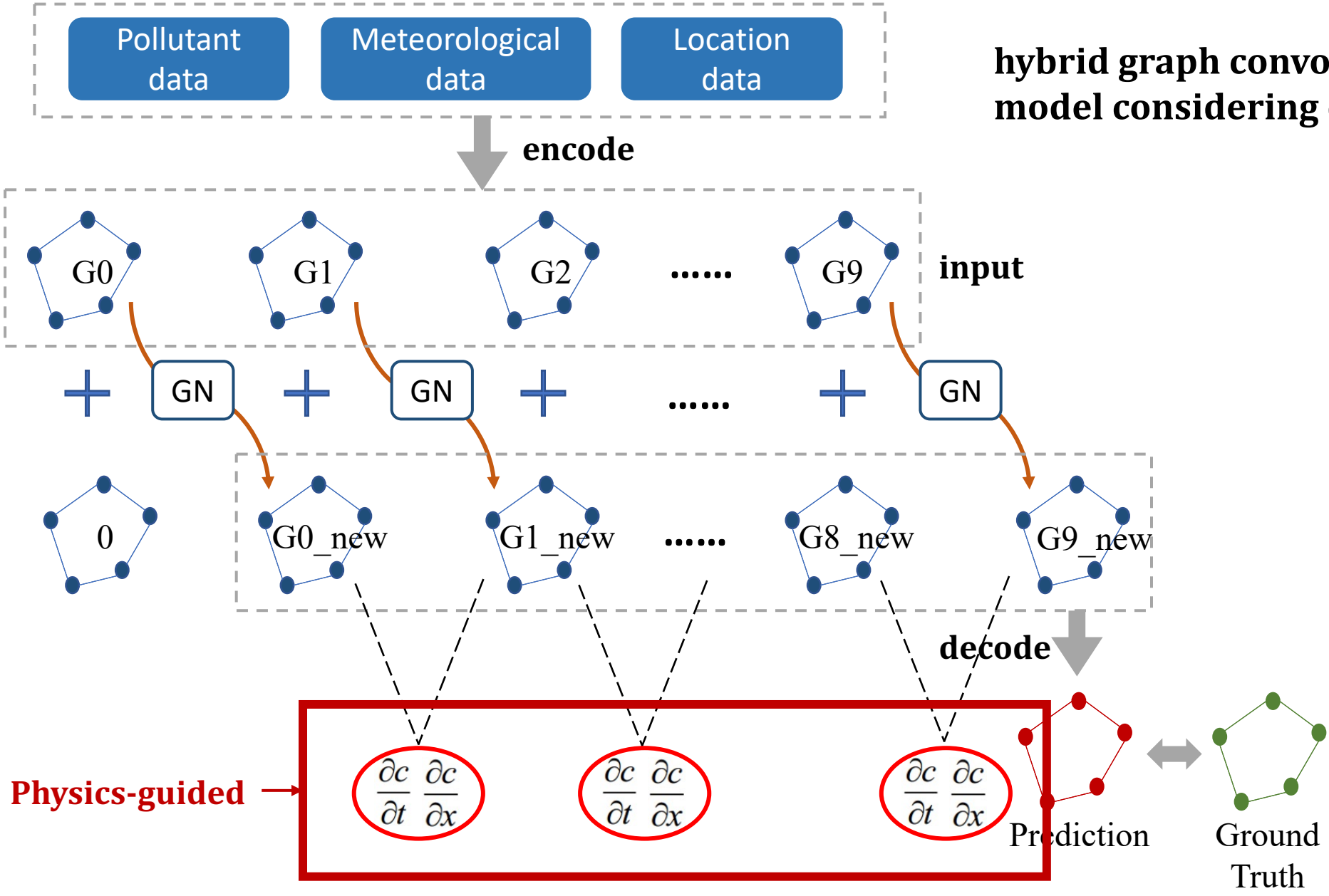


hybrid graph convolution-based model considering dynamic wind-field

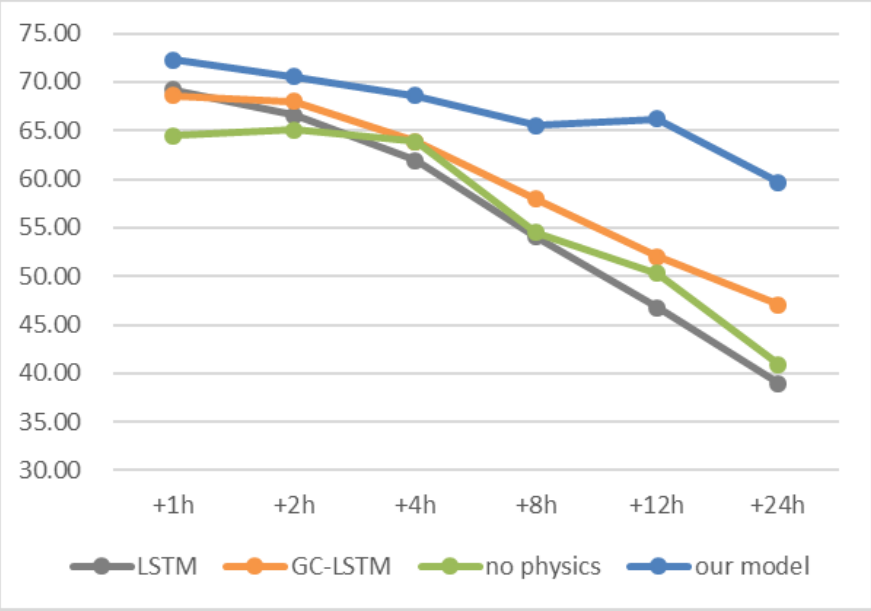
Zhou H , Zhang F , et al. Forecasting PM2.5 using hybrid graph convolution–based model considering dynamic wind–field to offer the benefit of spatial interpretability[J]. Environmental Pollution, 2021

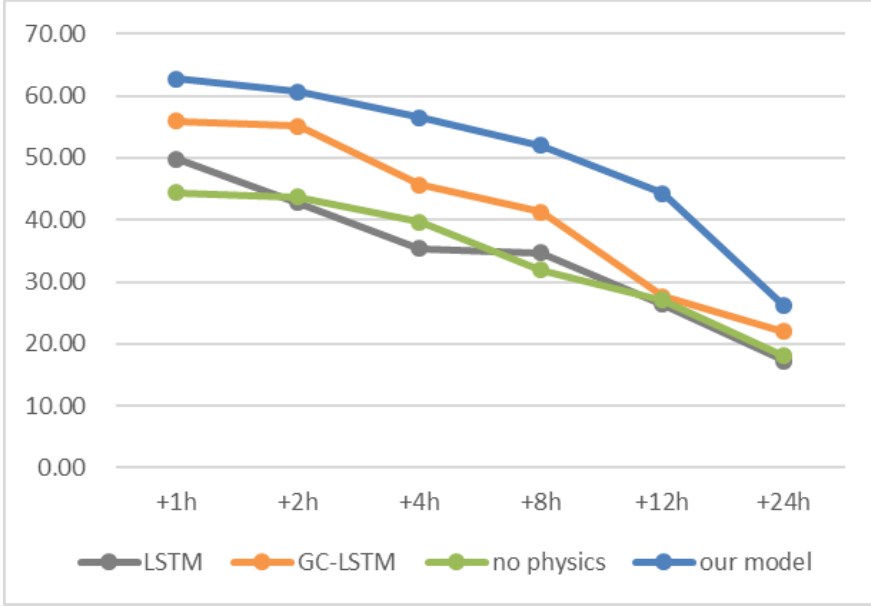
Result

Model		1	2	4	8	12	24
LSTM	rmse	20.6393	21.0103	22.3271	23.8861	25.1641	29.3749
	mae	15.2236	15.4459	16.2739	17.3312	18.1747	21.4094
	IA	0.8906	0.8850	0.8631	0.7988	0.7505	0.6026
	r	0.8266	0.8138	0.7776	0.7079	0.6506	0.5050
GC-LSTM	rmse	19.2963	19.8383	21.3861	23.4004	24.7533	28.5459
	mae	13.3595	13.7157	14.9543	17.1641	17.9145	21.4850
	IA	0.8806	0.8774	0.8591	0.8281	0.7852	0.7059
	r	0.8235	0.8168	0.7780	0.7284	0.6924	0.5583
GN-no-physics	rmse	19.2379	19.7214	21.0835	23.6588	25.3558	28.5466
	mae	13.0323	13.2661	14.4151	16.7451	18.4607	20.9568
	IA	0.8914	0.8853	0.8614	0.8033	0.7686	0.6560
	r	0.8325	0.8243	0.7950	0.7348	0.6864	0.5709
Our model	rmse	**18.1880**	**18.3571**	**19.6208**	**21.7959**	**23.3570**	**27.3578**
	mae	**12.1313**	**12.4879**	**13.5322**	**15.4026**	**16.7409**	**20.2831**
	IA	**0.9140**	**0.9087**	**0.8935**	**0.8670**	**0.8411**	**0.7863**
	r	**0.8532**	**0.8451**	**0.8198**	**0.7719**	**0.7324**	**0.6319**

0-35	Excellent	No effect on health
35-75	Good	Weak effects on the health of a very small number of susceptible people
75-115	Light pollution	Irritation symptoms in healthy people
115-150	Moderate pollution	Healthy people's heart and respiratory system are affected
150-250	Severe pollution	Significant increase in cardiopulmonary symptoms
250-500	extremelySevere pollution	Visible symptoms, disease onset

threshold=75



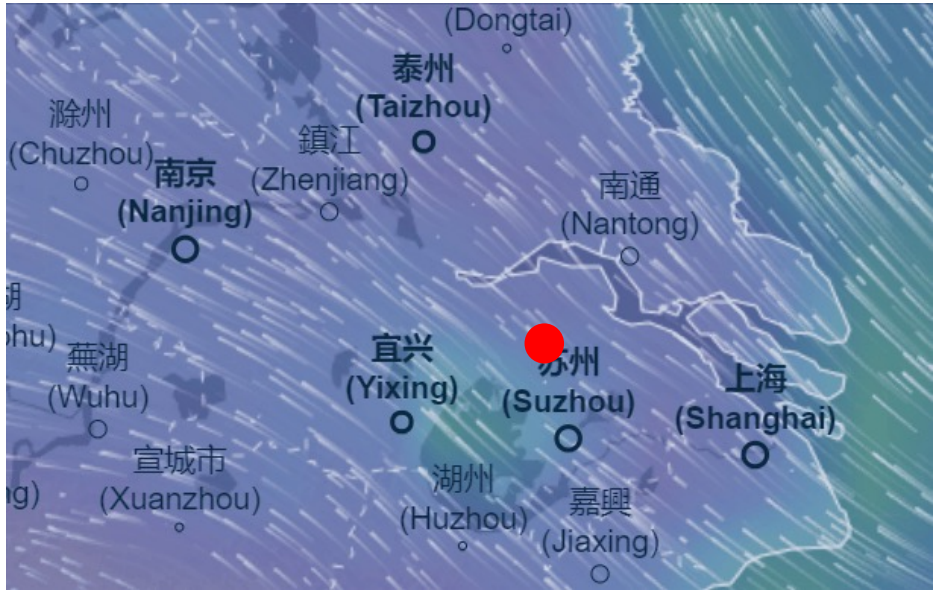


threshold=115

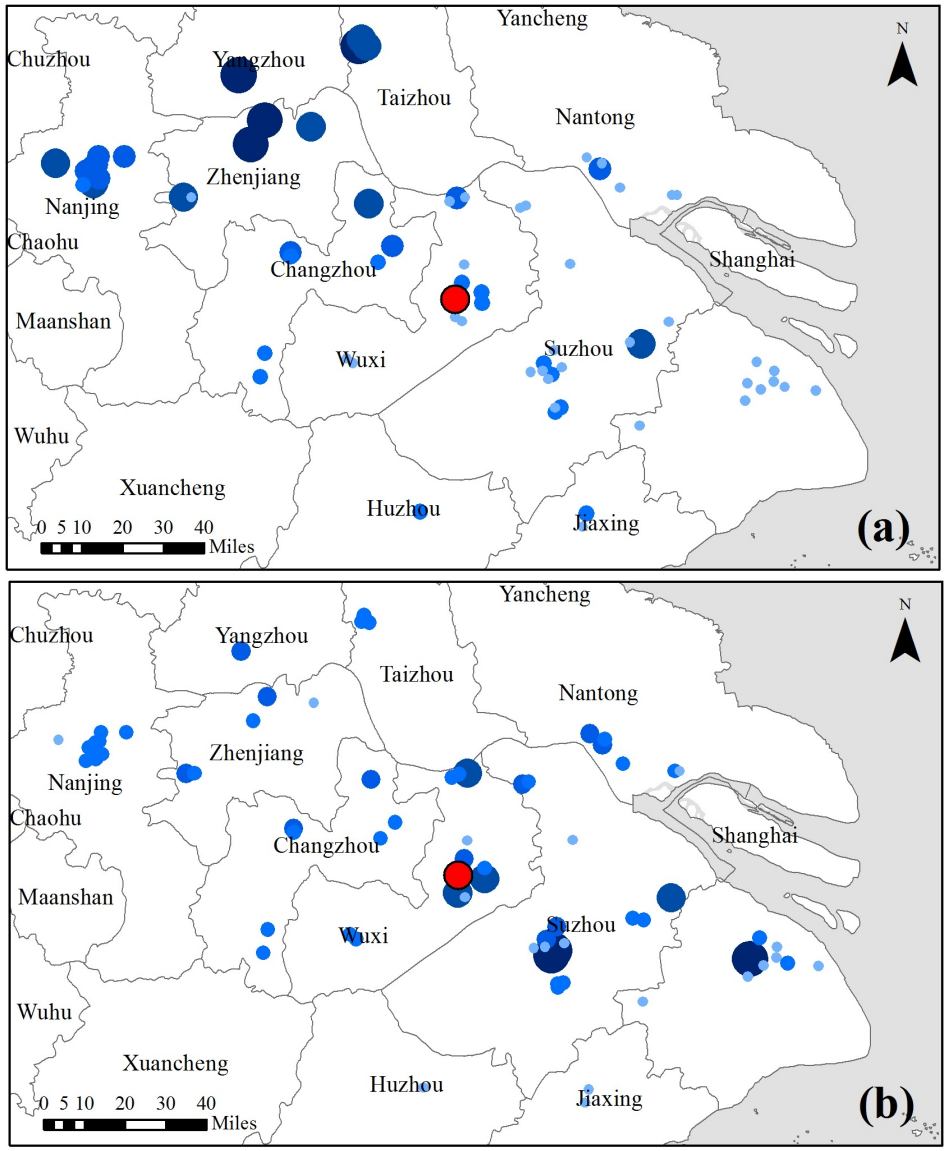
Zhou H , Zhang F , et al. Forecasting PM2.5 using hybrid graph convolution–based model considering dynamic wind–field to offer the benefit of spatial interpretability[J]. Environmental Pollution, 2021

Explain the model

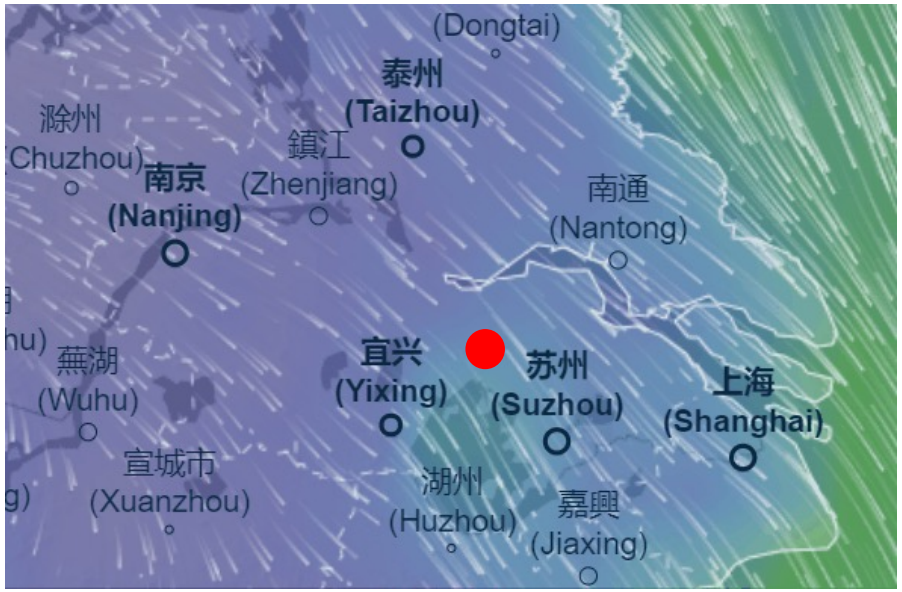
GNNEXPLAINER (Ying, Zhitao et al)



2016.08.01



Explain the model



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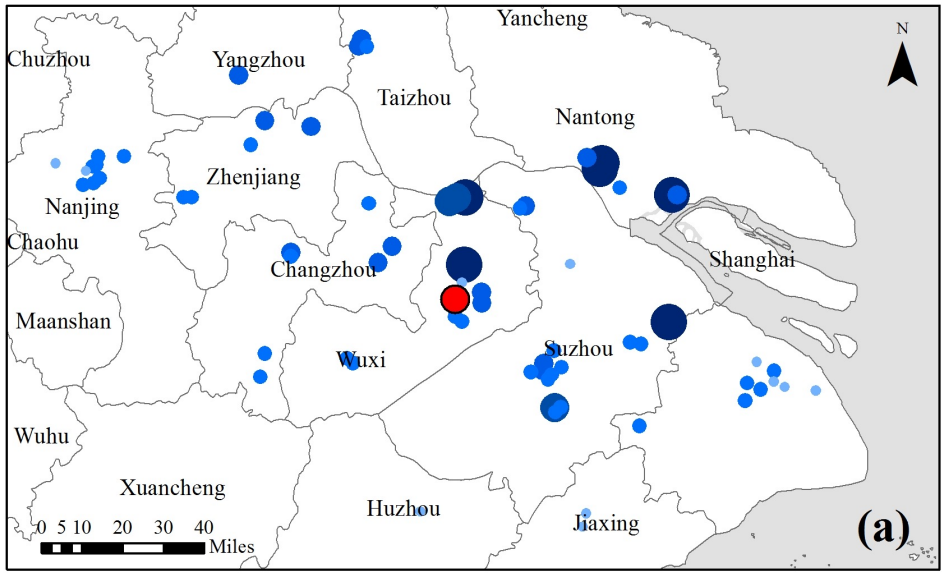
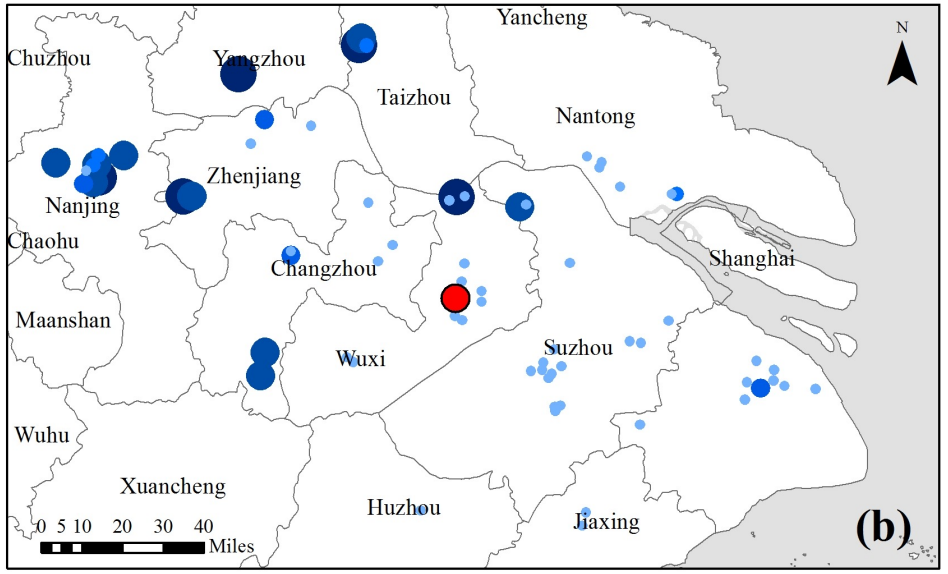
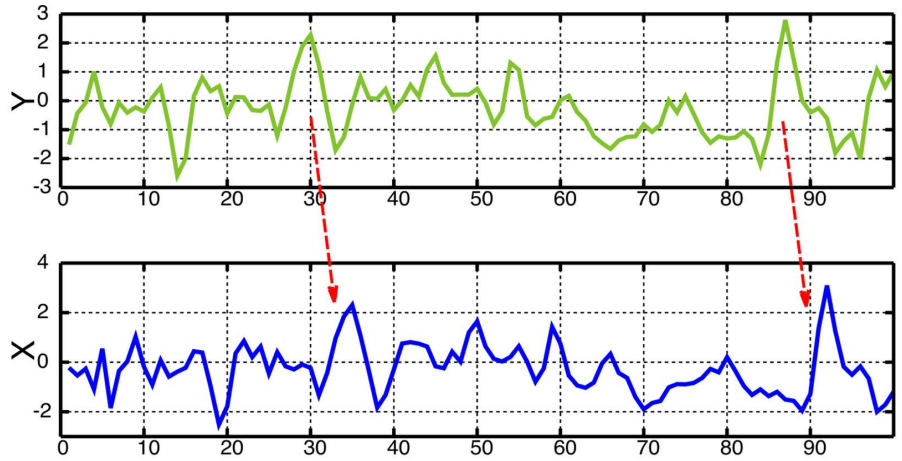


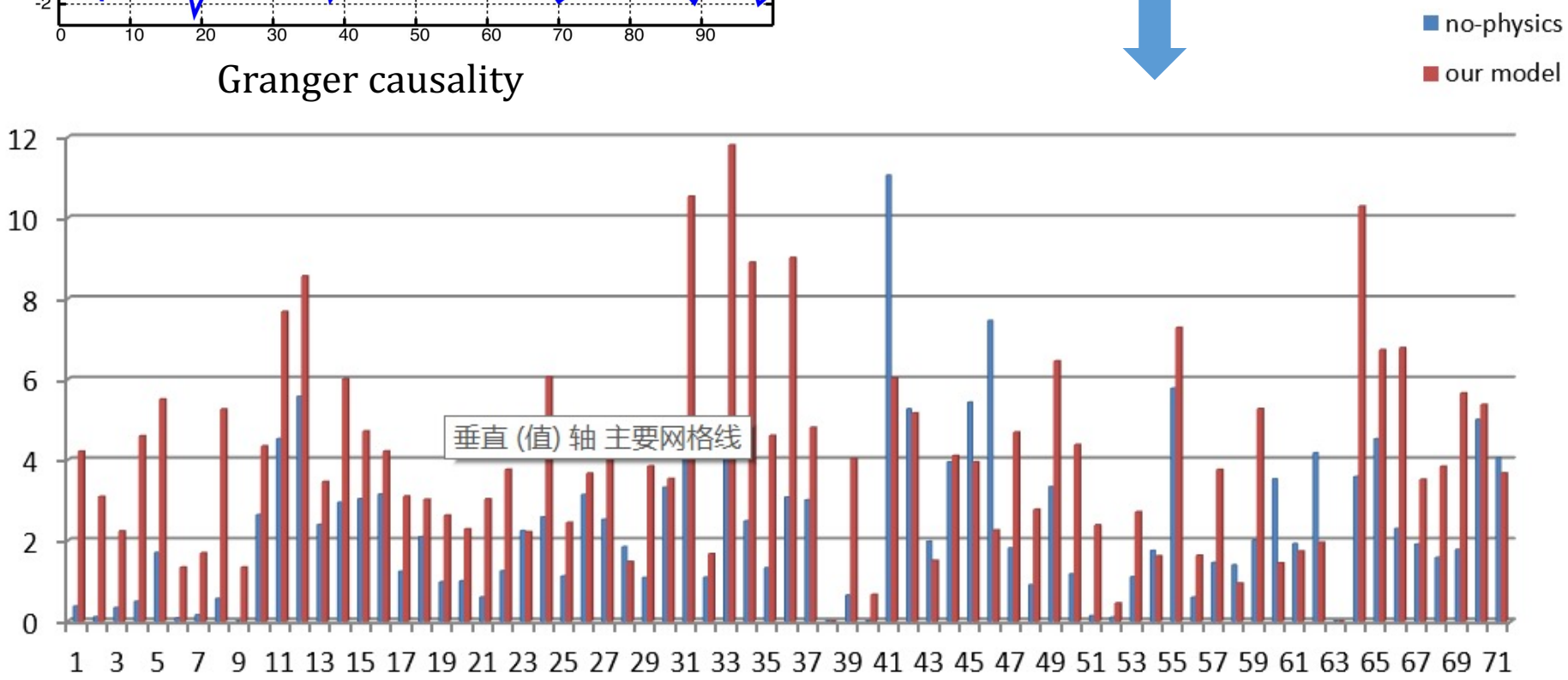


Explain the model



Granger causality

Granger causality
×
Explain Weight



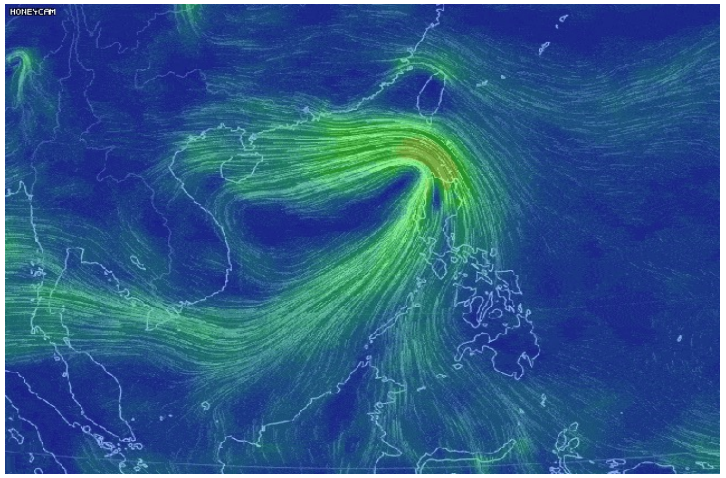
How to integrate theory-driven and data-driven models?

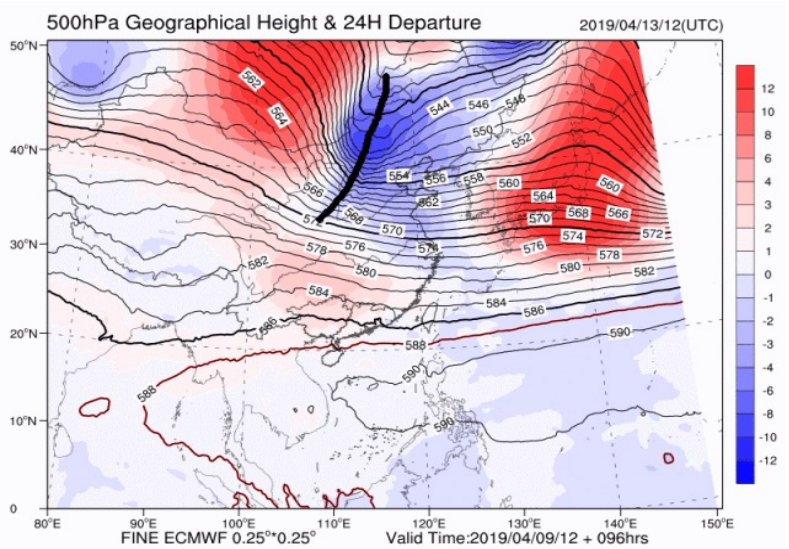
1. Optimizing theory-driven models with data-driven models

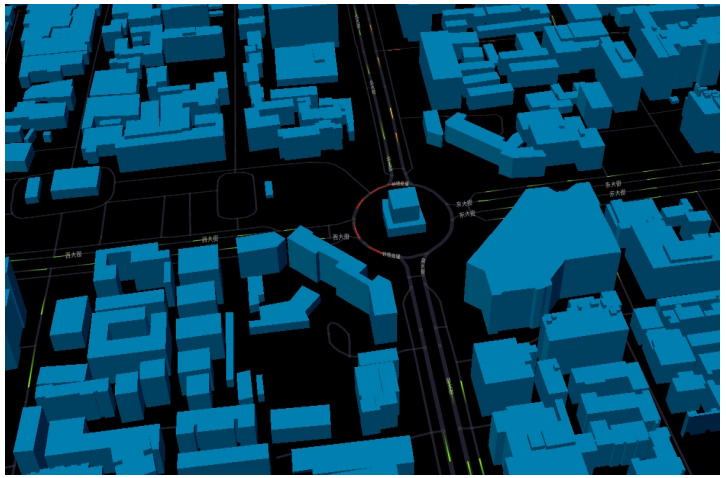
2. Theory-guided data driven models

3. **Data-driven prediction that uncovers dynamic patterns**

Dynamic System



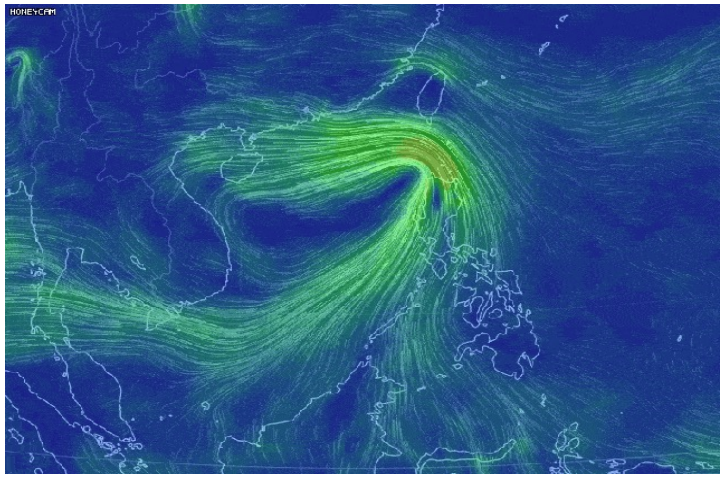


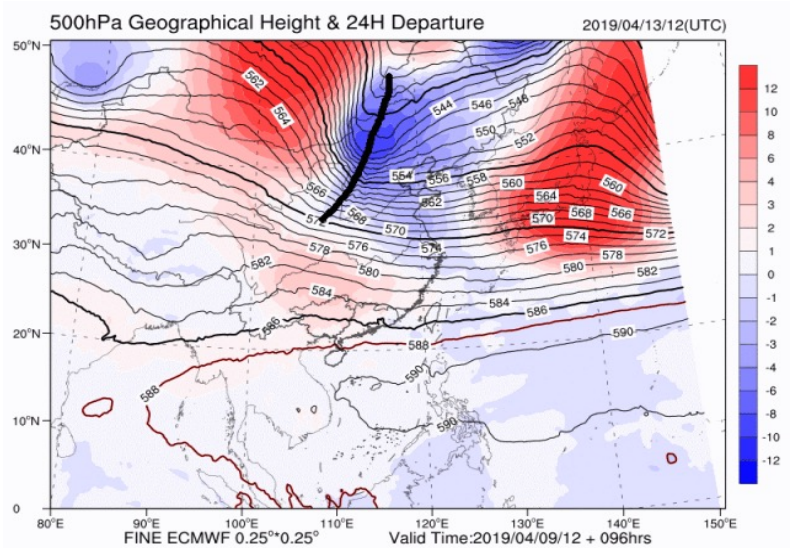


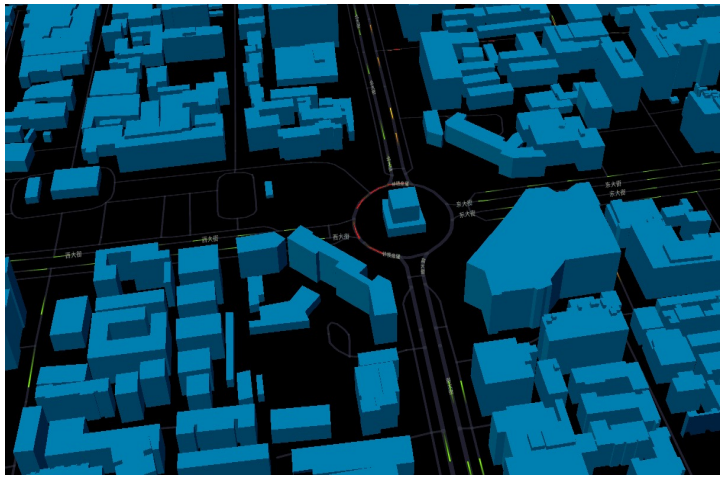
Dynamic System

Gaussian diffusion model

$$c(x,y,z)=\frac{Q}{4\pi u(D_yD_z)^{1/2}}\exp[-\frac{u}{4x}(\frac{y^2}{D_y}+\frac{z^2}{D_z})]$$







Dynamic System

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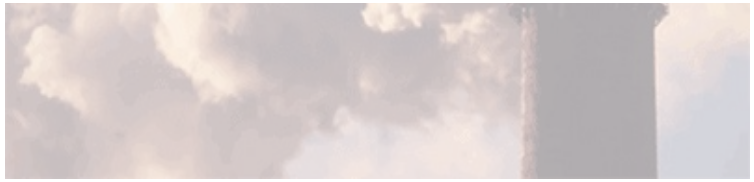
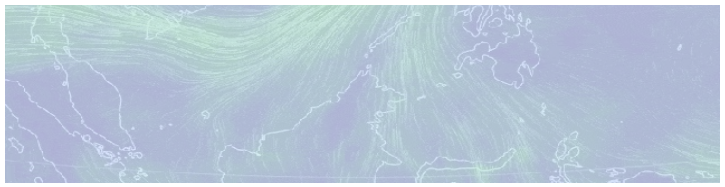
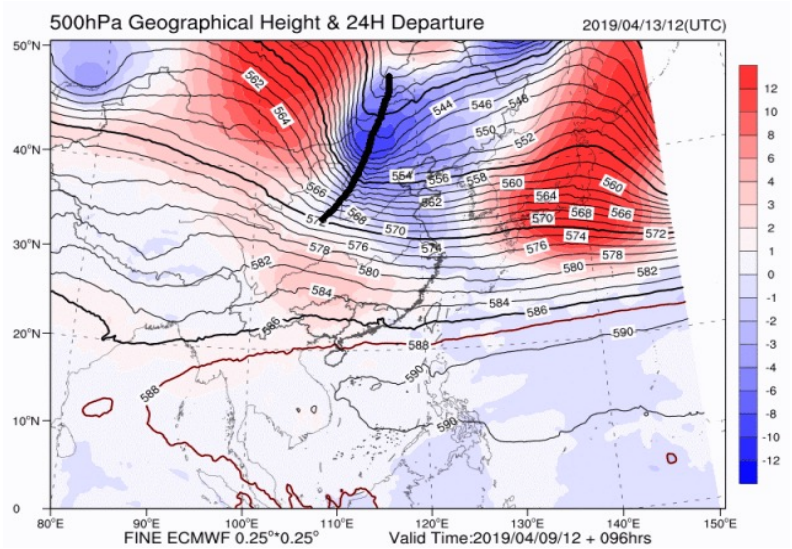
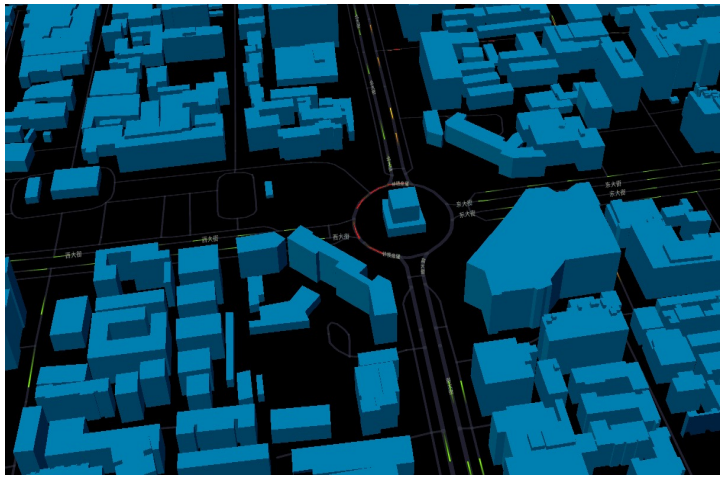


Navier-Stokes equation

$$\partial_t u+(u\cdot\nabla)u=-\nabla p+v\Delta u$$







Dynamic System

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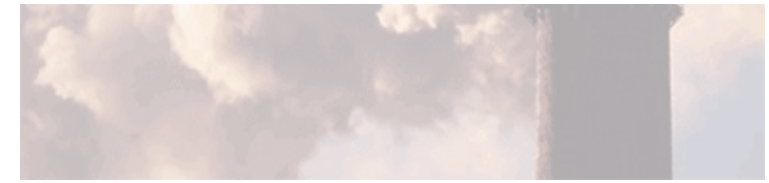

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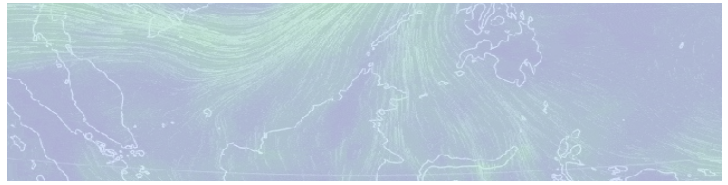
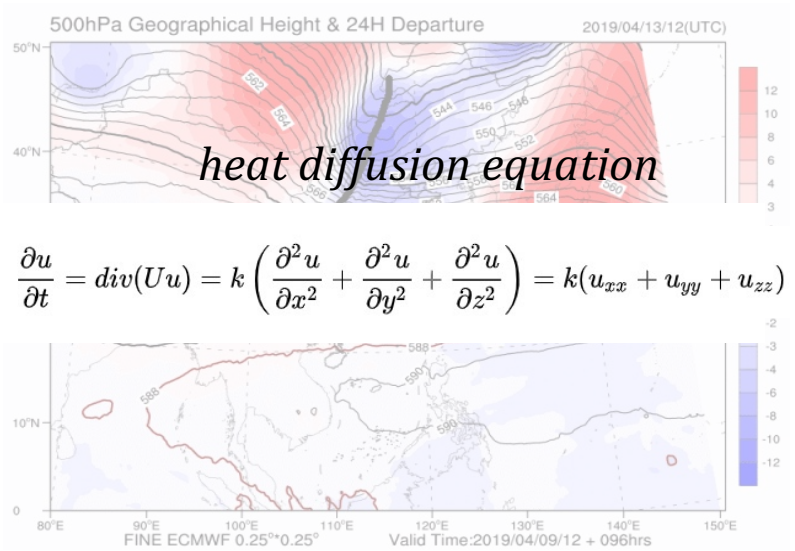
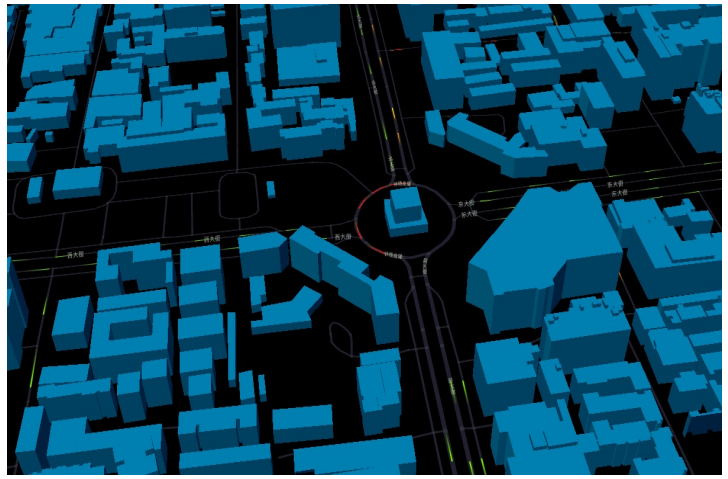




heat diffusion equation

$$\frac{\partial u}{\partial t}=div(Uu)=k\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}\right)=k(u_{xx}+u_{yy}+u_{zz})$$



Dynamic System

Gaussian diffusion model

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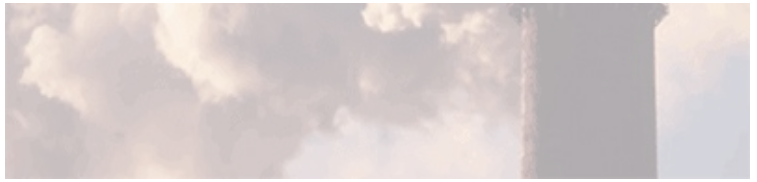

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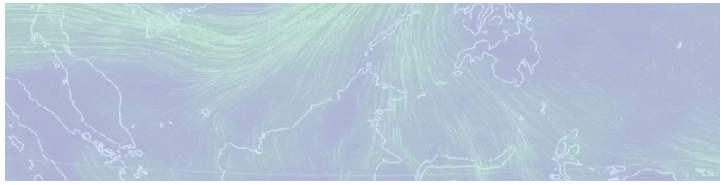

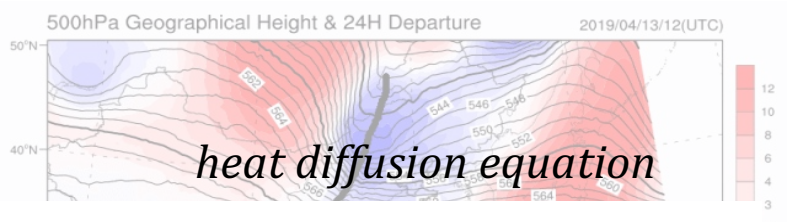

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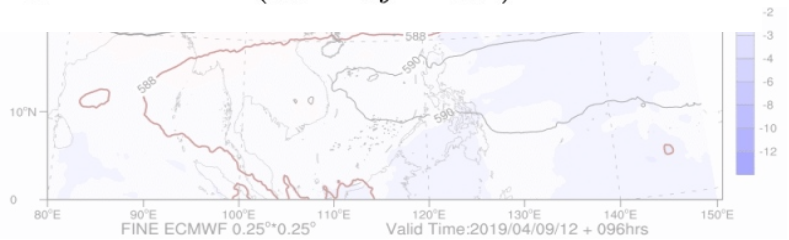
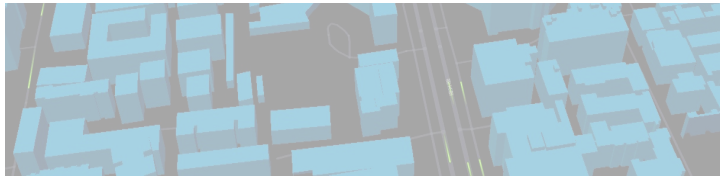


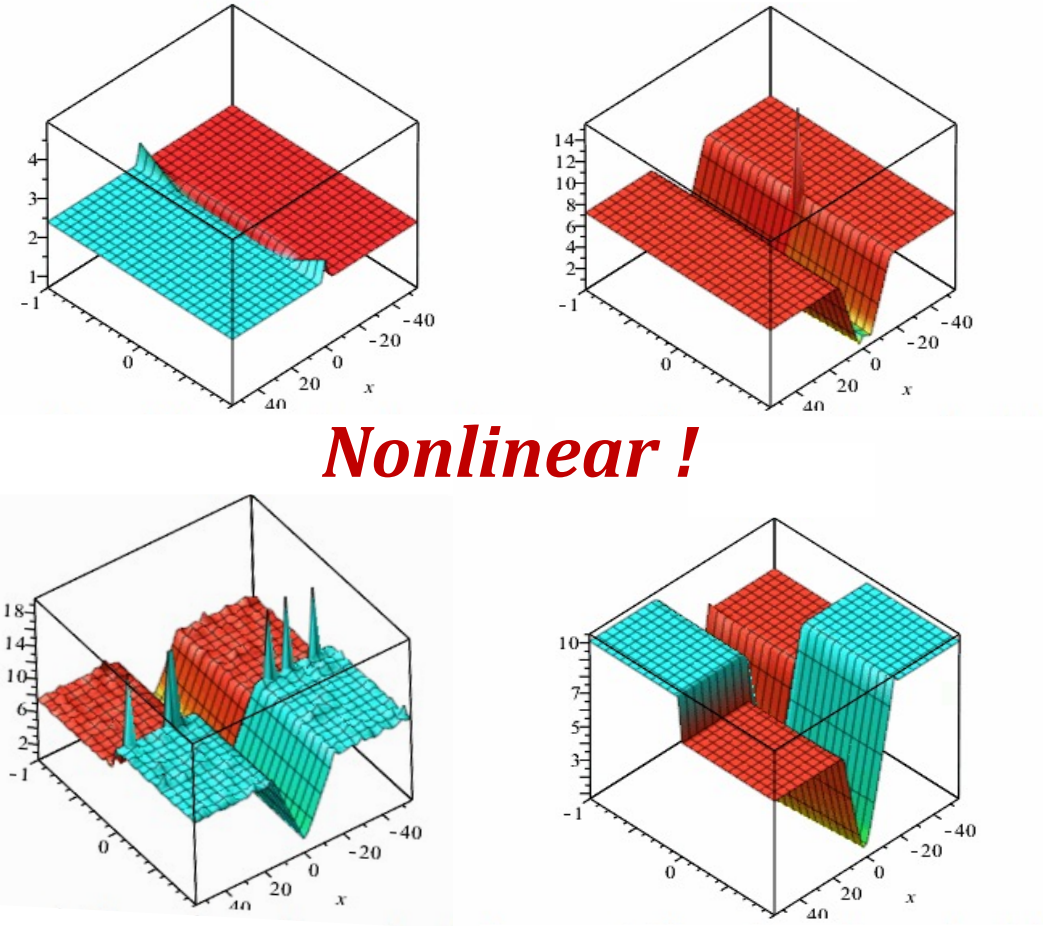
Galloping model

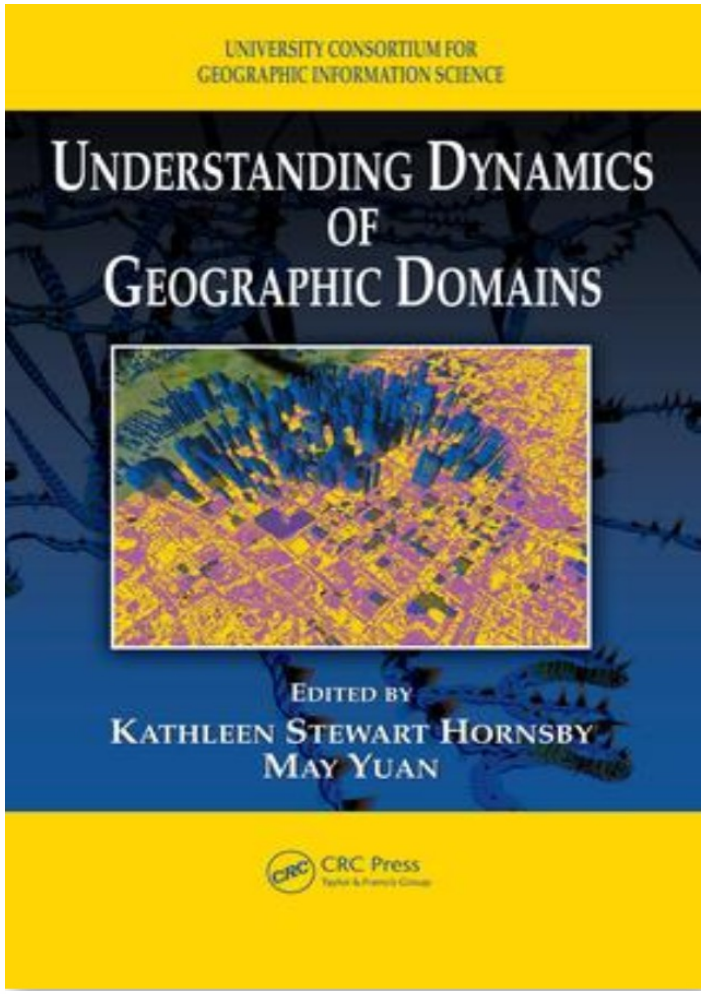
$$\ddot{x}_{n+1}(t+T)=\alpha[\dot{x}_n(t)-\dot{x}_{n+1}(t)]$$



Dynamic System

Different modes in spatio-temporal process





Data-driven forecasting for dynamical system

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A. M. Avila & I. Mezić

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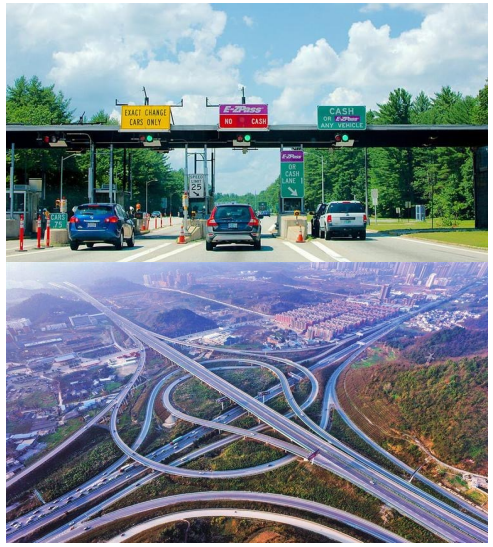
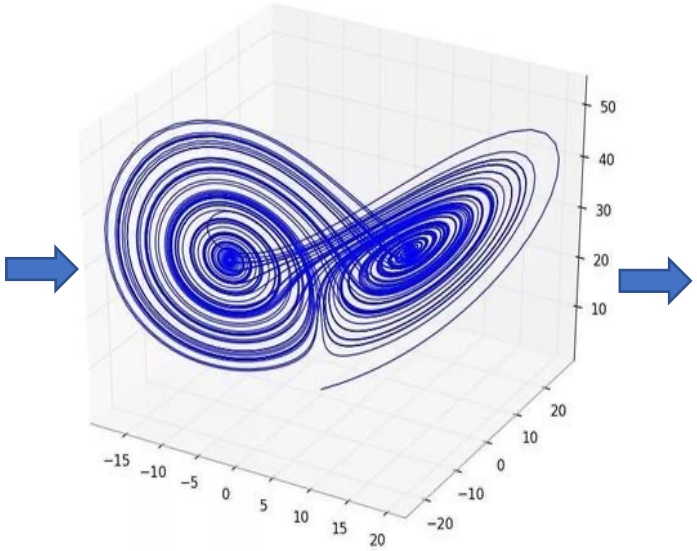
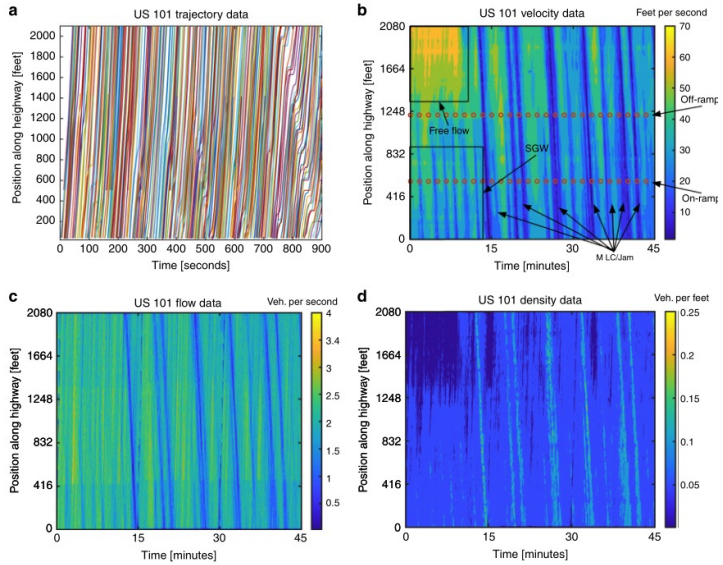






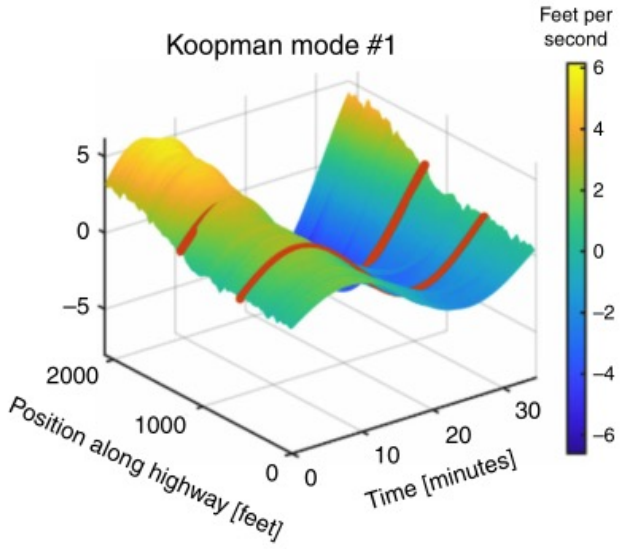
model-free

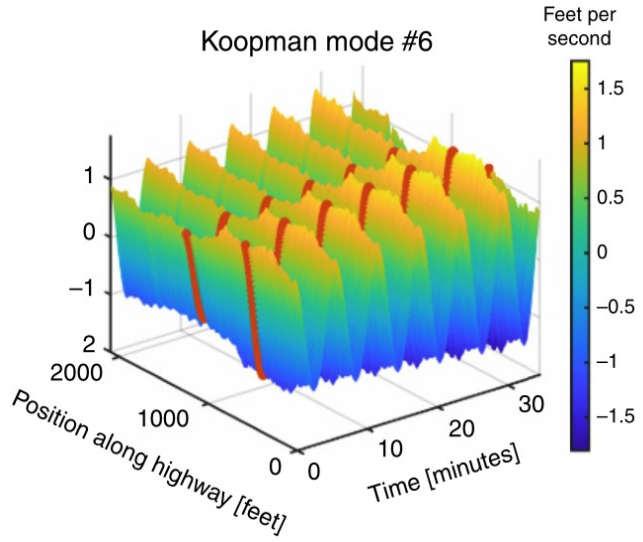
data-driven

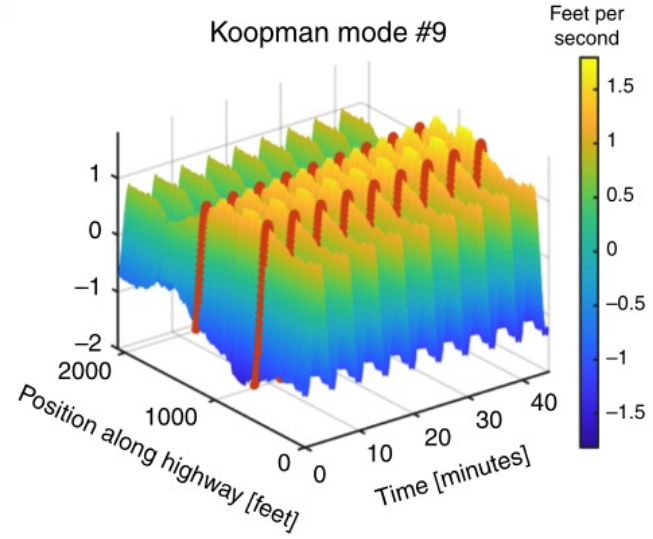
Koopman pattern decomposition

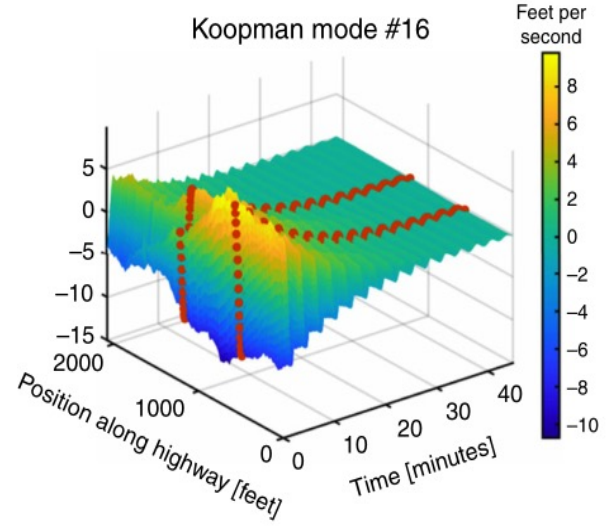
Data-driven forecasting for dynamical system

The Koopman modes uncover complex spatiotemporal wave structures that are hidden within traffic data.



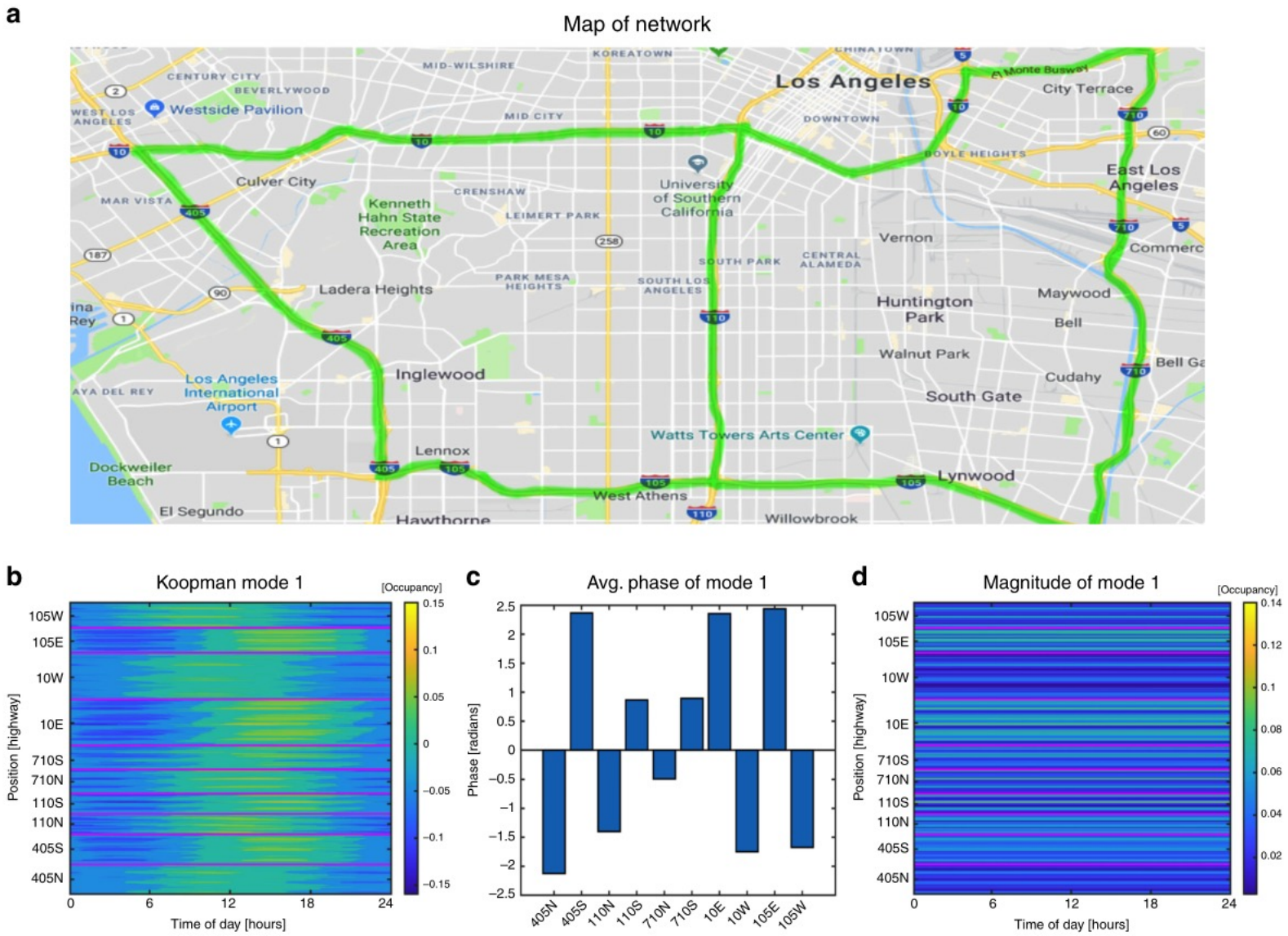






Data-driven forecasting for dynamical system

The 24-hour Koopman mode revealing the order of congestion within the network.



Conclusion

- Data-driven models will not replace theory-driven models, but strongly complement and enrich it.
- Data-driven models will benefit from plausible physically based relationships derived from the natural sciences.
- In the absence of theoretical guidance, data-driven results can guide the direction of future theoretical research

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