Graph diffusion model **for spatio-temporal graph generation**

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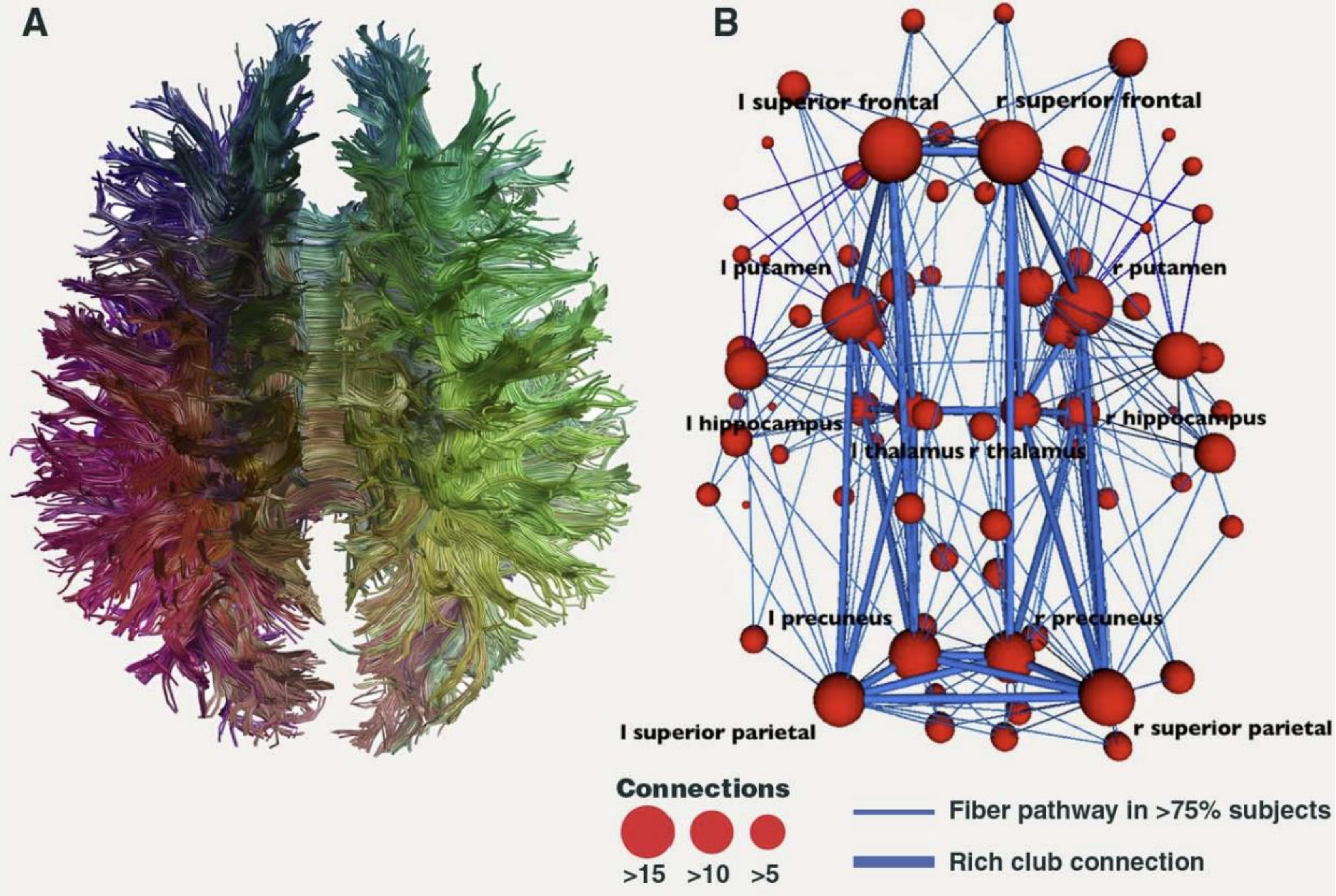
Research interest

1. Computational methods for bioinformatics
- Statistical models for sparse, hi-dim geometry of biological data
- Generative deep learning models

2. Medical image analysis
- Self supervised learning in multi-modality
- Universal medical image processing

3. Quantum computing
- Statistical algorithms inspired by adiabatic quantum computing
- Quantum analog of conventional machine learning algorithms



A
B
l superior frontal
r superior frontal
l putamen
r putamen
l hippocampus
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l precuneus
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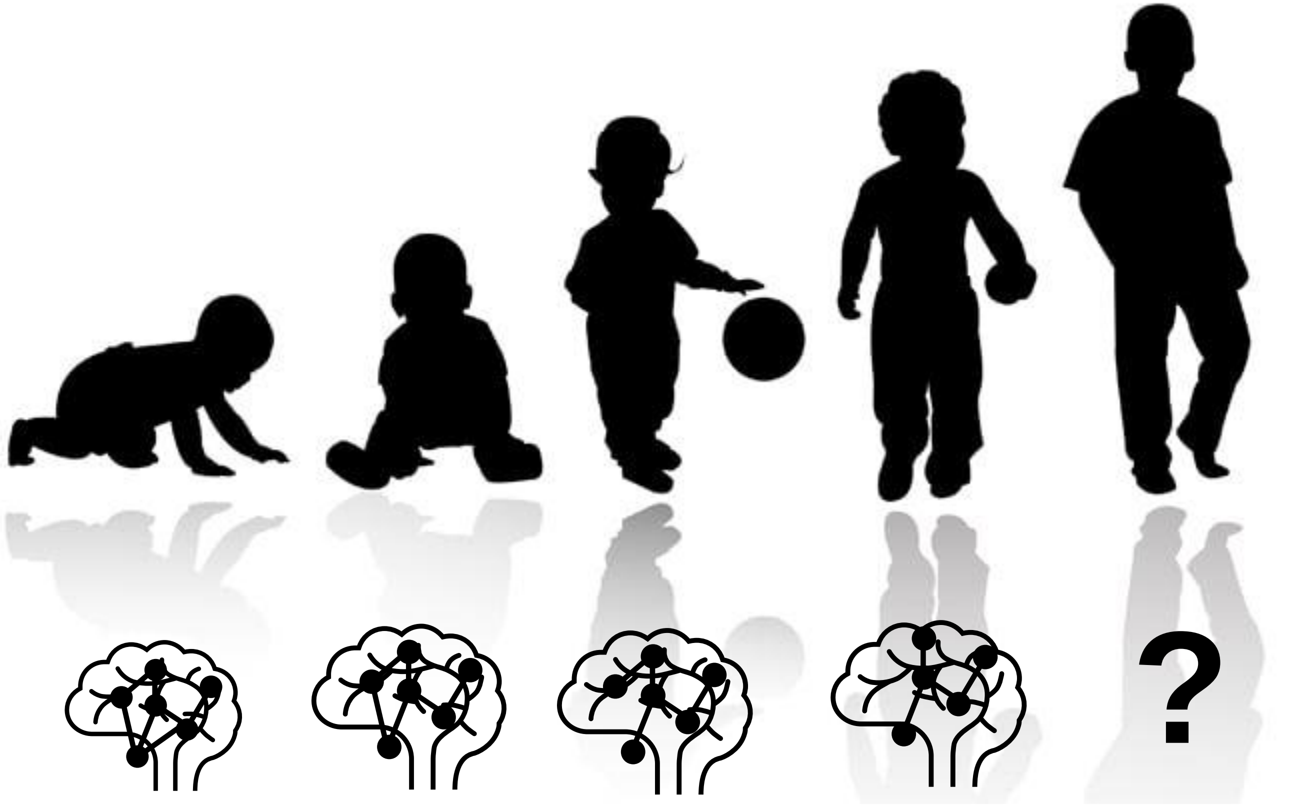
l superior parietal
r superior parietal
Connections
>15
>10
>5
Fiber pathway in >75% subjects
Rich club connection



Story begins from

<u>Dynamic</u> graph
<u>Series</u> of dynamic graph
<u>Generating</u> series of dynamic graph

Systematic approach:

Classify, Regress, and Generate

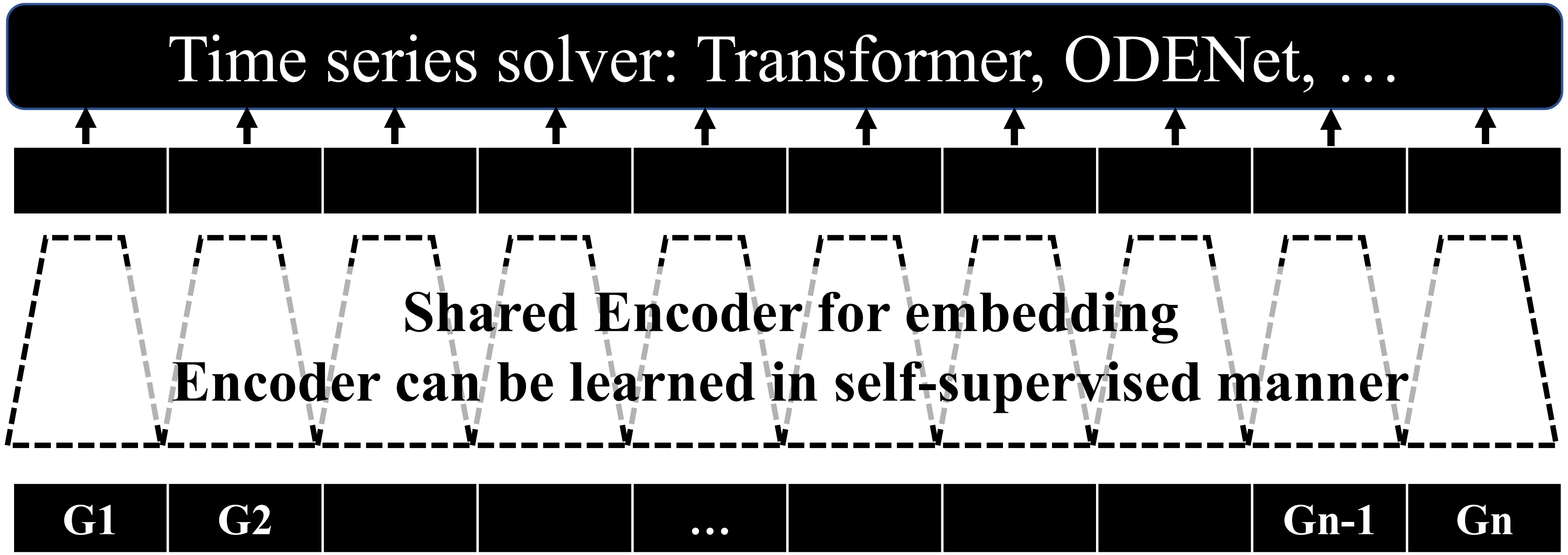
Naïve spatio-temporal approach

Somehow encode spatial data.
Provide embedding to transformer.

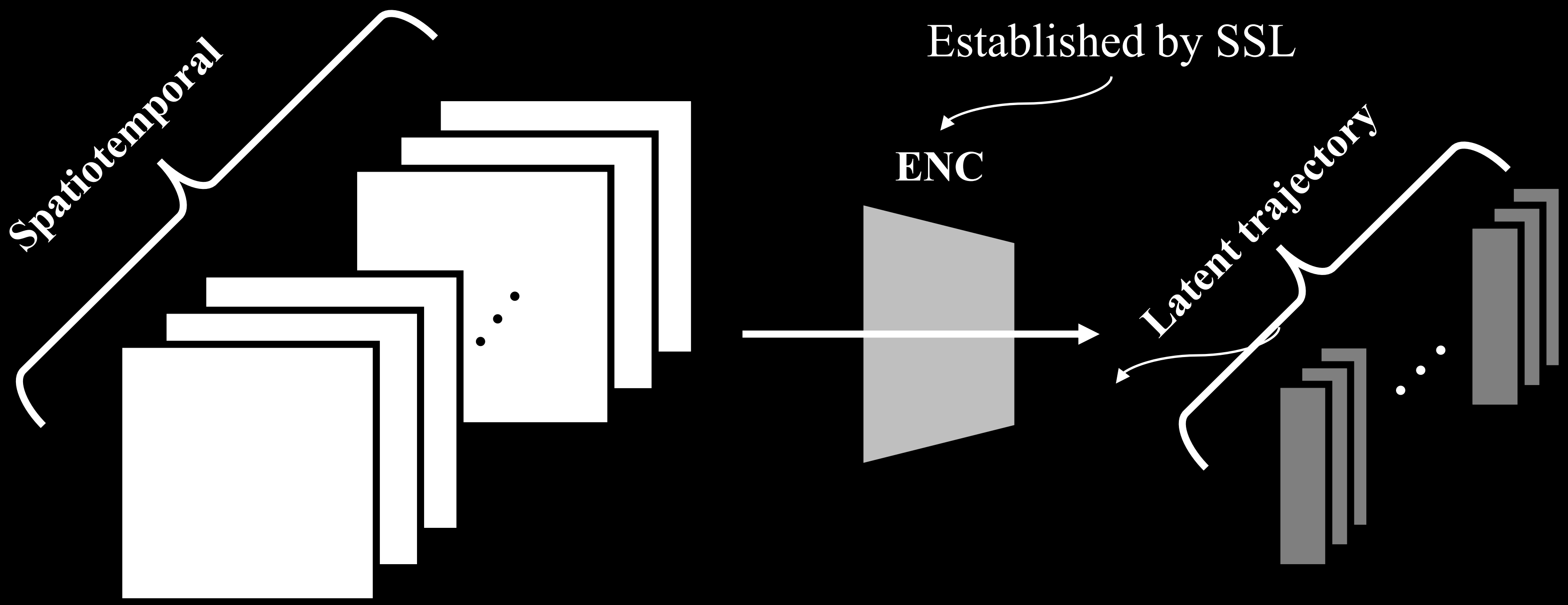
Naïve spatio-temporal approach

$$\mathbf{h}_t = \mathbf{f}_{\mathrm{ENC}}(\mathbf{G}_t) \ (t=1, \ldots, T)$$
$$\text{prediction} = \mathbf{g}_{\mathrm{TSsolver}}(\|_t \, \mathbf{h}_t)$$

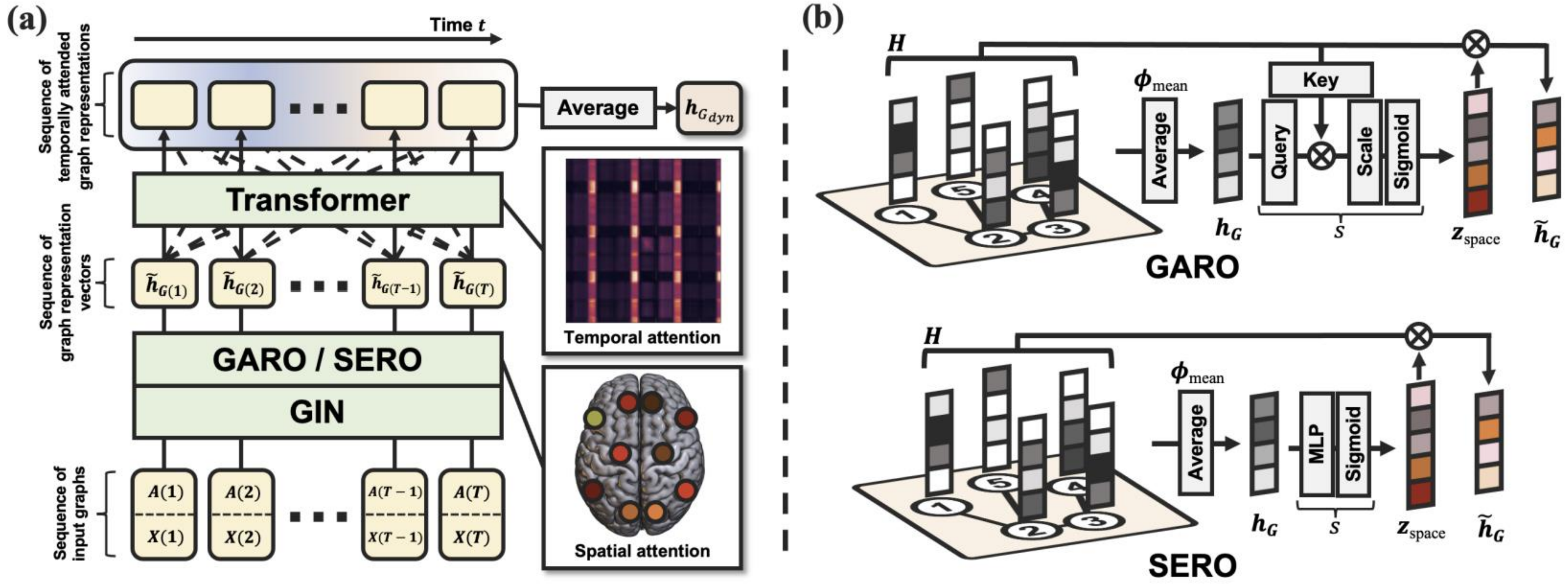
Naïve spatio-temporal approach



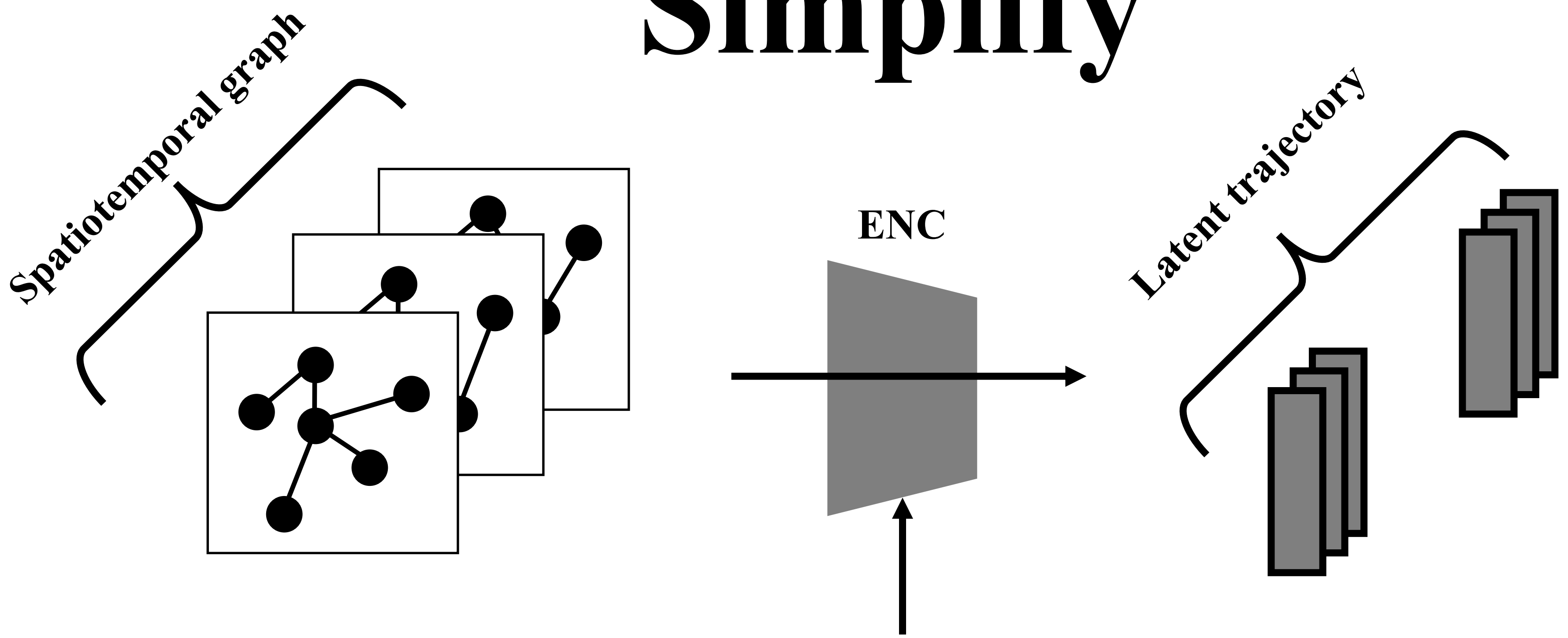
Image



Kim et al.
(NIPS 2021)

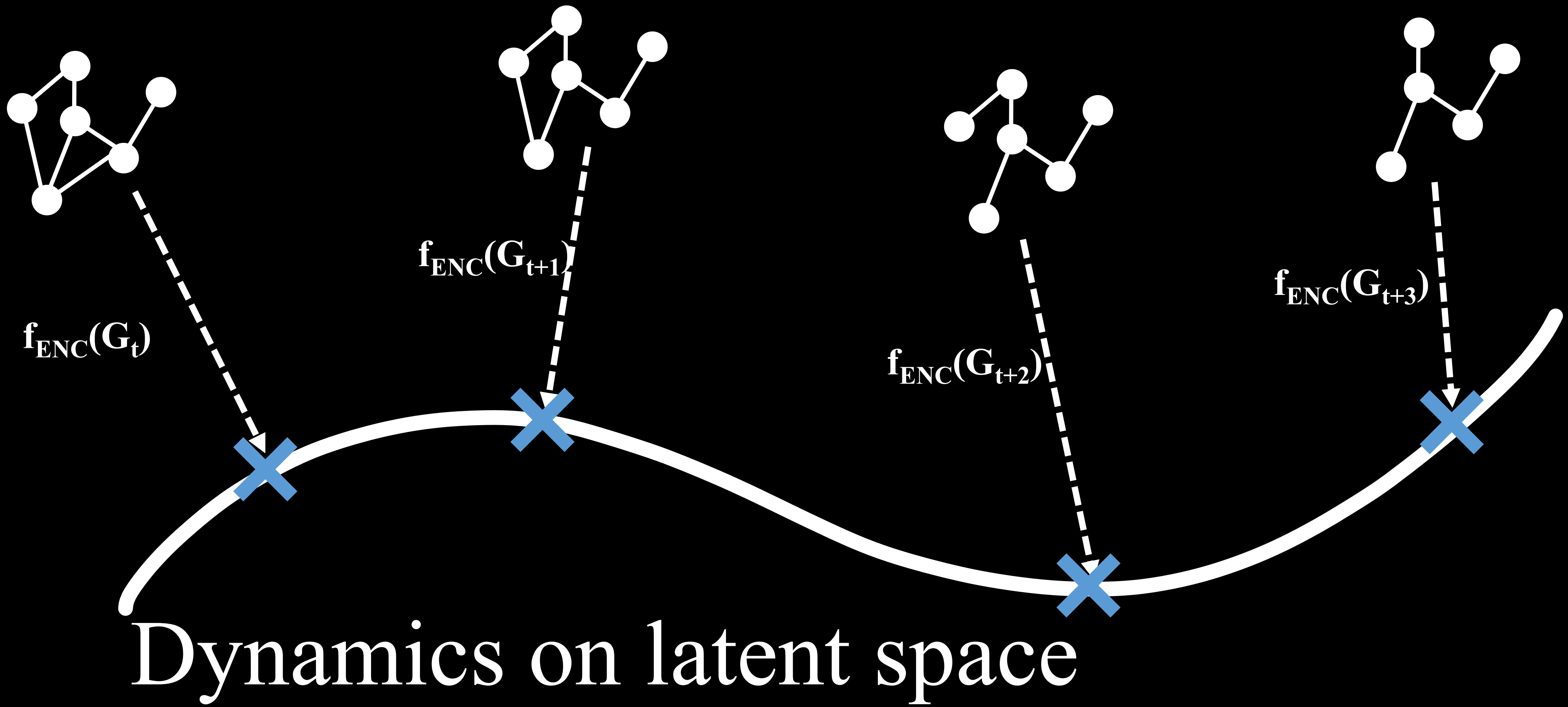


Simplify



SSL?
Generative model?
One-step approach?

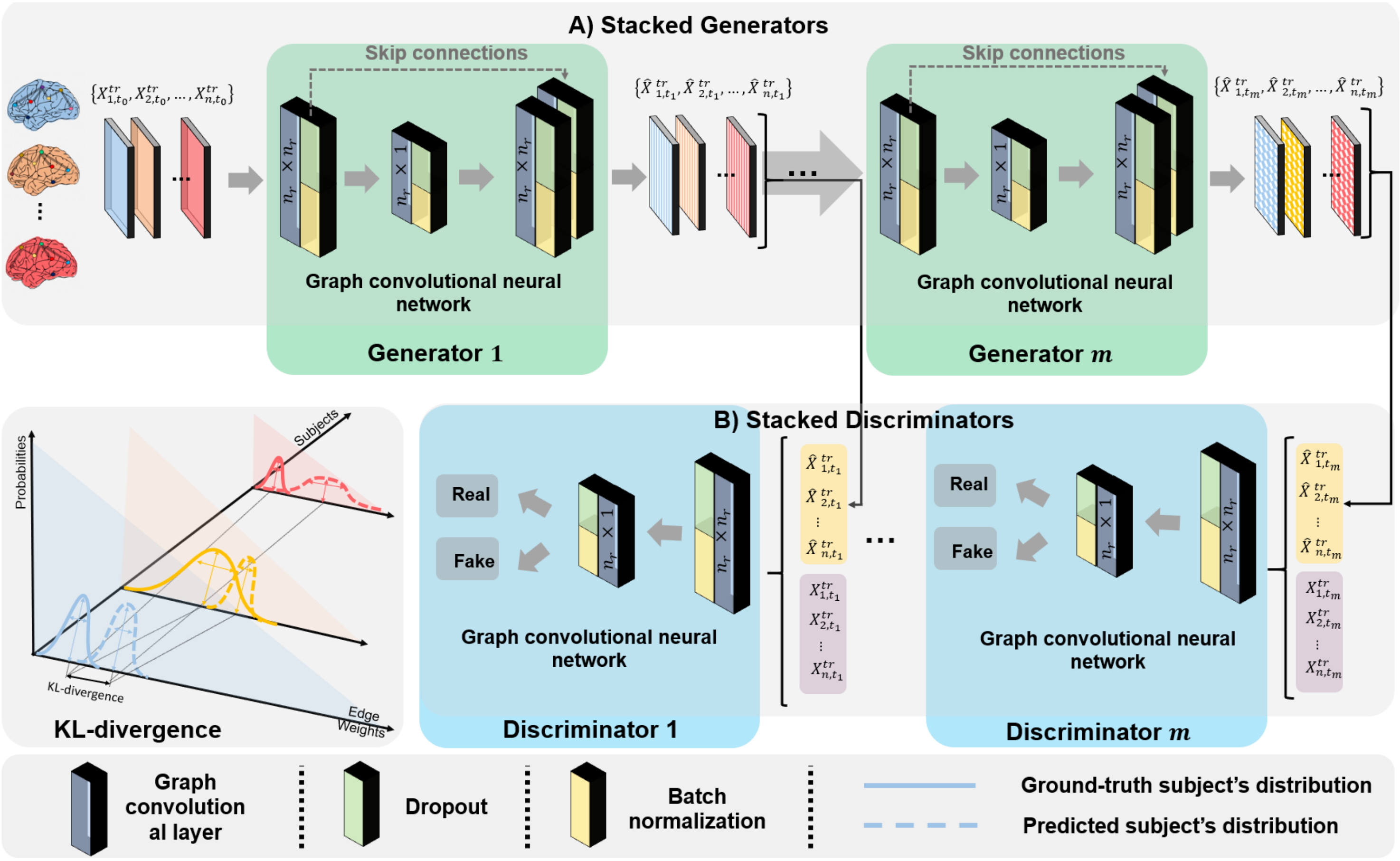
Shared encoder + TS model



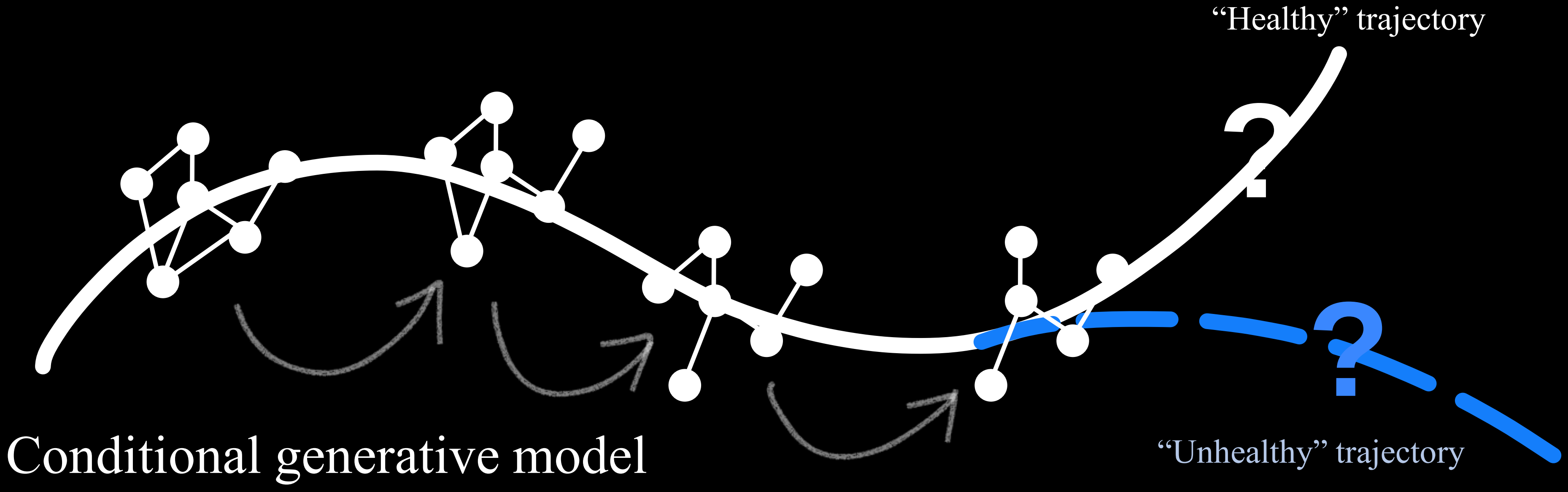
Applicable to
Spatiotemporal Graph Generation?

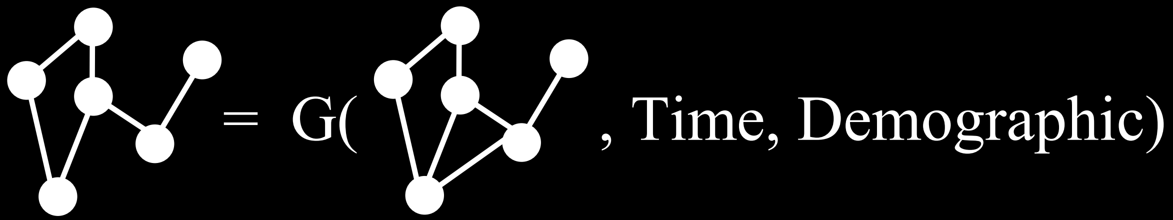
Autoregressive

Nebli et al. (PRIME 2020)



Autoregressive





Converting forecasting problem to Conditional generation problem

Regazzoni et al. 2023 Apr

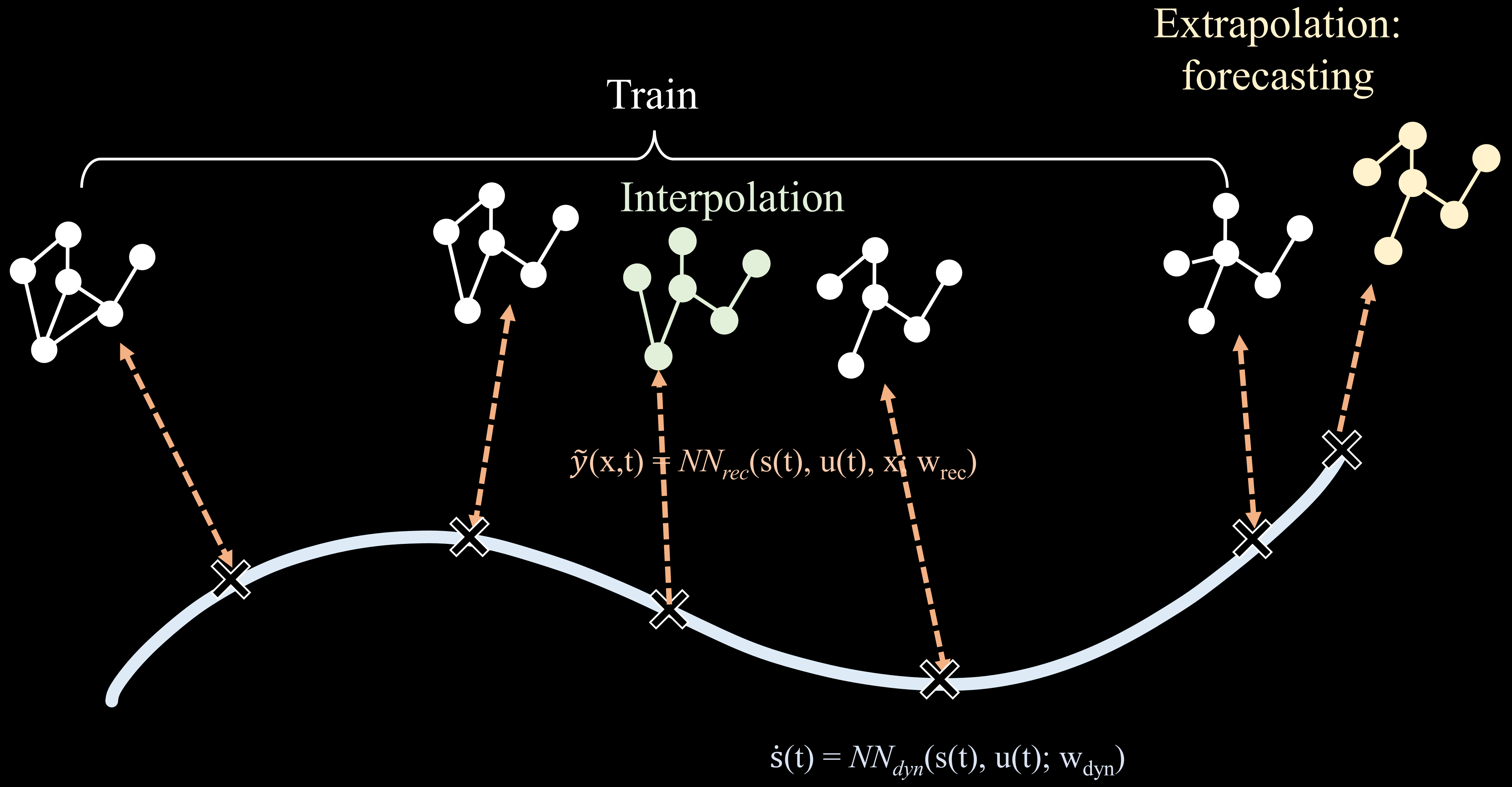
Latent Dynamics Networks (LDNets): learning the intrinsic dynamics of spatio-temporal processes

Components

Latent Dynamics Model NN_{dyn}

Reconstruction(generative) Model NN_{rec}

$$\dot{s}(t) = NN_{dyn}(s(t), u(t); w_{dyn})$$
$$\tilde{y}(x,t) = NN_{rec}(s(t), u(t), x; w_{rec})$$



Extrapolation:
forecasting
Train
Interpolation
$\tilde{y}(x,t) = NN_{rec}(s(t), u(t), x; w_{rec})$
$\dot{s}(t) = NN_{dyn}(s(t), u(t); w_{dyn})$

Remaining questions

$$\dot{s}(t) = NN_{dyn}(s(t), u(t); w_{dyn})$$
$$\tilde{y}(x,t) = NN_{rec}(s(t), u(t), x; w_{rec})$$

Select dynamics model: domain-specific?

Select generative model: AE? GAN? Diffusion?

Graph Diffusion is gaining attention

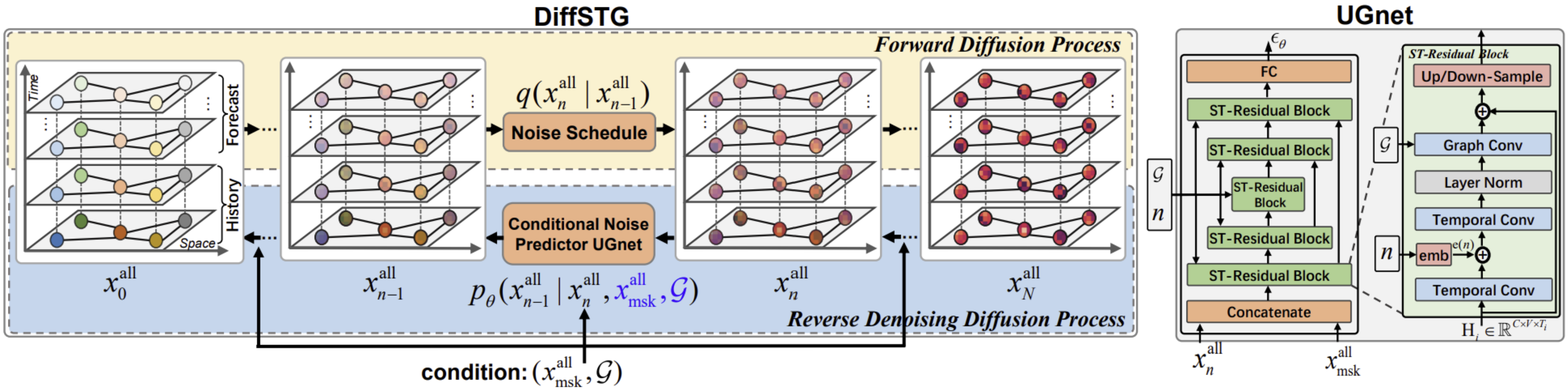
Brief introduction:

Will be detailed @ GUG blogs ☺

SMLD	**DDPM**	**DDPM**
EDP-GNN	**DiGress**	**GRAPHARM**
Upper triangular part of adj. matrix	Node feature & edge attribute	Row of adj. matrix (autoregressive)

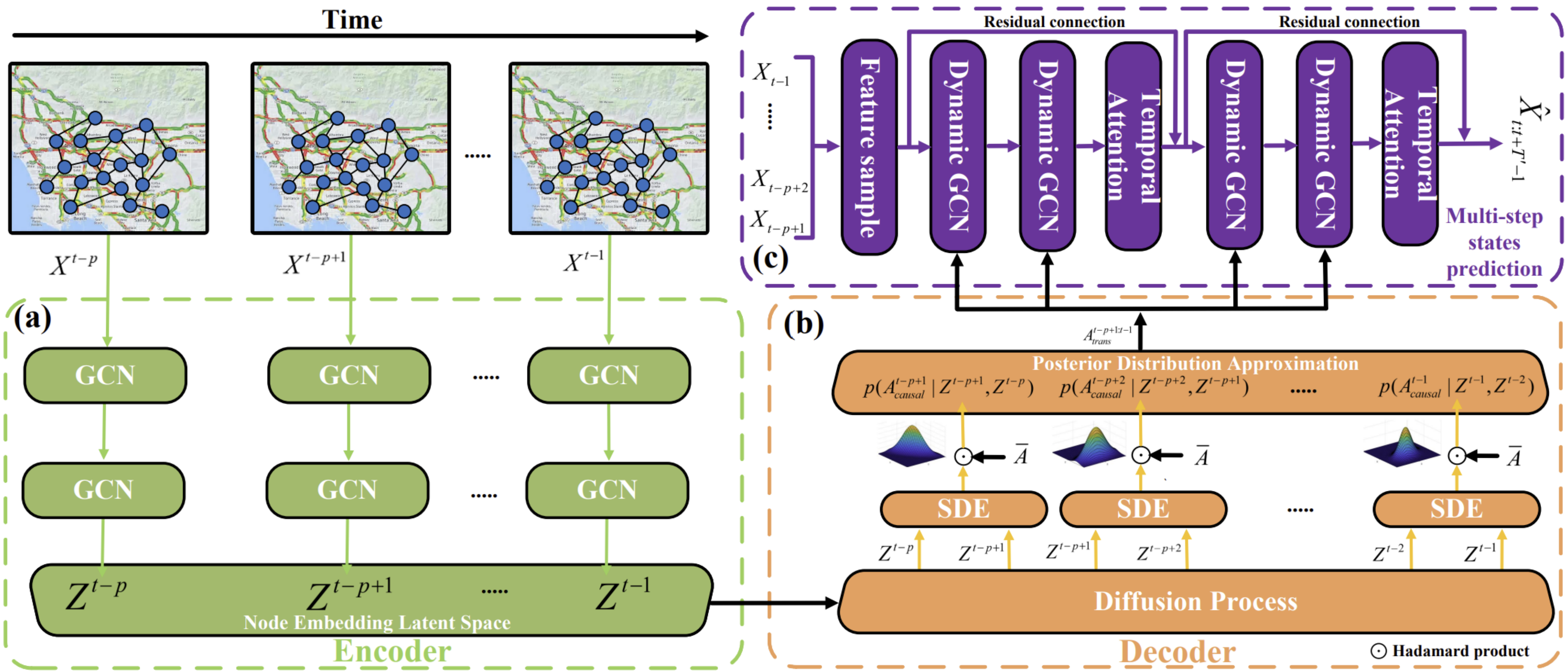
Wen et al.(2023)

Probabilistic Spatio-Temporal Graph Forecasting with Denoising Diffusion Models



Liang et al.(2023)

Diffusion-Variational Graph Neural Network(DVGNN) for Spatio-temporal Forecasting

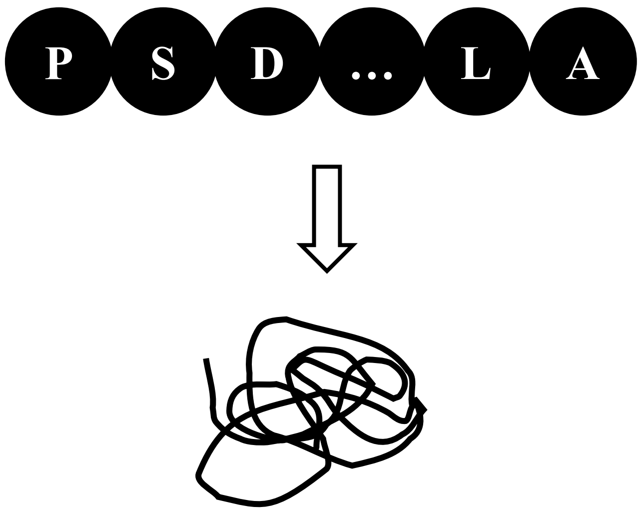


Questions, Please

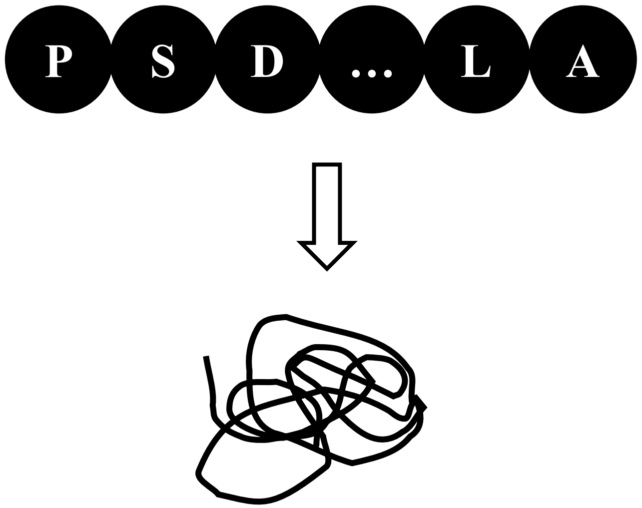
Appendix

AlphaFold
RoseTTAFold

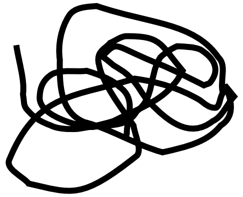
Protein folding



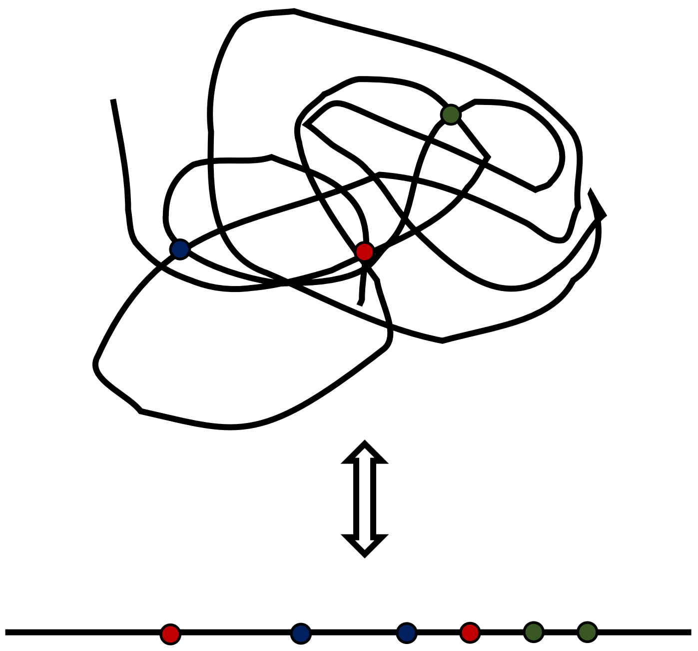
Where is graph?



3D structure is graph

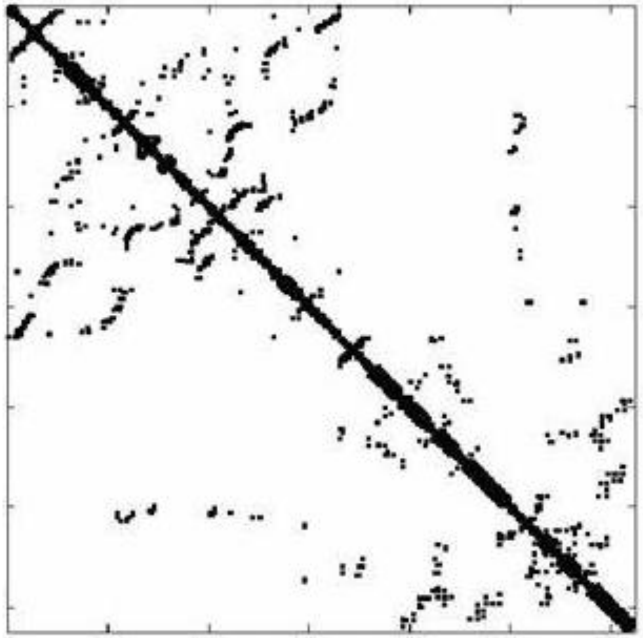


Contact Map Estimation

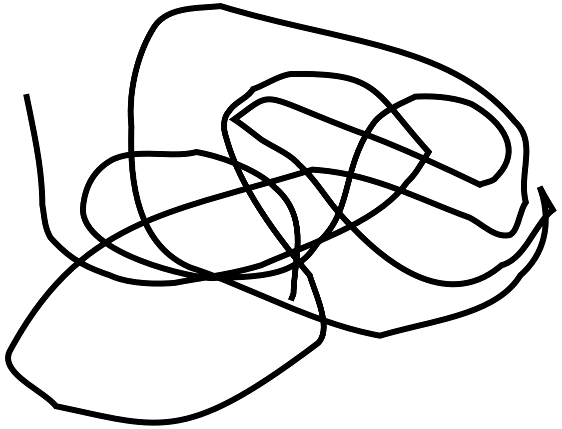


Not Isomorphism
Machine Learning fills the gap:
learning Riemannian manifold that protein contact map exists

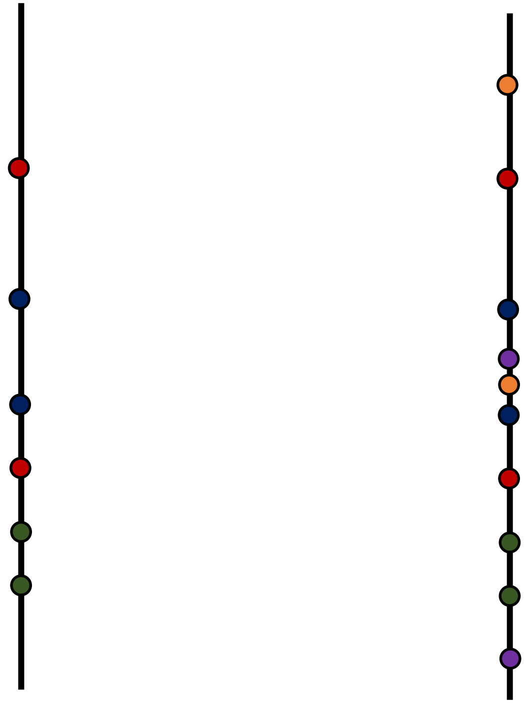
Graph or Image: AlphaFold vs. RoseTTAFold



Is protein folding solved?



Estimation of 3D structure requires high-resolution contact map

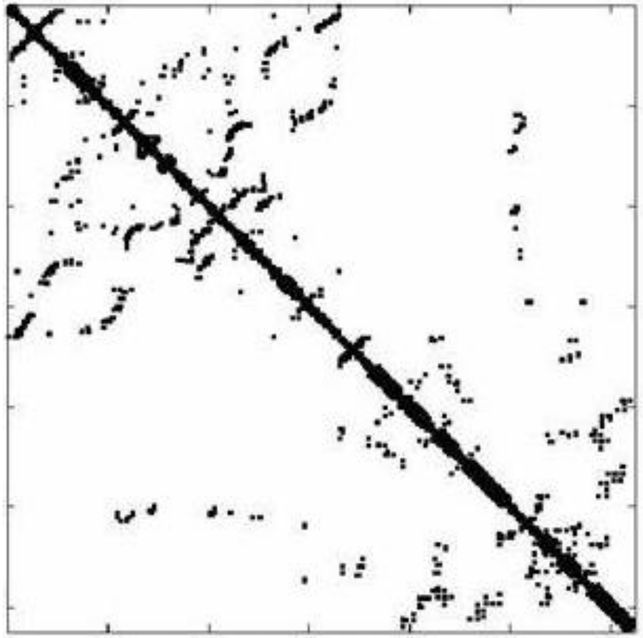


Given data ***Sparse***

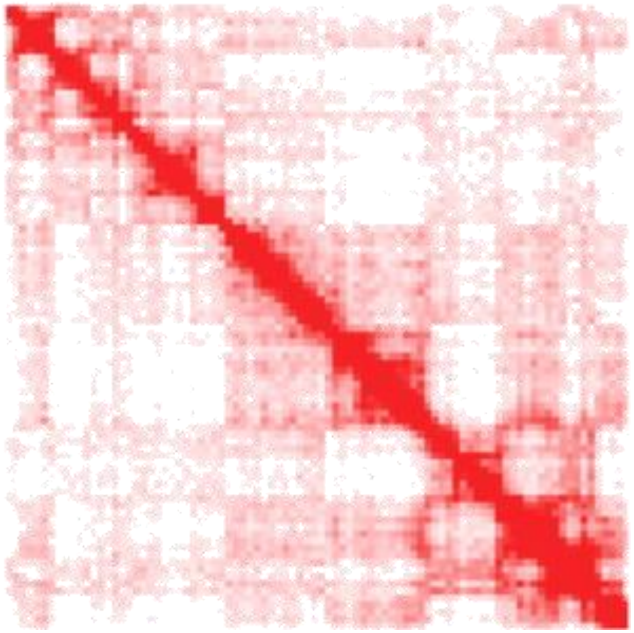
Required ***Dense***

Graph
Super-Resolution!

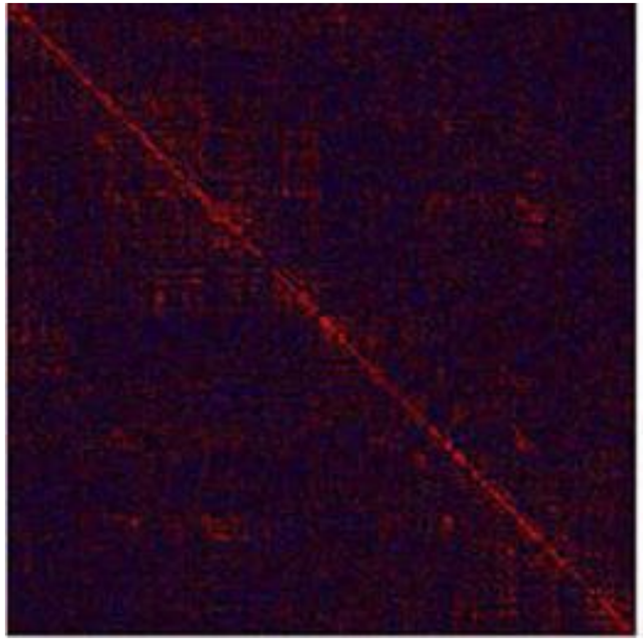
Analogy



Contact map of Protein

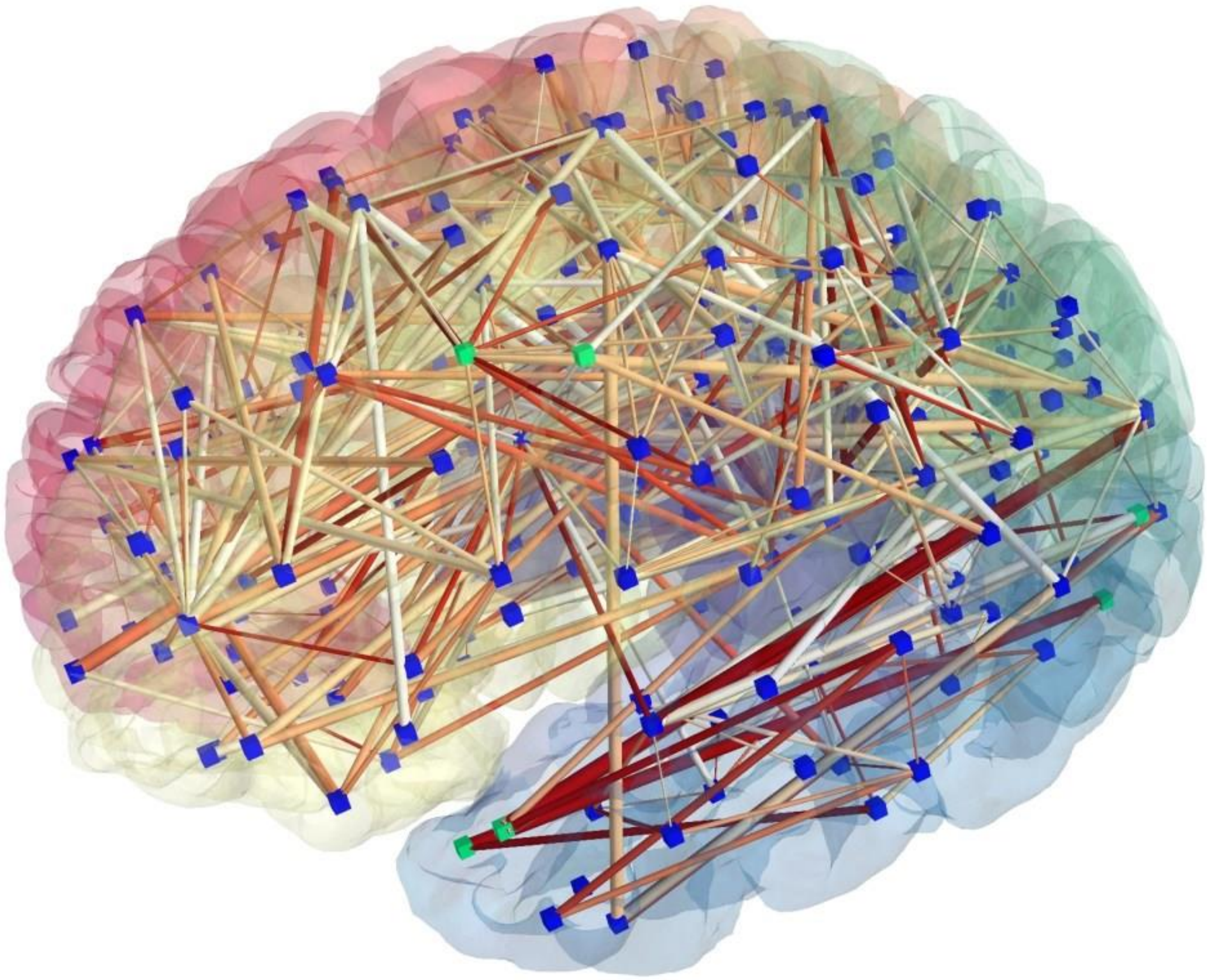


Contact map of Chromatin



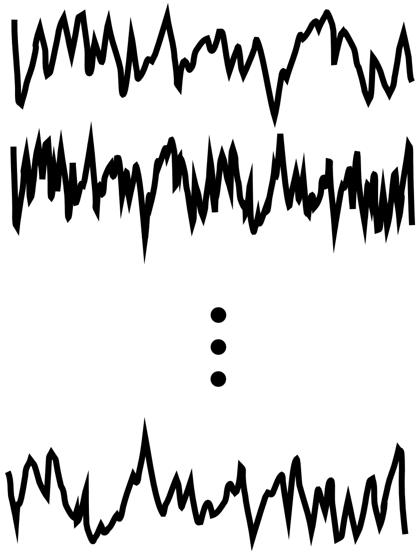
Connectivity matrix of Human Brain

Dynamic graph: brain connectome



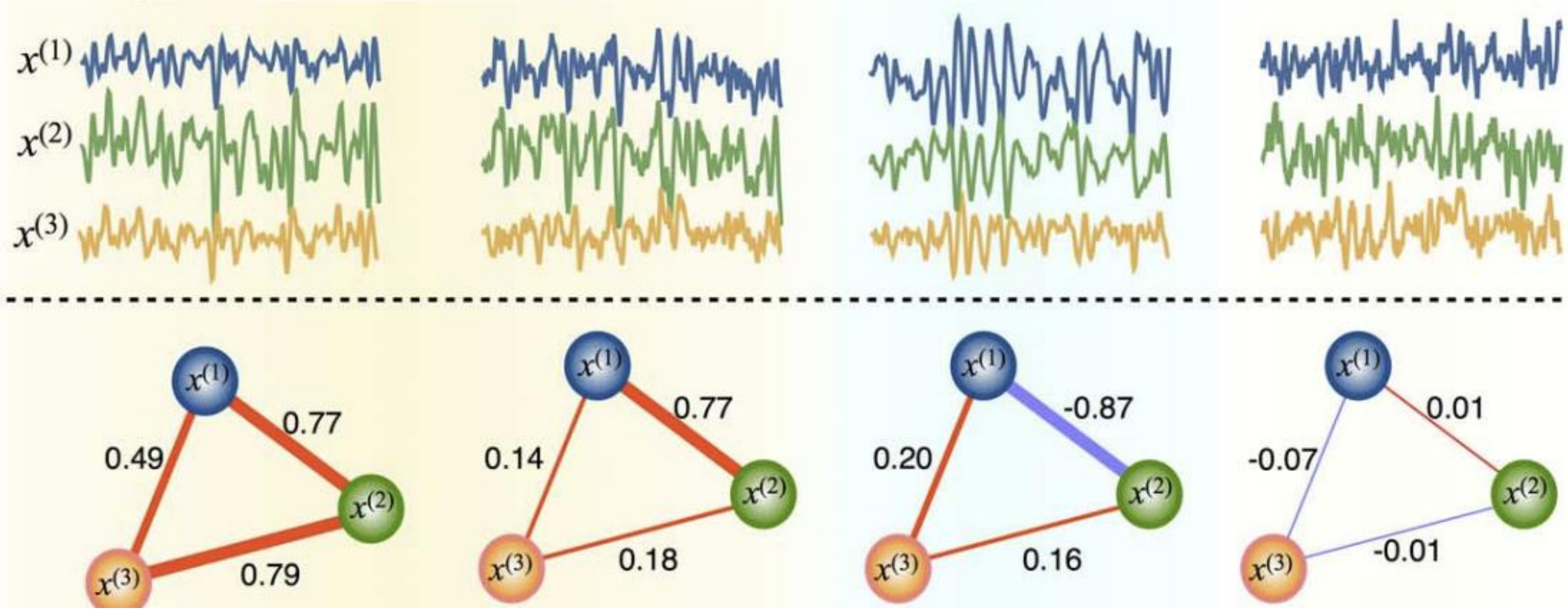
Signal

(fMRI BOLD, EEG)

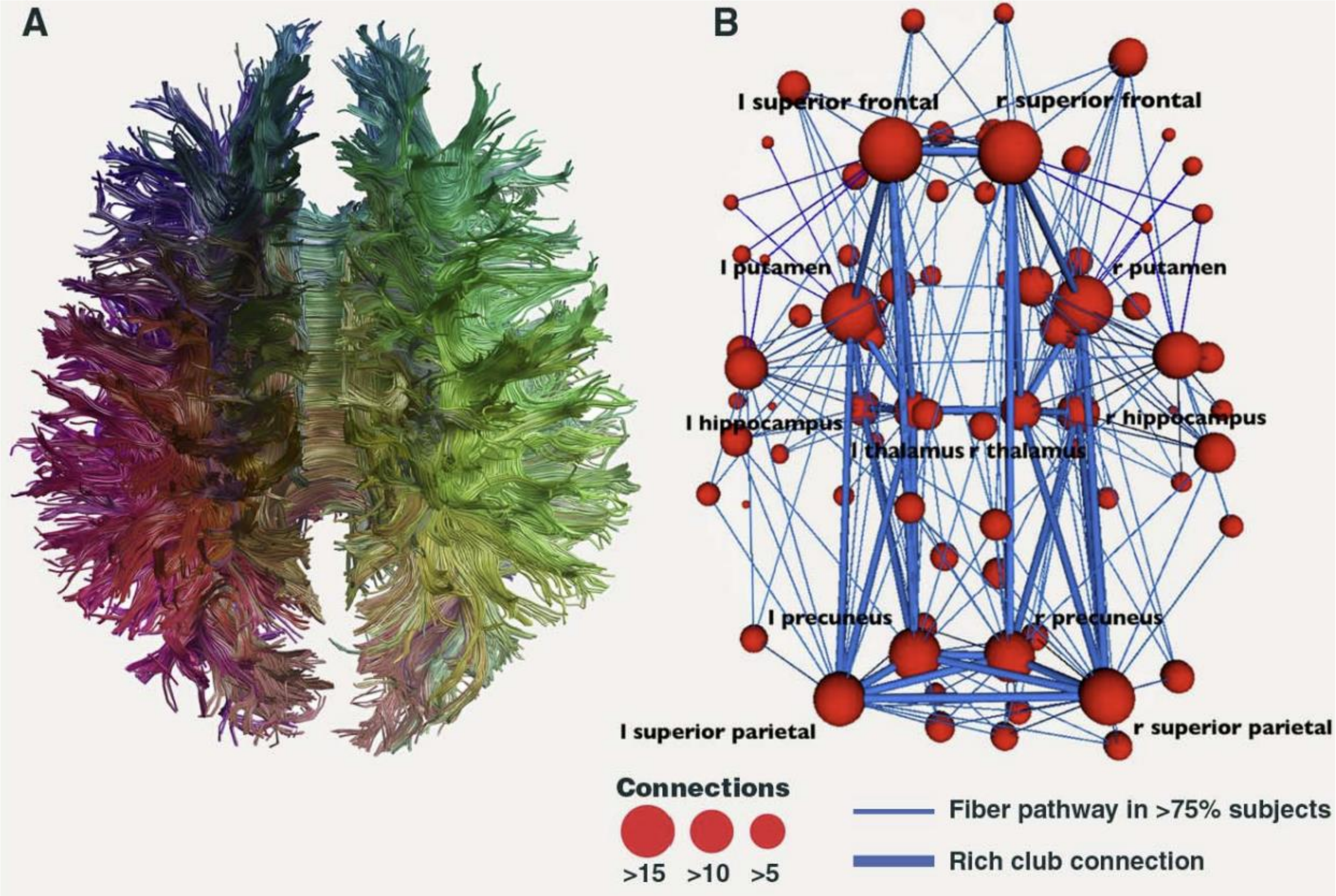


How you will construct Graph with this data?

Correlation as graph weights



Weight of edge E(x(i), x(j)) = Corr(x(i), x(j))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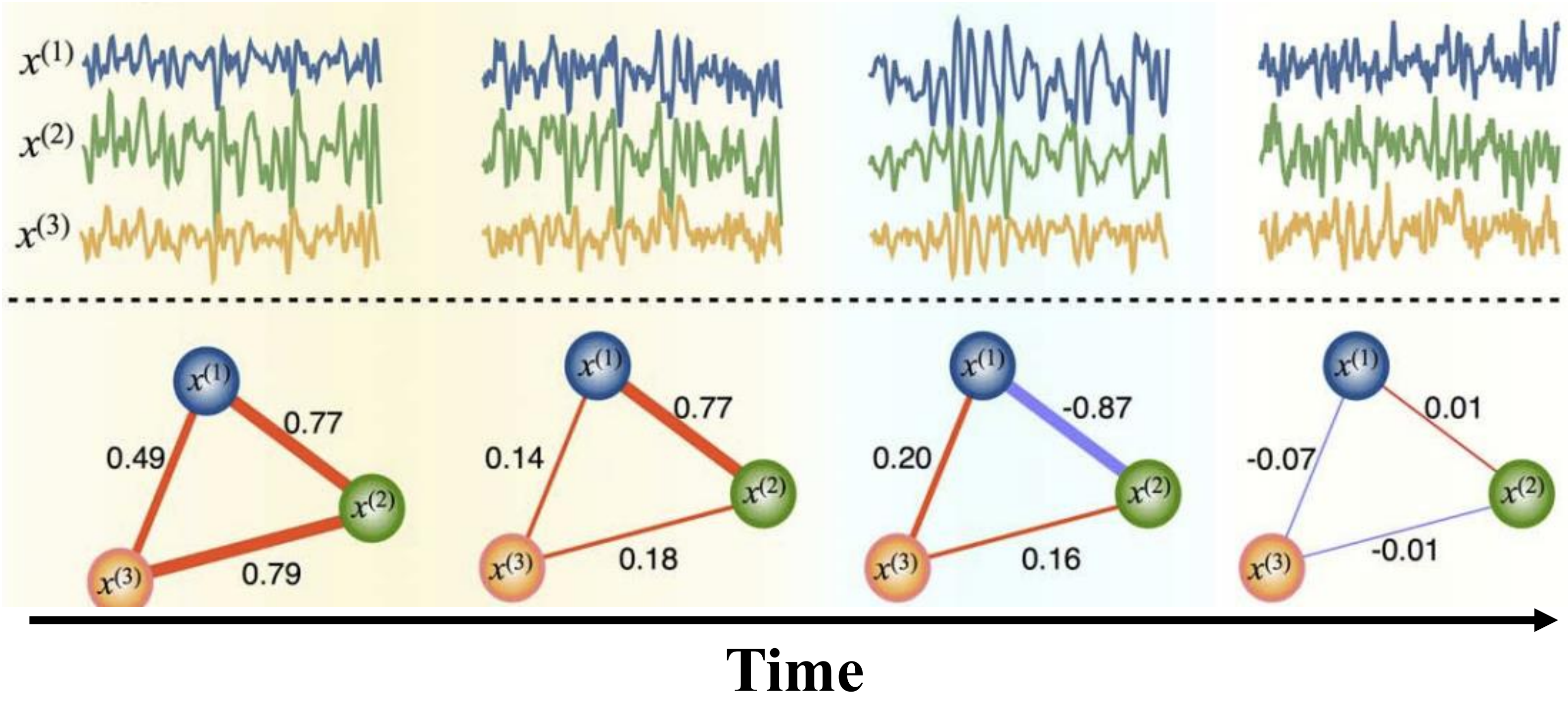
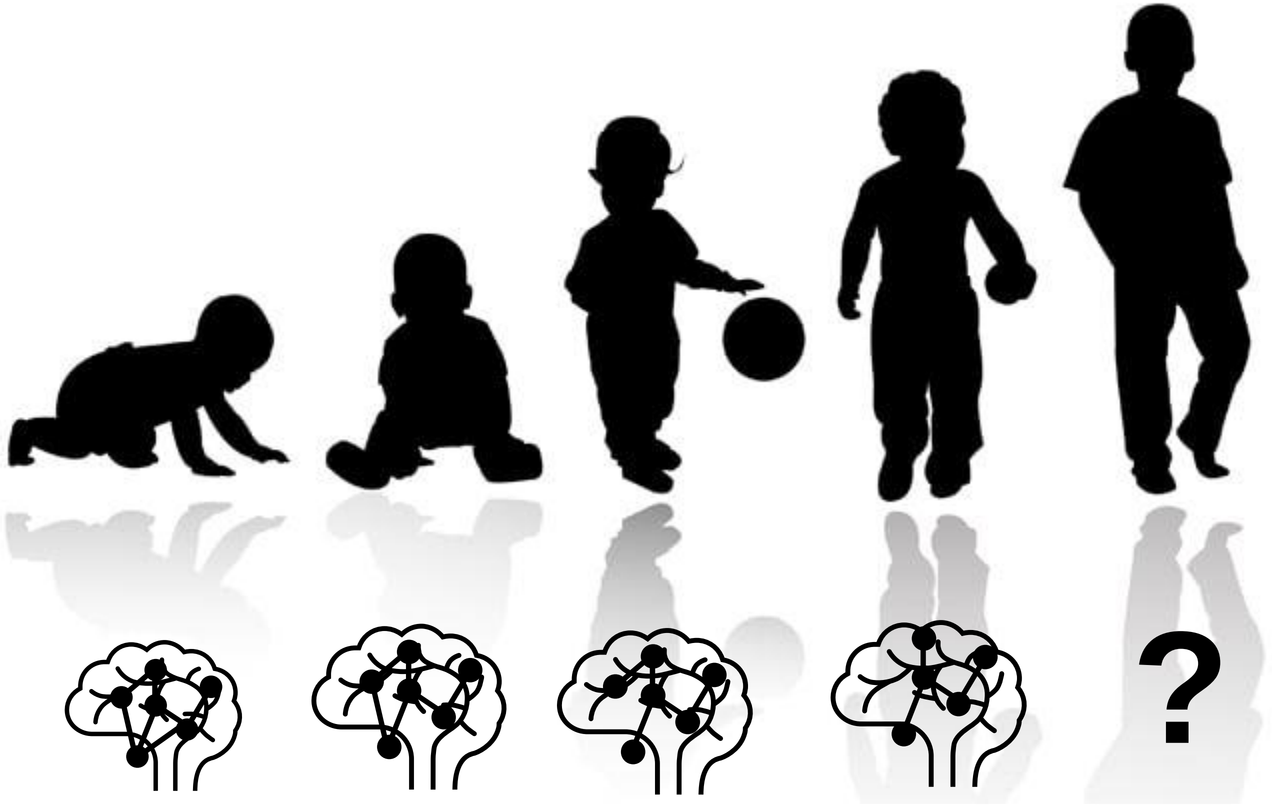
Spatio-Temporal approach is natural





Spatiotemporal?

① Brain ROI location matters

② Brain development; time series of <u>graph:</u>

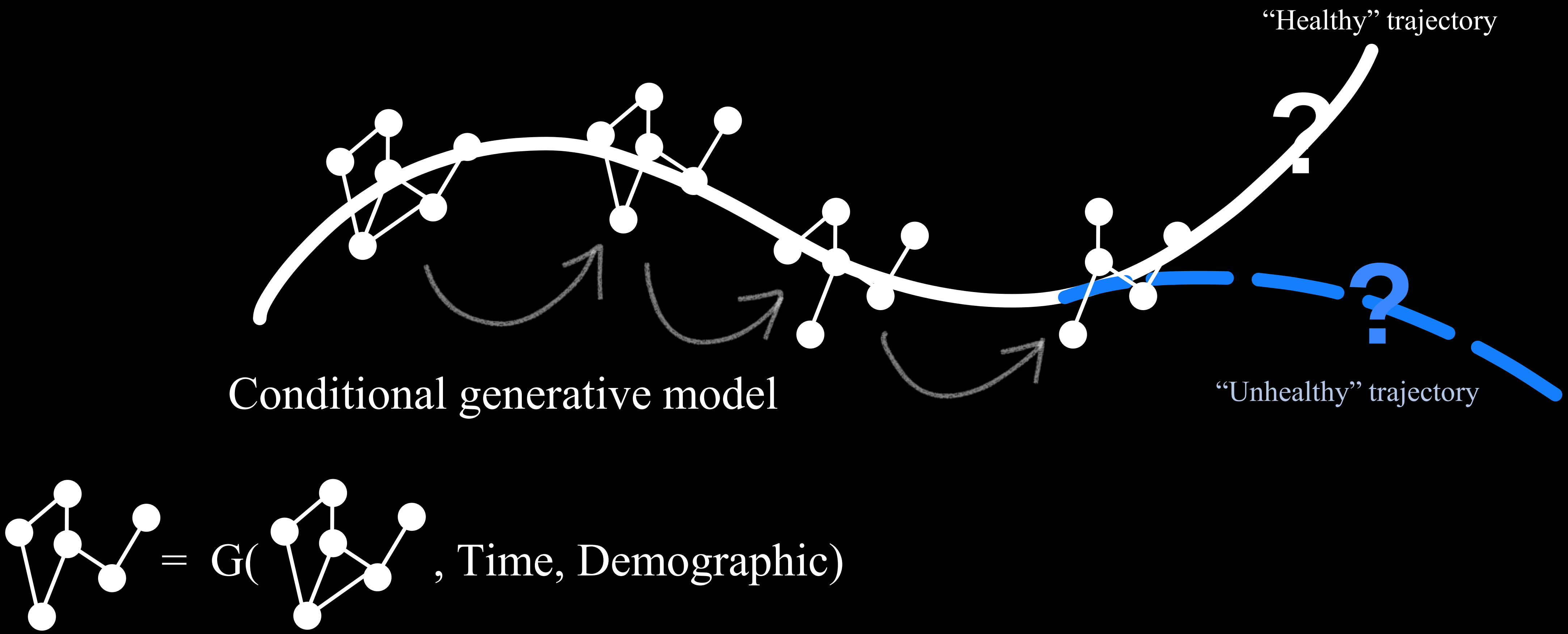
* <u>Differ with dynamic graphs</u>

We argue

Graph generation naturally fits on series of graph;
* in terms of predicting future graph dynamics
* not solving classification or regression problem

Usually more straightforward and information-rich.

Predicting future brain graph



Predicting future brain graph

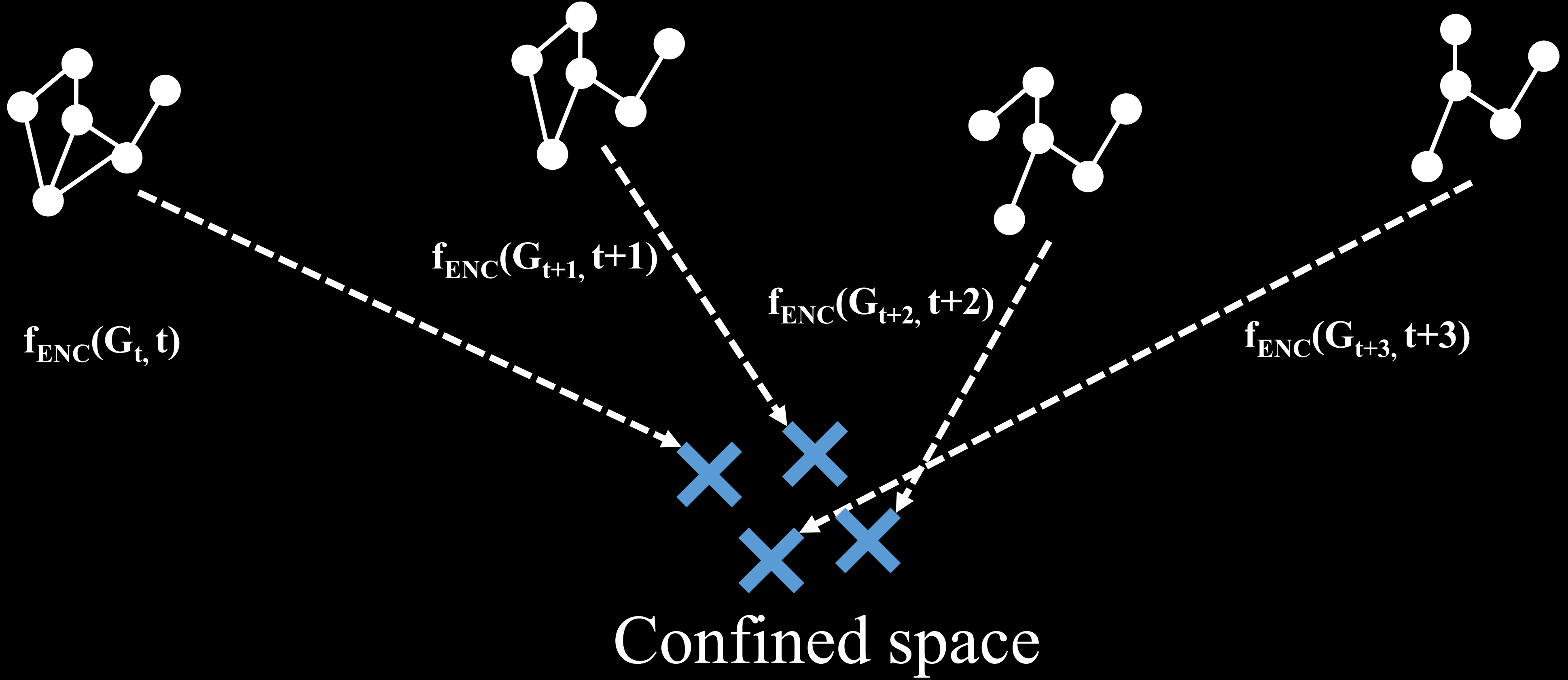
Brain graph
Temporal factor
Demographic factor

Conditional generative model
G(●, t, d)

Good match with diffusion model

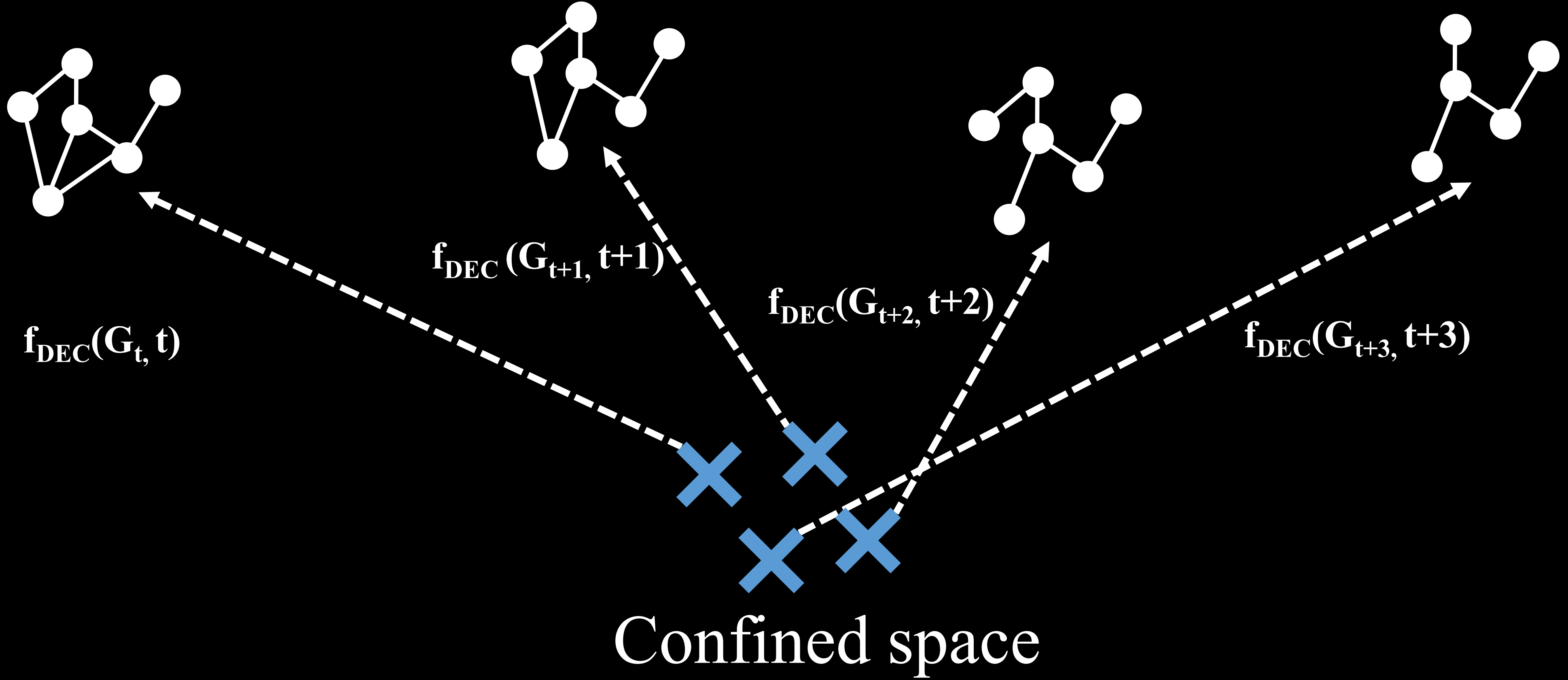
Graph Encoder Latent Dynamics Model Graph Decoder

T-dependent encoder?

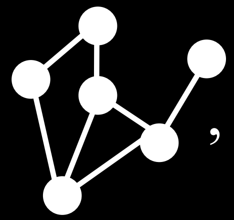


Graph Encoder Latent Dynamics Model Graph Decoder

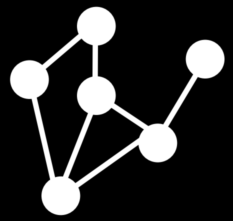
T-dependent decoder?



T-dependent enc/decoder

$L = f_{ENC}($  $, T)$

Conditional Generation

 $= f_{DEC}(L, T), L \sim$ Gaussian

Encoder/decoder

We missed a relationship