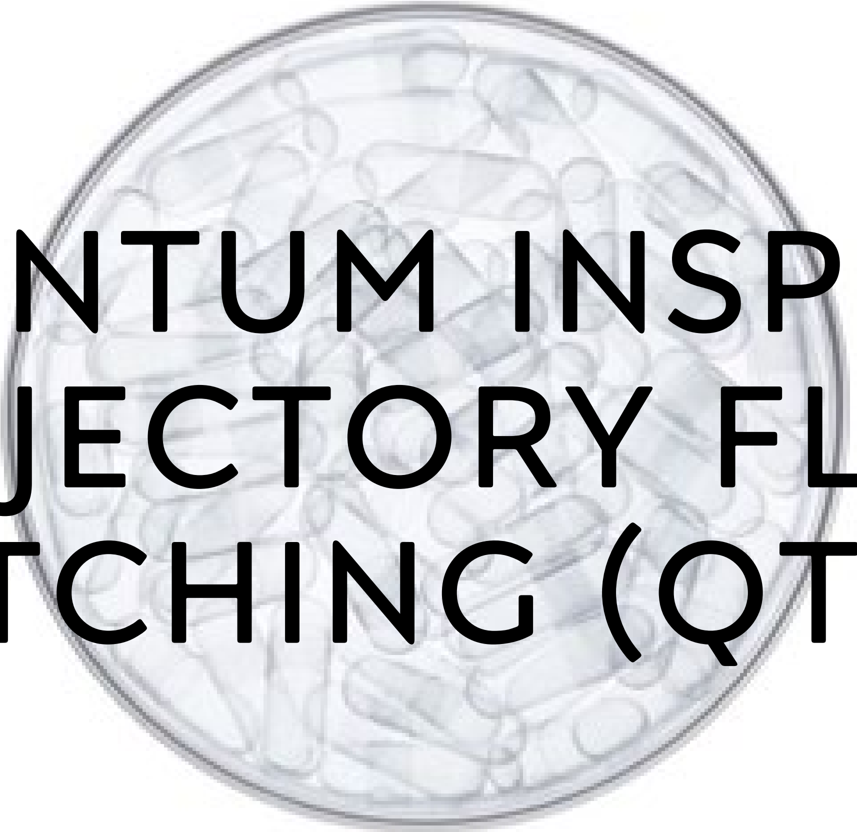


QUANTUM INSPIRED TRAJECTORY FLOW MATCHING (QTFM)

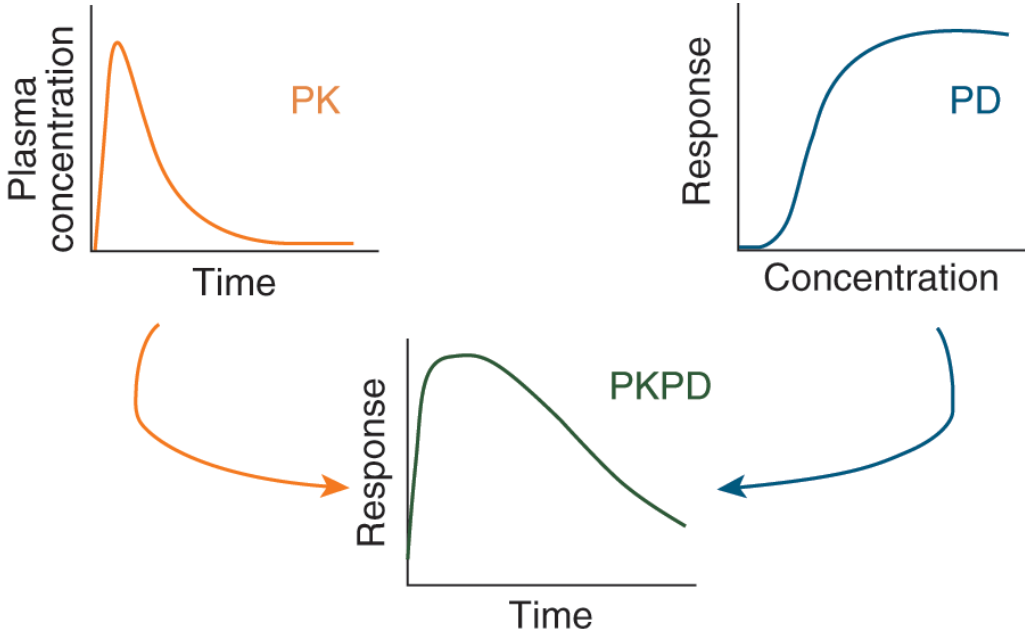
LOCO QUANTUM TEAM

Ran Xue, Zhuo Cao, Mira Sharma and Zhongyi Jiang

OUTLINE

- PK/PD PROBLEM
- TRAJECTORY FLOW MATCHING
- QUANTUM INSPIRED TFM
- RESULTS & OUTLOOK
- OUR TEAM

PK/PD PROBLEM



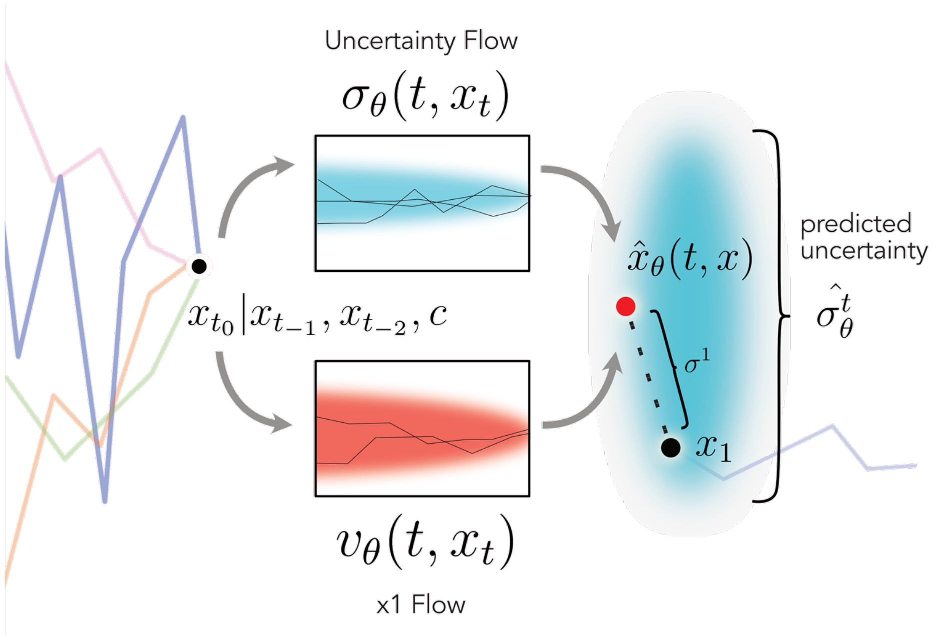
A dynamical system to be understood with limited clinical data.

OUR APPROACH

Quantum inspired - trajectory flow matching (TFM)

WHY TFM?

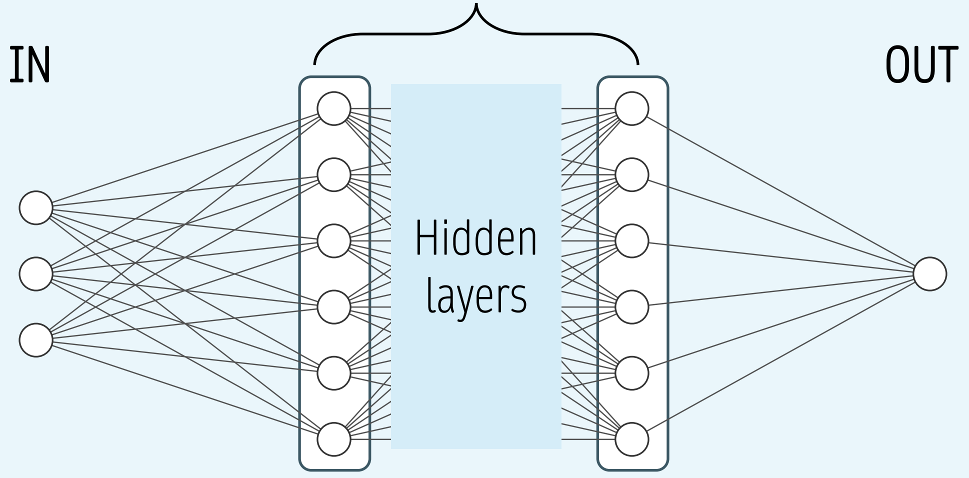
- MOTIVATION:
  - Clinical data (i.e. time-series of bio-marker) = **irregular, limited, noisy.**
  - Conventional models (RNN, neural ODE/SDE) struggle with irregular sampling and simulations overhead.
- CORE IDEA:
  - TFM learns a **continuous time-flow field** from the patient trajectories (irregularly sampled data).
  - Training process is **simlutation-free** i.e. no need of back-propagation.
  - The learned flow field (i.e. how bio-markers evolve over time) enables continuous-time inference.



TFM MODEL INSTANCE

- Preditct the instantaneous velocity $v_\theta(t, x_t)$ and future observations.

The conventional approach:



w neurons per hidden layer

The core differential equation:

$$\dot{x}_t = v_\theta(t, x_t)$$

[1] Xi Z. et al., Trajectory Flow Matching with Applications to Clinical Time Series Modeling arXiv: 2410.21154v2 (2025)

WHERE QUANTUM IS APPLIED

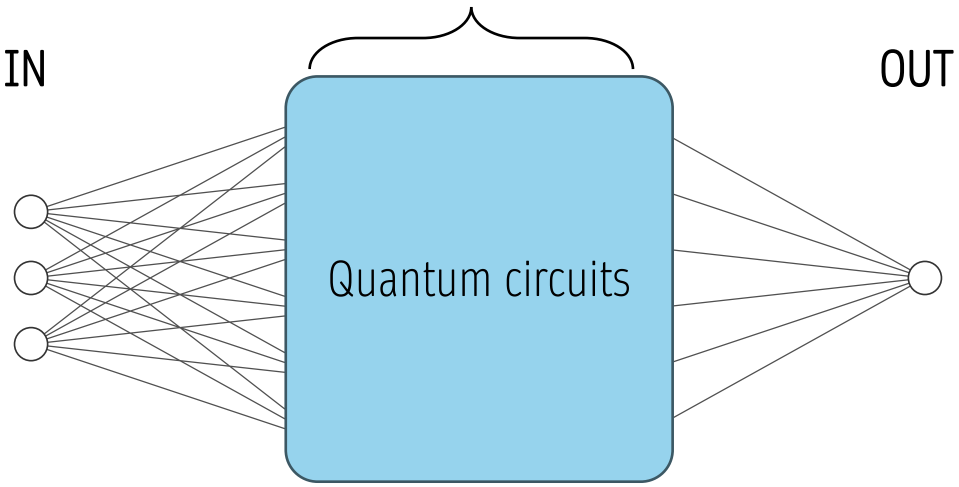
MOTIVATION:

- "Hidden layers" become layers of **shallow variational quantum circuit.**
- Quantum systems encode correlations and interference naturally i.e. **capturing complex and coupled nonlinearities**.
- Quantum dynamics are inherently **continuous and unitary evolutions**.

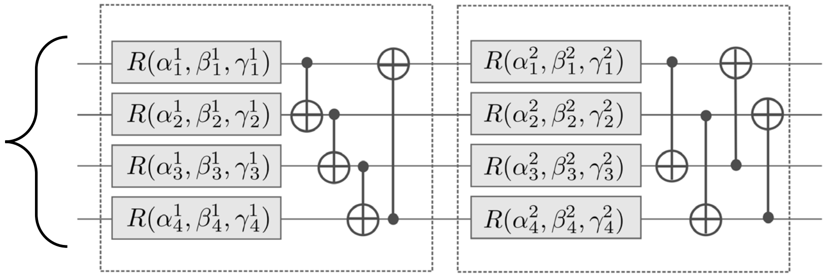
Quantum inspired approach:

Amplitude encoding + pairweise entanglements

~~Linear + SELU activation~~



w neurons per hidden layer → $N_{qubit} = \log_2 w$



Inspired by quantum!

PyTorch

ADVANTAGES OF USING QUANTUM (INSPIRED) METHOD

Comparing to conventional methods:

- ✓ Fewer trainable parameters
  - ✓ Faster convergence with less data
  - ✓ Less prone to overfitting
- ✓ Uses **quantum nonlinearity**

  → effective activation
- ✓ Uses **quantum nonlocality**

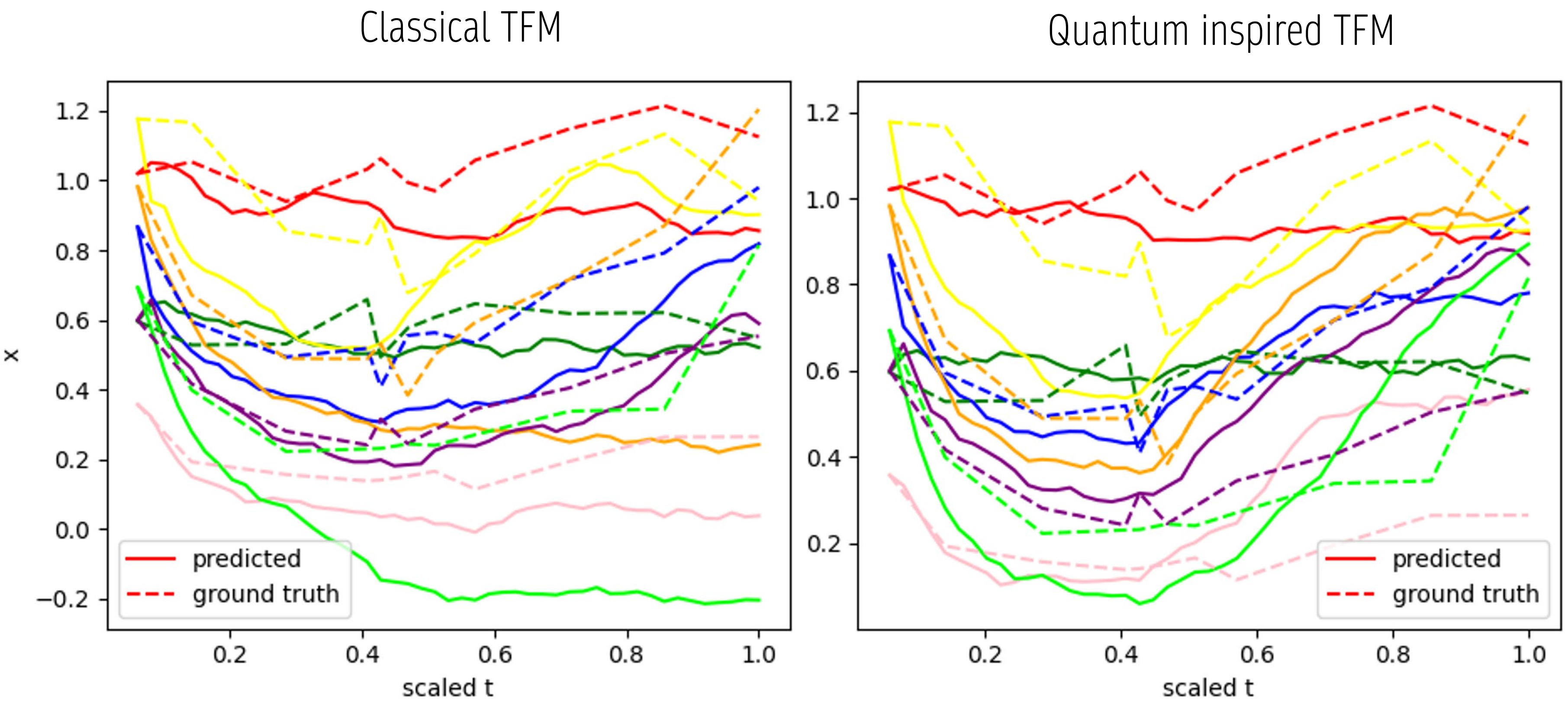
  → powerful feature entanglement

Comparing to Quantum Simulators

- ✓ Faster inference
- ✓ Lower cost
- ✓ Suitable for algorithm validation and prototyping

RESULTS

CLASSICAL VS. QUANTUM



- Trainable parameters: **3,522 → 450**
- Validation MSE losses: **0.0708 → 0.0237**

GENERALIZABILITY & SCALABILITY

Training dataset

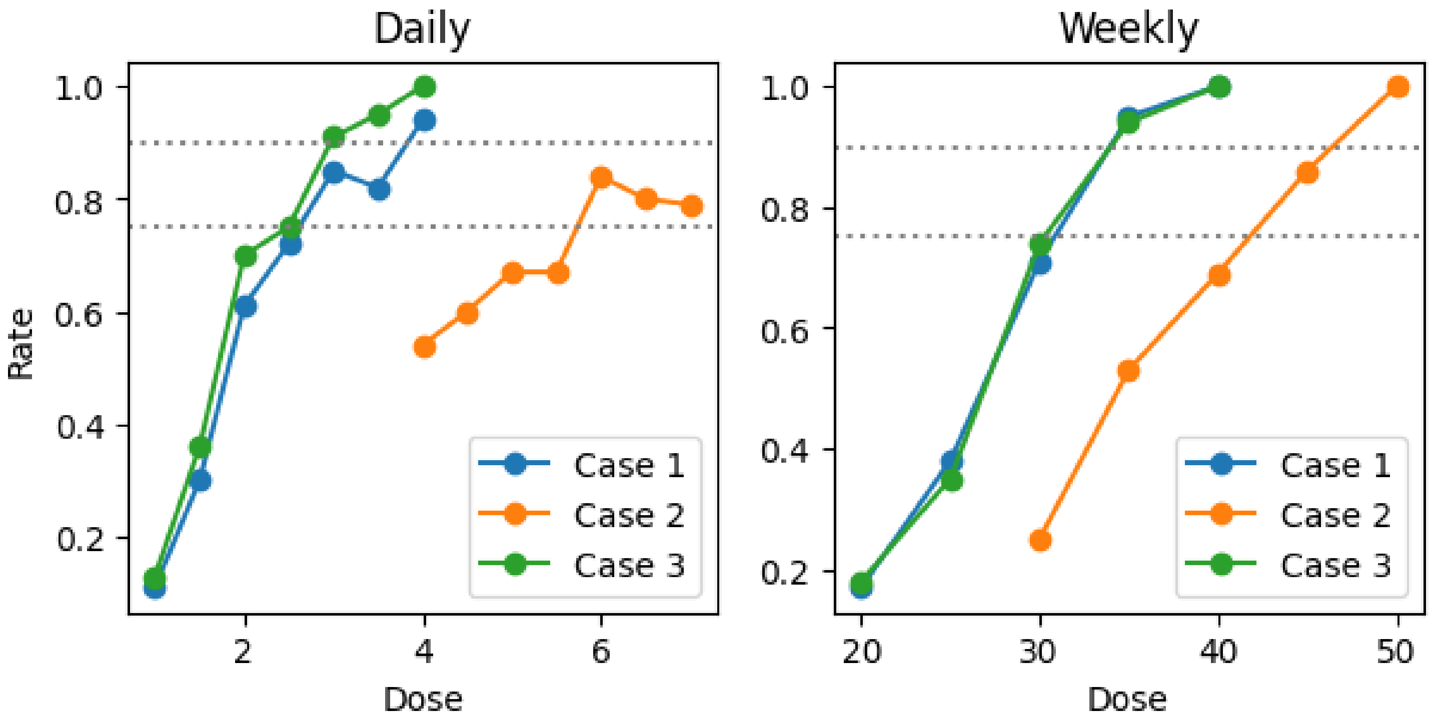
Case 1: similar to the given data

Case 2: larger body weight

Case 3: avoid concomitant medication

Success rate vs dose level

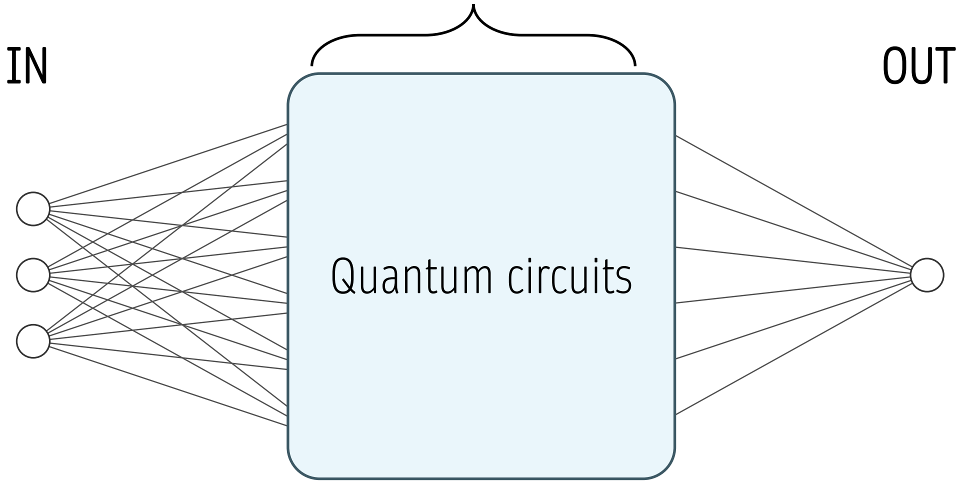
Successfully suppressed bio-marker below the clinical threshold

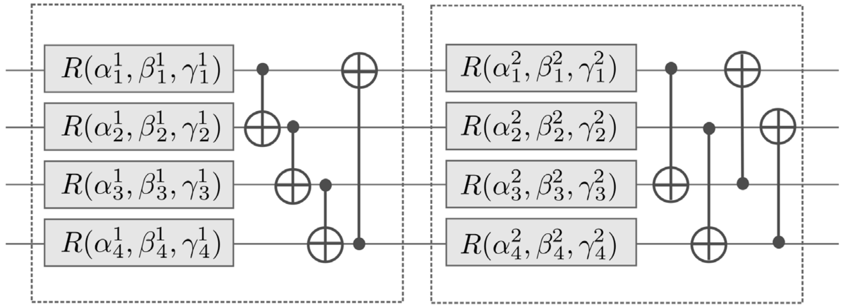


SUMMARY

Amplitude encoding + pairweise entanglements

~~Linear + SELU activation~~





- Trajectory accuracy: **MSE reduced** from 0.07 to 0.02, i.e. by **70%**.
- Parameter efficiency: trainable parameters of QTFM has only about **10%** of the classical TFM.

PLAN FOR PHASE 2

Completeness of existing algorithm

- Extended experiments for uncertainty estimations.
- Fit PK and PD seperately, in addition to the joint modeling.

- Try neural ODE based training scheme.

Algorithmic benchmarking

- Performance benchmarking of quantum inspired algorithms against classical baselines.
- Analyze computational efficiency, scalability, etc.

Exploration of new approach

- Hardware efficiency enhancement.
- Incorporate physics-informed constraintes.

LoCoQ

LoCo Quantum @ LinkedIn

THANK YOU

OUR TEAM

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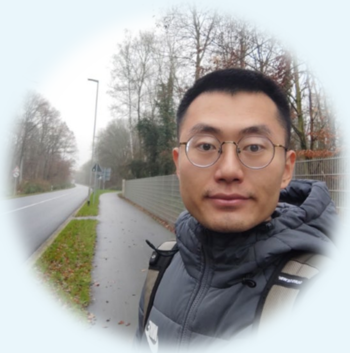
Generative &
explainable AI

Dr. Mira Sharma
from RWTH Aachen
Quantum algorithm,
Spin qubits hardware
& device modeling



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