



AI4SE Working Group

January 30, 2022

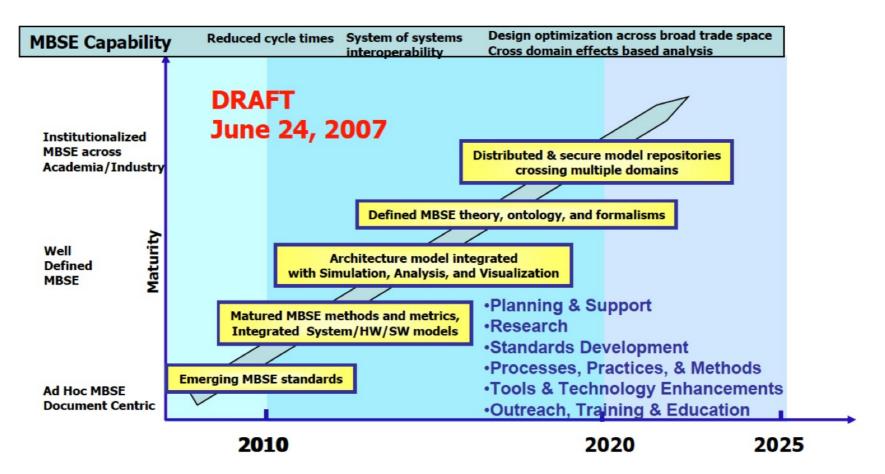
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Acknowledgements: Leonard Petnga, Parastoo Delgoshaei, Maria Coelho, Mark Blackburn. **Collaborations:** NIST, National Cancer Institute, DoD / SERC.

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Motivation: Vision for MBSE Capability ...



Notice: Use of AI Implied. No mention of Data Mining, Machine Learning

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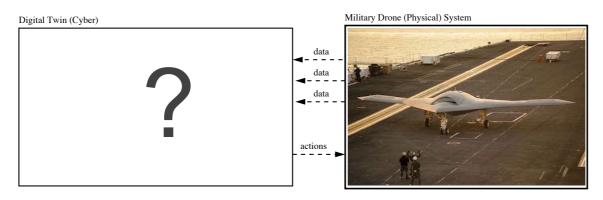
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Motivation: Vision for MBSE Capability ...



Definition of Digital Twin (2000 – today)

• Virtual representation of a physical object or system that operates across the system lifecycle (not just front end).



Required Functionality

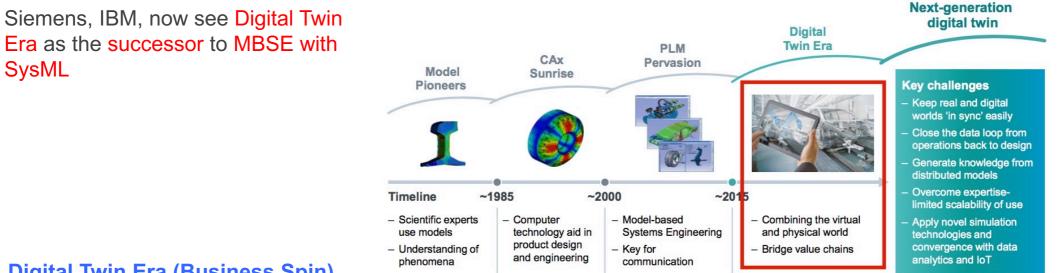
- Mirror implementation of physical world through real-time-monitoring and synchronization of data with events.
- Provide algorithms and software for observation, reasoning and physical systems control.

Many Application Domains

• NASA, manufacturing processes, building operations, personalized medicine, smart cities, ...

Importance and Timeliness (Why?)

Business Drivers (Why this project is timely?)



Digital Twin Era (Business Spin)

- New methods and tools for model-centric engineering.
- New operating system environments for observation, reasoning and physical systems control. •
- Superior levels of system performance, agility, economy, etc.

Technical Implementation (2020, Google, Apple, Amazon, Siemens, IBM ...)

Al and ML will be deeply embedded in new software and algorithms. •

Proposed Approach (Why?)



Definition of AI and ML

- AI: Knowledge representation and reasoning with ontologies and rules. Construction of semantic graphs, executable event-based processing, multi-domain reasoning.
- ML: Modern neural networks (closely related to signal processing of data streams). Data Mining. Input-to-output prediction, Learn structure and sequence. Identify objects, events, anomalies. Remember stuff.

AI/ML Strengths and Weaknesses

State-of-the-art AI and ML technologies are **fragmented** in their capability:

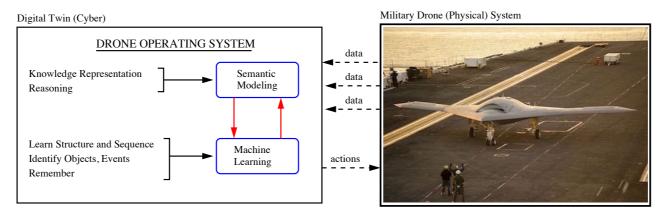
- Al provides a broad view of concepts needed for reasoning. Decision making processes are transparent; semantic graphs are flexible.
- Semantic reasoning is decision making in-the-moment (no memory).
- Data mining algorithms can organize information from large data sources.
- ML procedures developed to solve very specific tasks.
- ML decision making procedures lack transparency.
- ML procedures can identify anomalies (events) in streams of data.

Proposed Approach (What's New?)



Digital Twins (What's New?)

• Explore design of digital twin architectures that support AI and ML formalisms working sideby-side as a team.



Key Research Challenge

• How to design digital twin elements and their interactions to support: (1) methods and tools for modelcentric engineering, and (2) digital twin operating system environments for observation, reasoning, control.

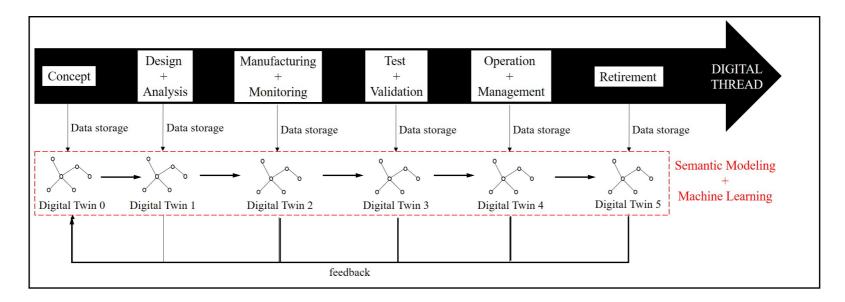
Project Success (What does it look like?)

• Knowledge to guide architectural development of future digital twins enabled by AI / ML technology.





AI4SE: Cradle-to-Grave Lifecycle Support (Digital Threads)



Observation: A lot of model-centric engineering boils down to representation of systems as graphs and sequences of graph transformations punctuated by decision making and work / actions.

Reasonable Starting Point: Understand the range of possibilities for which machine learning of graphs and their attributes support and enhance activities in model-centric engineering and systems operation.

Digital Twin Architecture (2017-2022)



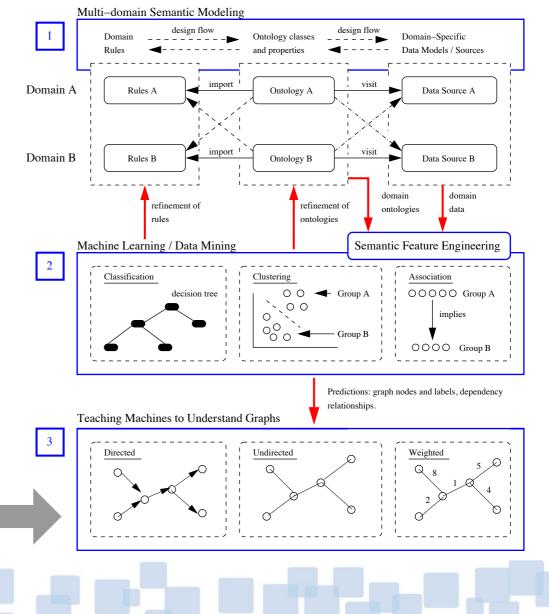
• **Step 1:** Multi-Domain Semantic Modeling

- **Step 2:** Semantic Modeling + Data Mining
- Step 3: Teaching Machines to Understand Graphs

What will the machine learning do?

Maria Coelho's PhD Research

Explore opportunities for teaching machines to understand graphs.



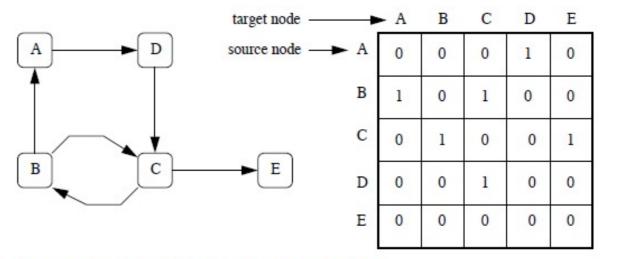
Classical Graph Models and Graph Analysis



A **graph** is defined as G = (V, E), where V is a set of vertices (i.e. nodes), E = set of edges, and each edge is formed from pair of distinct vertices in V.

Traditional Approach to Graph Analysis (Euler, 1735)

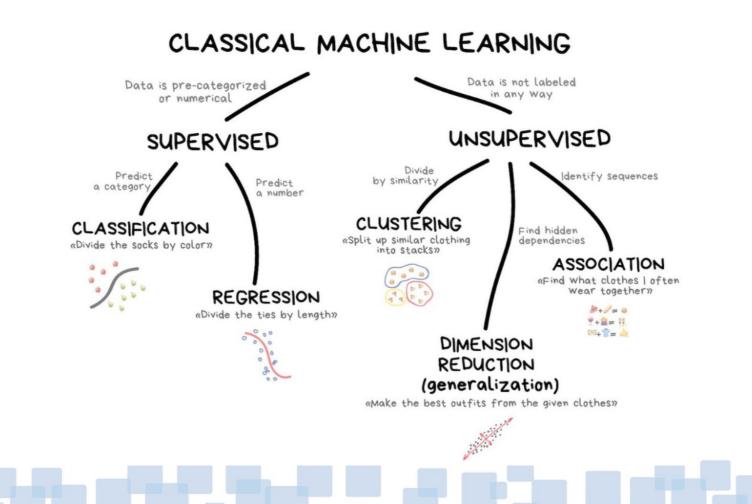
- Traditional approaches to graph modeling employ adjacency matrices.
- Topology properties can then be extracted through graph analysis tasks: e.g., connectivity analysis, traceability analysis, cycle detection.



Machine Learning



Algorithms that use statistics to learn patterns and hidden insights in data without being explicitly programmed for it.

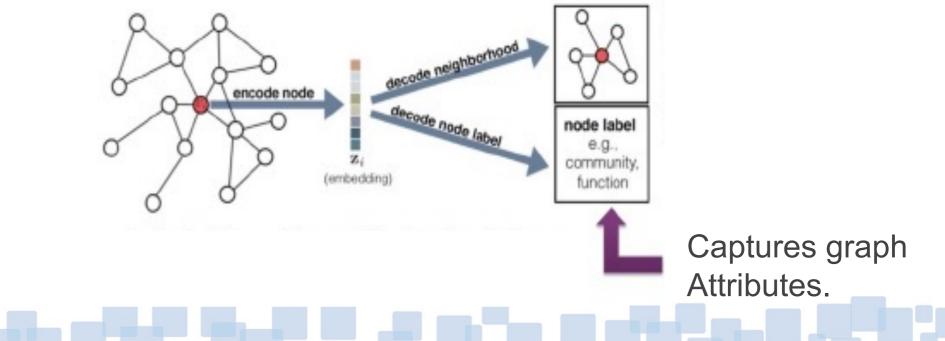


Graph Analytics



Machine Learning Approach to Graph Analytics

- Adjacency matrices suffer from data sparsity, high-dimensionality, and a lack of support for capturing graph attributes.
- Surge in graph embedding approaches.
- Output vectors are statistical, should be interpreted as graph analytics.
- Learned embeddings could advance various downstream learning tasks:
 - Node Classification
 - Node Clustering
 - Anomaly Prediction
 - Attribute Prediction
 - Link Prediction
 - Recommendation
 - ➤ Etc.





Recent Research at UMD, 2021

Frame Graph Learning as a Binary Classification Problem

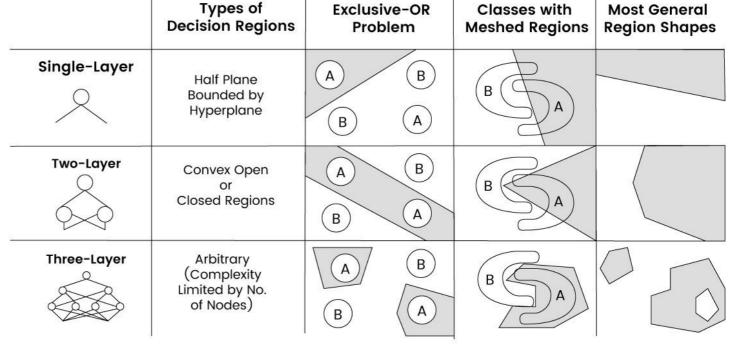
Network Architecture for Classification

One Region

- > One Hidden Layer
- Hidden Layer Size = number of hyperplanes required to form region
- Output neuron

Many Regions

- Two Hidden Layers
- Hidden Layer 1 Size = number of hyperplanes required to form regions
- Hidden Layer 2 Size = number of regions
- Output neuron



Source: Lippmann, R., 1987

Key Observation: Input-output relations (logic) can be framed in terms of node-to-node connectivity in a graph. It's only a question of interpretation!

Directed Line Problem (One Region)

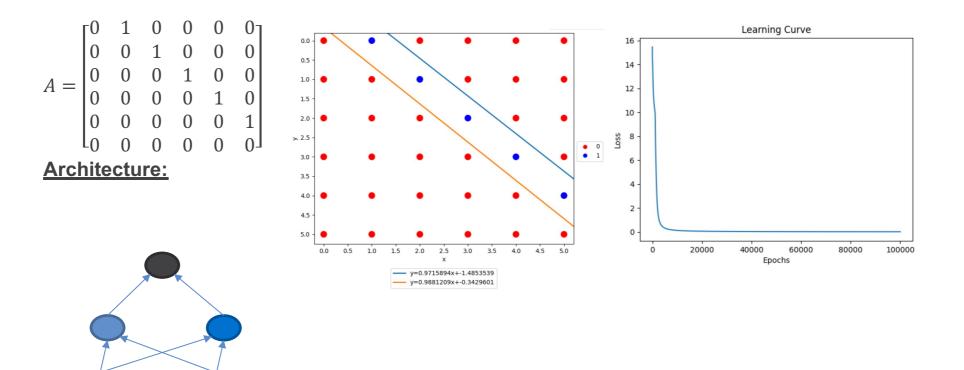


Topology:

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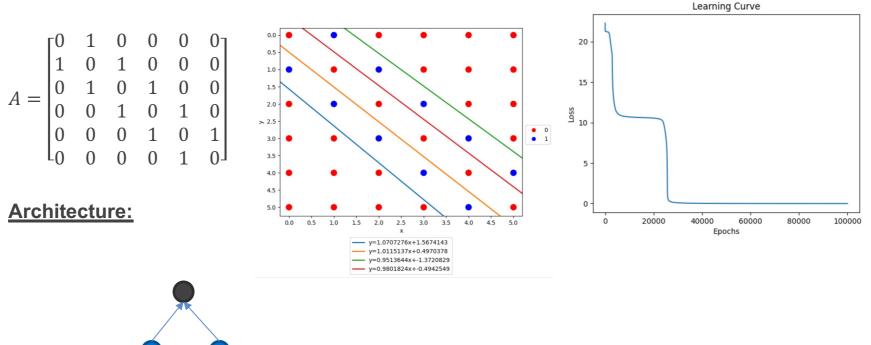


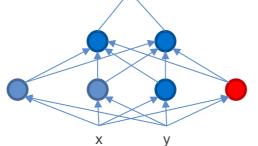
Line Problem (Multiple Regions)



Topology:



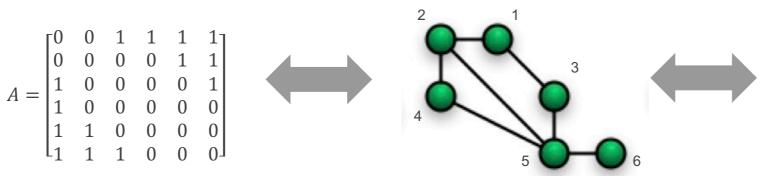






Graph Mesh Problem

Topology:

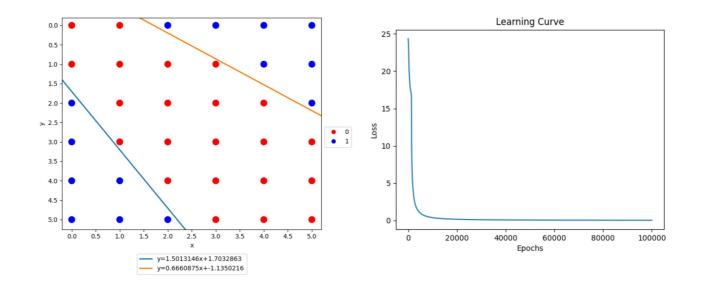


Key Benefit: Good physical intuition.

Architecture:

Х

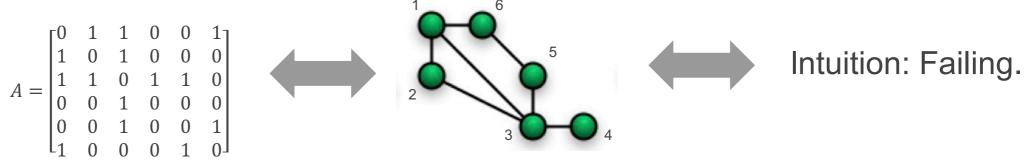
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Graph Mesh Problem



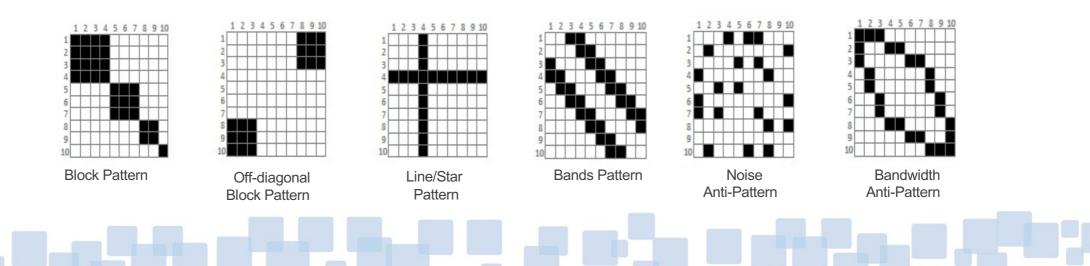
Topology:



Architecture:

Visually hard to determine required architecture, **need for matrix reordering approach.**

Matrix Reordering: Automation to Reveal Visual Patterns

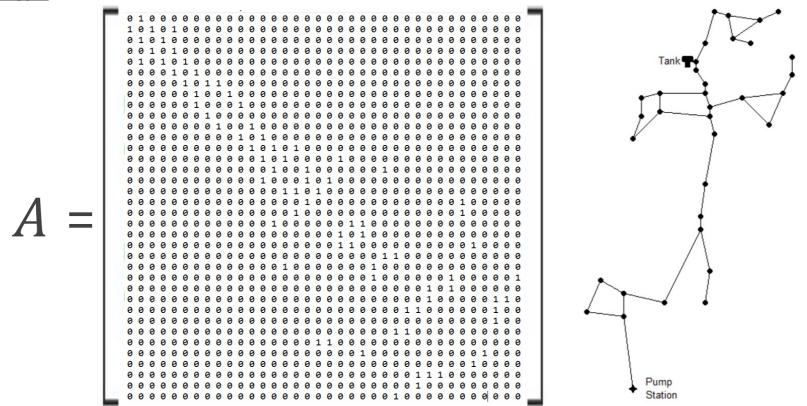


Matrix Reordering for Graph Learning



Example: Water Distribution Network

Topology:

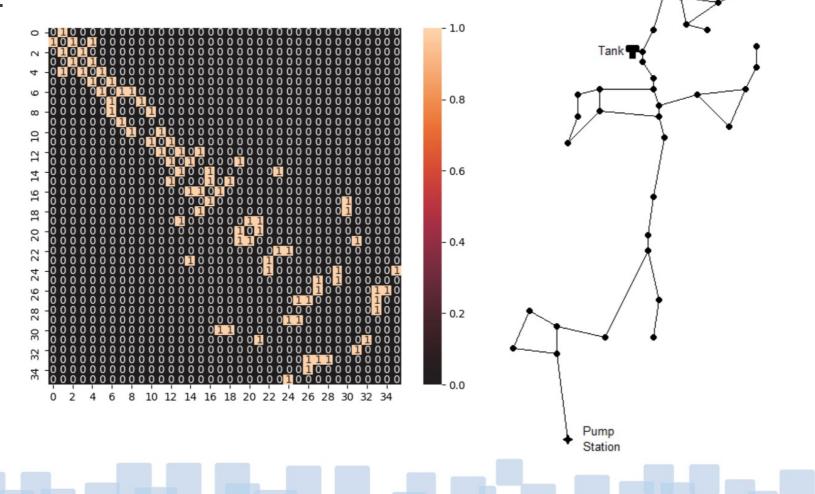


Matrix Reordering for Graph Learning



Water Distribution Network

Heatmap:

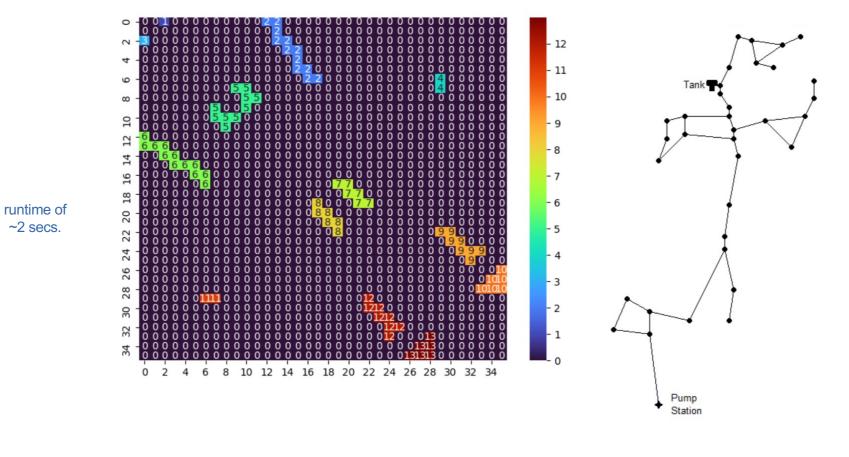






Matrix Reordered Water Distribution Network

Traveling Salesman:



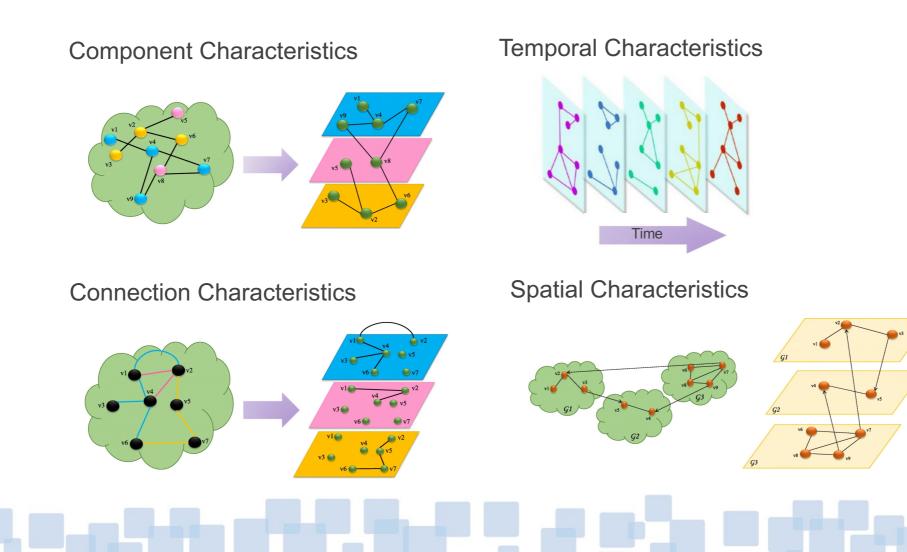
Current Research, 2021-2022.



Transition to Networked Decomposition and Incremental Learning of Multi-Domain Graphs

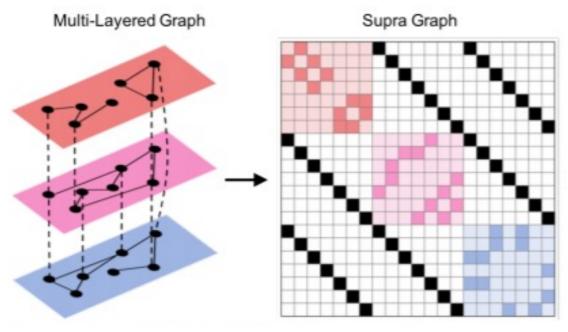


Attribute-Driven Decomposition of System Graphs





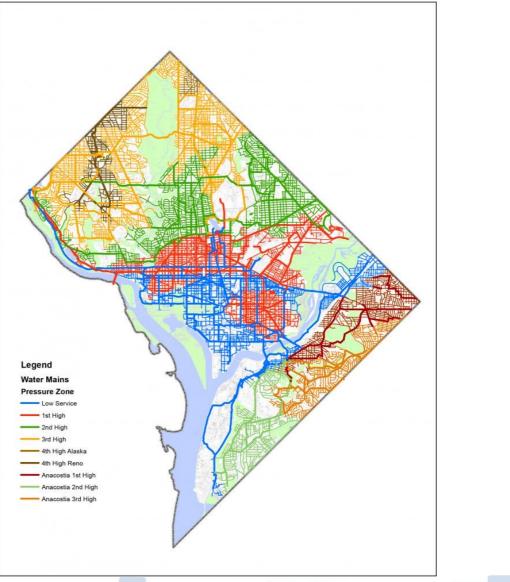
Supra Graph Framework: Support for multi-layer / multi-domain graphs, graph zones, viewpoints, etc.



Shanthamallu et al., 2019

Example: Washington DC Water Network

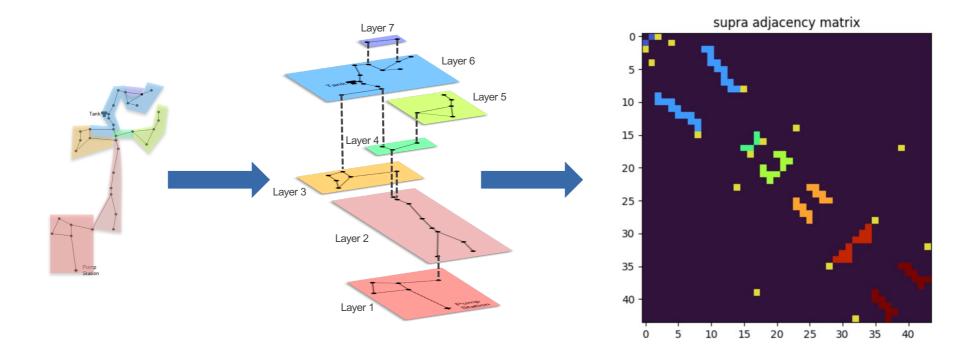
- Washington DC's drinking water is distributed by elevation levels.
- Distribution network is divided into "pressure zones".





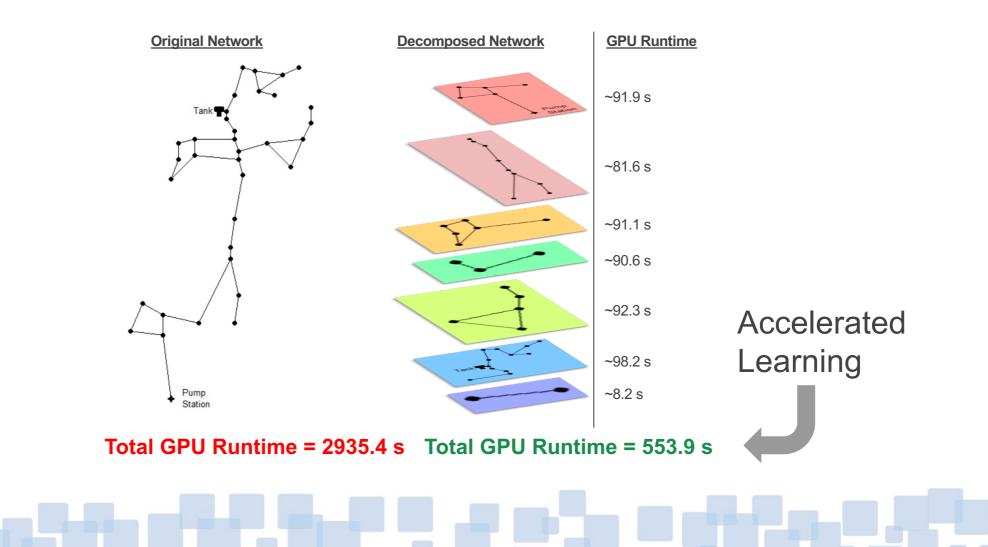


Water Network Decomposition into Graph Layers





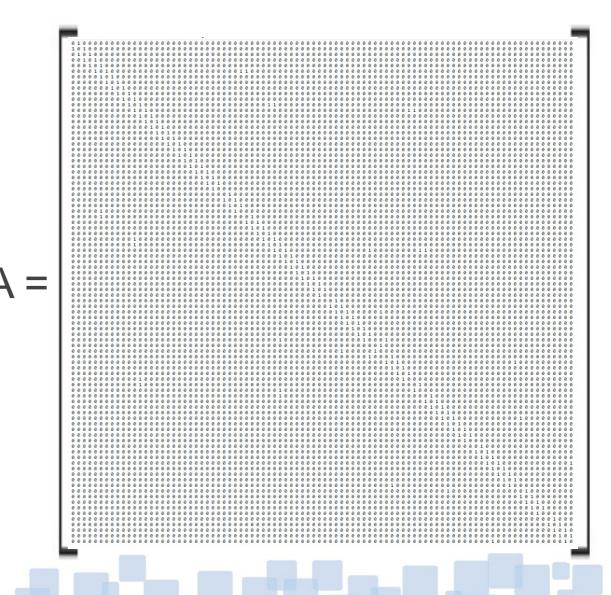
Incremental Learning of Network / Graph Zones





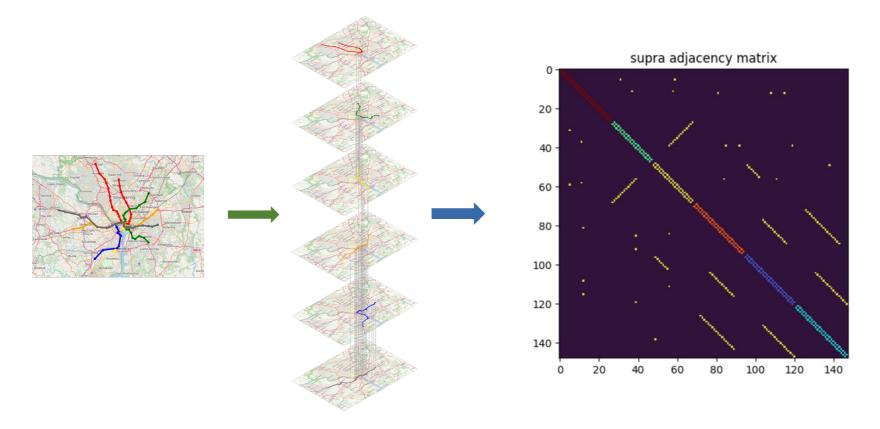
Washington DC Metro System Network





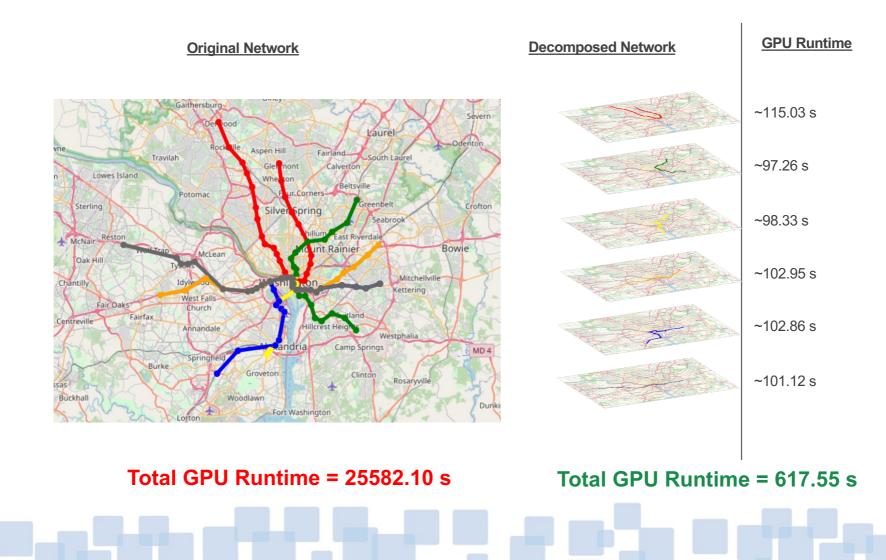


Washington DC Metro System Network





Accelerated Learning of Network / Graph Zones



Results and Future Work

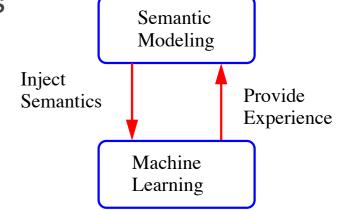


Results: Teaching Machines to Understand Graphs

- Small graphs that have static graph topologies.
- Formulae for synthesis of neural network architectures and incremental learning.
- Modeling of attributed multi-domain graphs.

Next Steps: Focus on AI-ML Collaboration in Digital Twins

- Understand mechanisms of AI ML interaction.
- Reasoning with events, time and space.
- Dynamic graph topologies.
- Inject semantics into Machine Learning.







Questions?

Contact Information

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References



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