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Temporal Graph Neural Networks with GraphNeuralNetworks.jl



Google Summer of Code

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GraphNeuralNetworks.jl

A graph neural network Julia package based on the Flux.jl.

Among its features:

- Standard graph convolutions
- Batched graph support
- Custom layer creation
- GPU computing via CUDA.jl
- Graphs.jl integration
- Various ML task examples
- Heterogeneous and temporal graphs

Installation `pkg> add GraphNeuralNetworks`

Gender classification in brain networks

Gender classification is the problem of determining the category of the graph, in this case female and male.

Temporal Brain Networks Dataset

The networks are obtained from resting-state fMRI data.

Nodes: 102 brain regions

Edge weights: region activity correlations

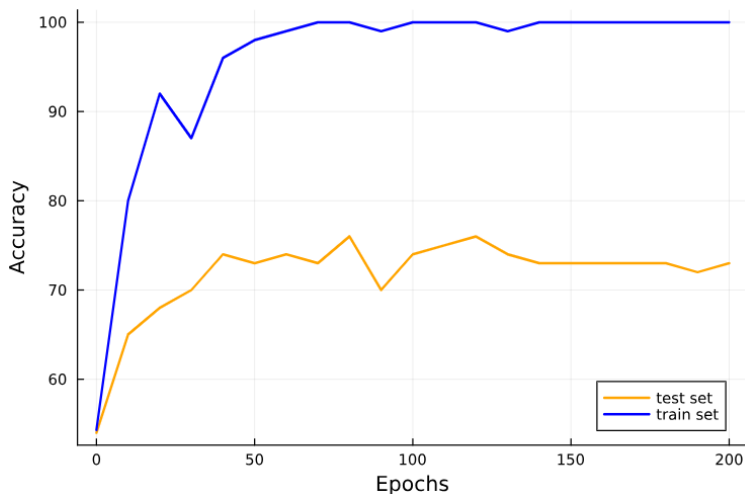
Node features: concatenation of one-hot encoding and mean activation of a node

Graph features: one-hot encoding of the gender

Model

- Graph Isomorphism Network for every snapshot $X' = f_{\theta}([(1 + \epsilon)I_N + A]X)$ where f_{θ} is a Multi Layer Perceptron
- Global pooling (mean) on node dimension
- Global pooling (mean) on time dimension
- A fully connected layer

Results



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Temporal graphs

Real-world dynamic networks (social, transportation, brain) are modeled as sequences of static graphs.

Traffic prediction example

Traffic forecasting is the problem of predicting future **traffic trends** on a road network given historical traffic data.

METR-LA Dataset

It contains traffic data from 207 sensors in highways of Los Angeles County.

Nodes: sensors

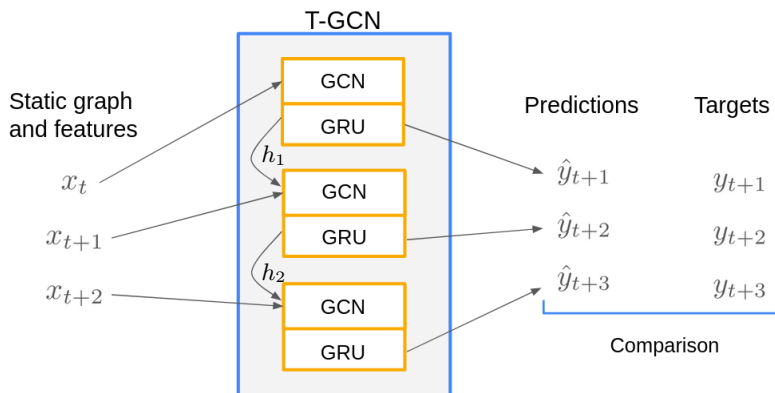
Edge weights: distances between the sensors

Node features: traffic speed and time of the day

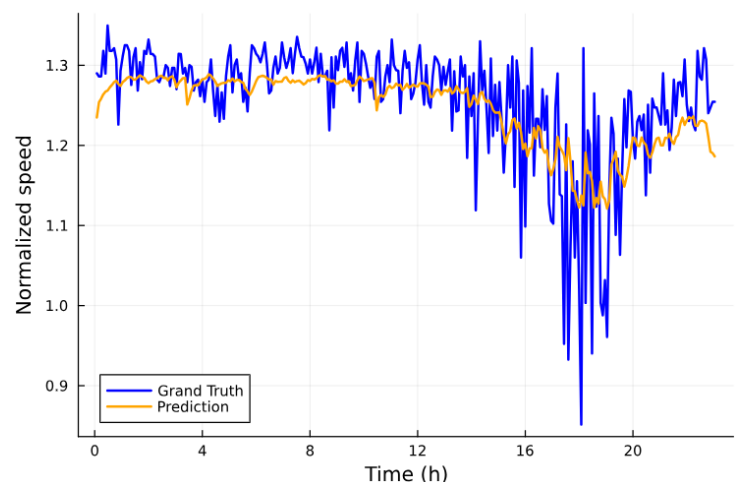
T-GCN Model

It is a recurrent model and a cell is composed of:

- Graph Convolutional Network to model spatial dependence
- Gated Recurrent Unit to model temporal dependence



Results



References

"T-GCN: A Temporal Graph Convolutional Network for Traffic Prediction"

Zhao et al.

"Diffusion Convolutional Recurrent Neural Network: Data-driven Traffic Forecasting" Li et al.

"How Powerful are Graph Neural Networks?", Xu et al.

<https://summerofcode.withgoogle.com/archive/2023/projects/vbQaqNYW>

<https://github.com/CarloLucibello/GraphNeuralNetworks.jl>