2022
Annual INCOSE
international workshop
HYBRID EVENT
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Jan 29 - Feb 1, 2022

AI4SE Working Group

January 30, 2022

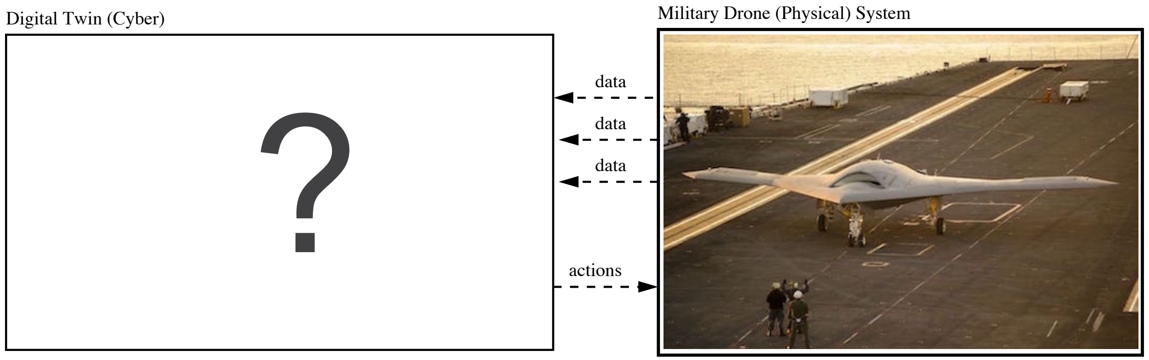
Dr. Mark Austin, Department of Civil Engineering,
University of Maryland, College Park.

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

Motivation: Digital Twins

Definition (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.

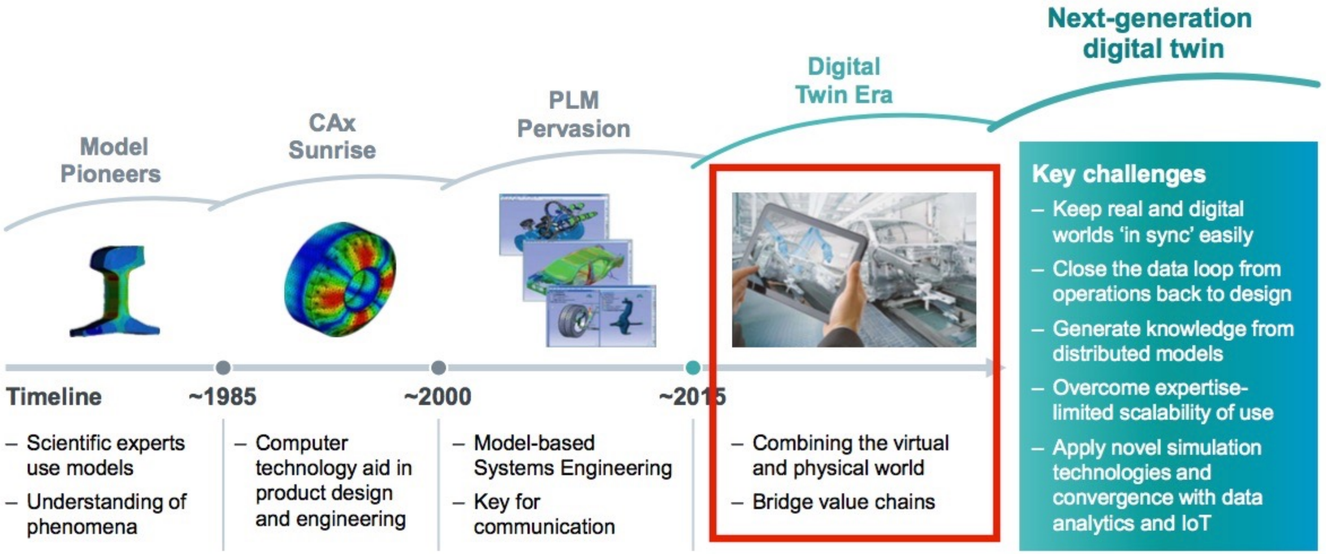
Many Application Domains

- NASA, manufacturing processes, building operations, personalized medicine, smart cities, …

Importance and Timeliness (Why?)

Business Drivers (Why this project is timely?)

Siemens, IBM, now see Digital Twin Era as the successor to MBSE with SysML



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 …)

- AI 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

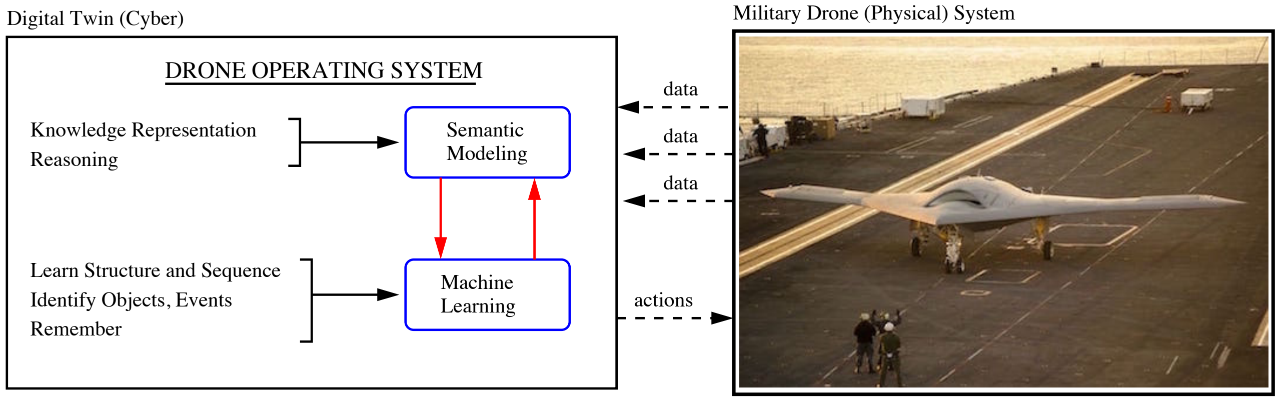
State-of-the-art AI and ML technologies are fragmented in their capability:

- AI 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 side-by-side as a team.



Key Research Challenge

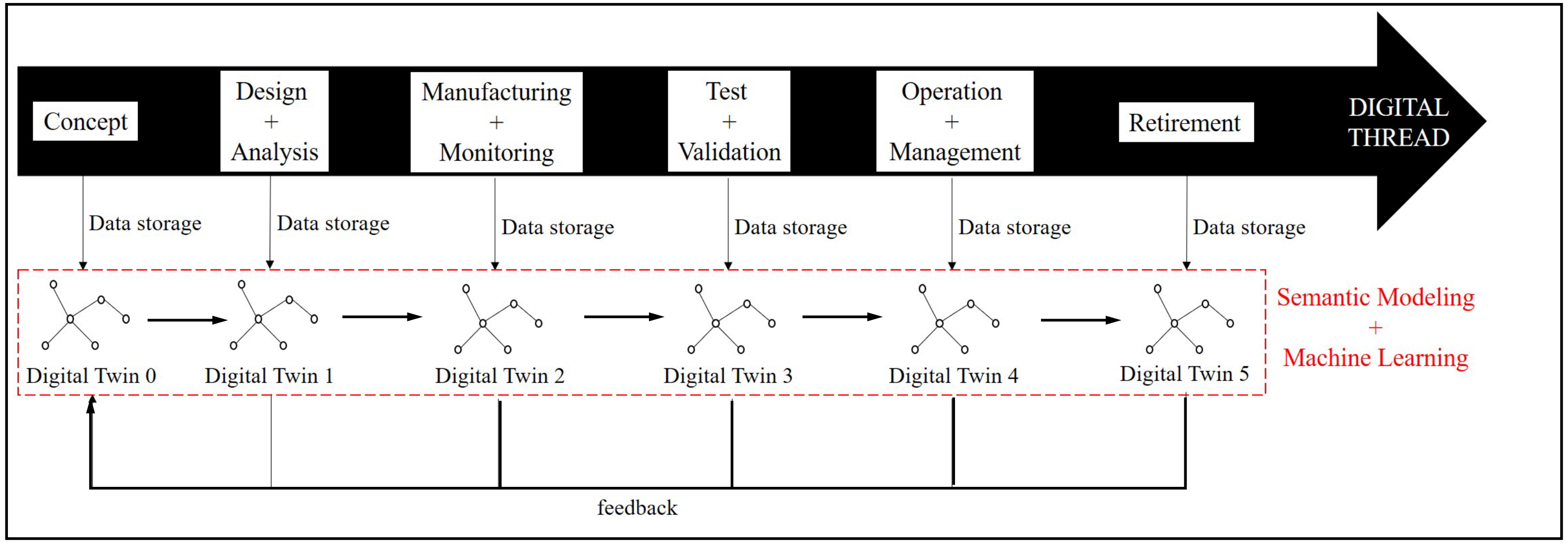
- How to design digital twin elements and their interactions to support: (1) methods and tools for model-centric engineering, and (2) digital twin operating system environments for observation, reasoning, control.

Project Success (What does it look like?)

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

Digital Twins → Digital Threads (What?)

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.

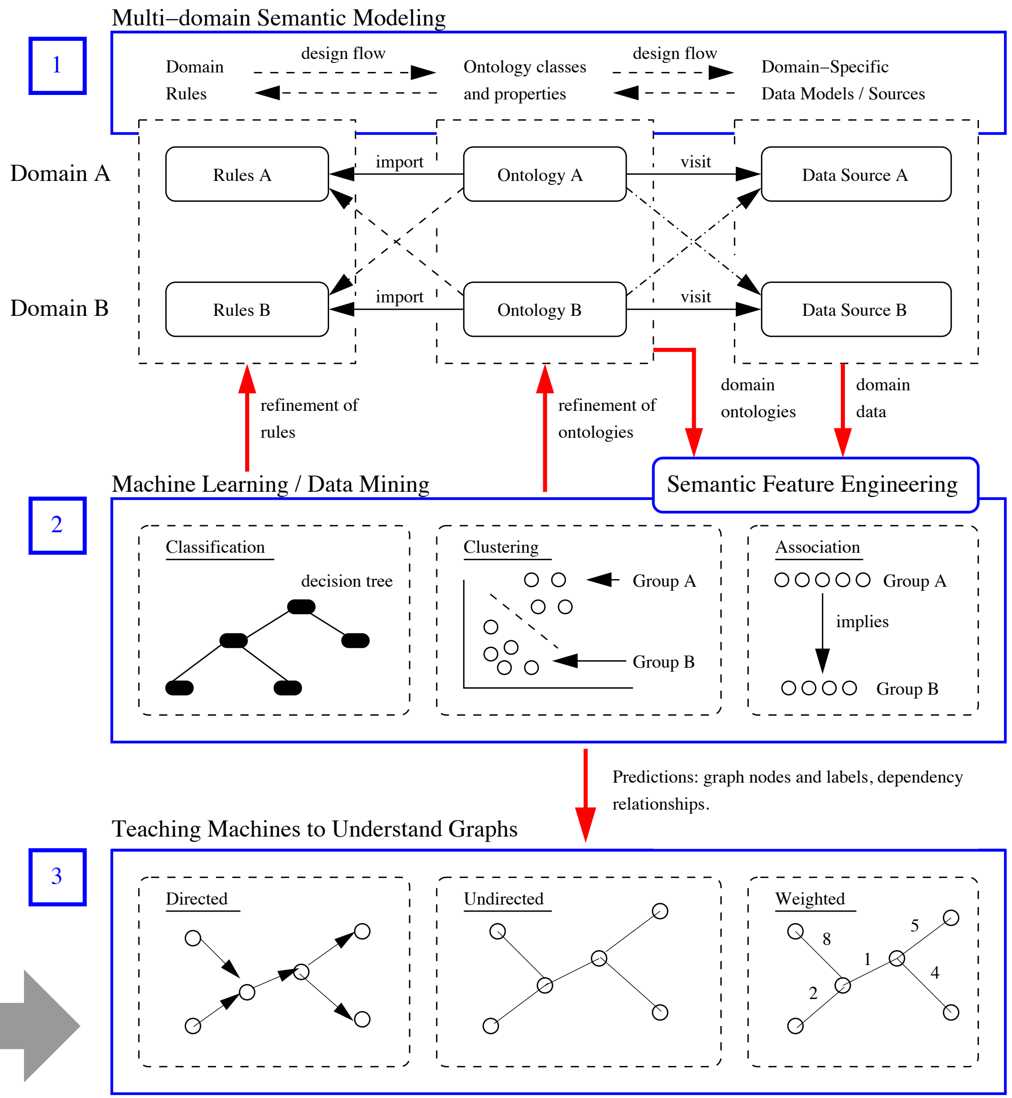
Digital Twin Architecture (2017-2022)

- **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.

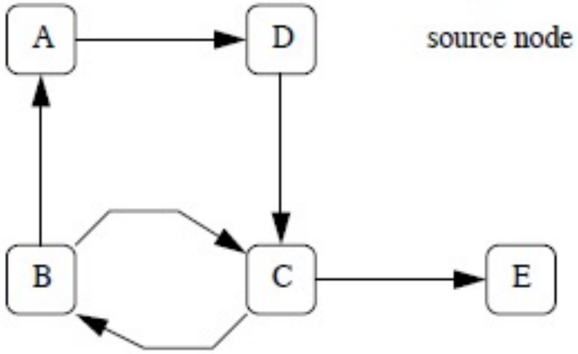


Classical Graph Models and Graph Analysis

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

- 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.

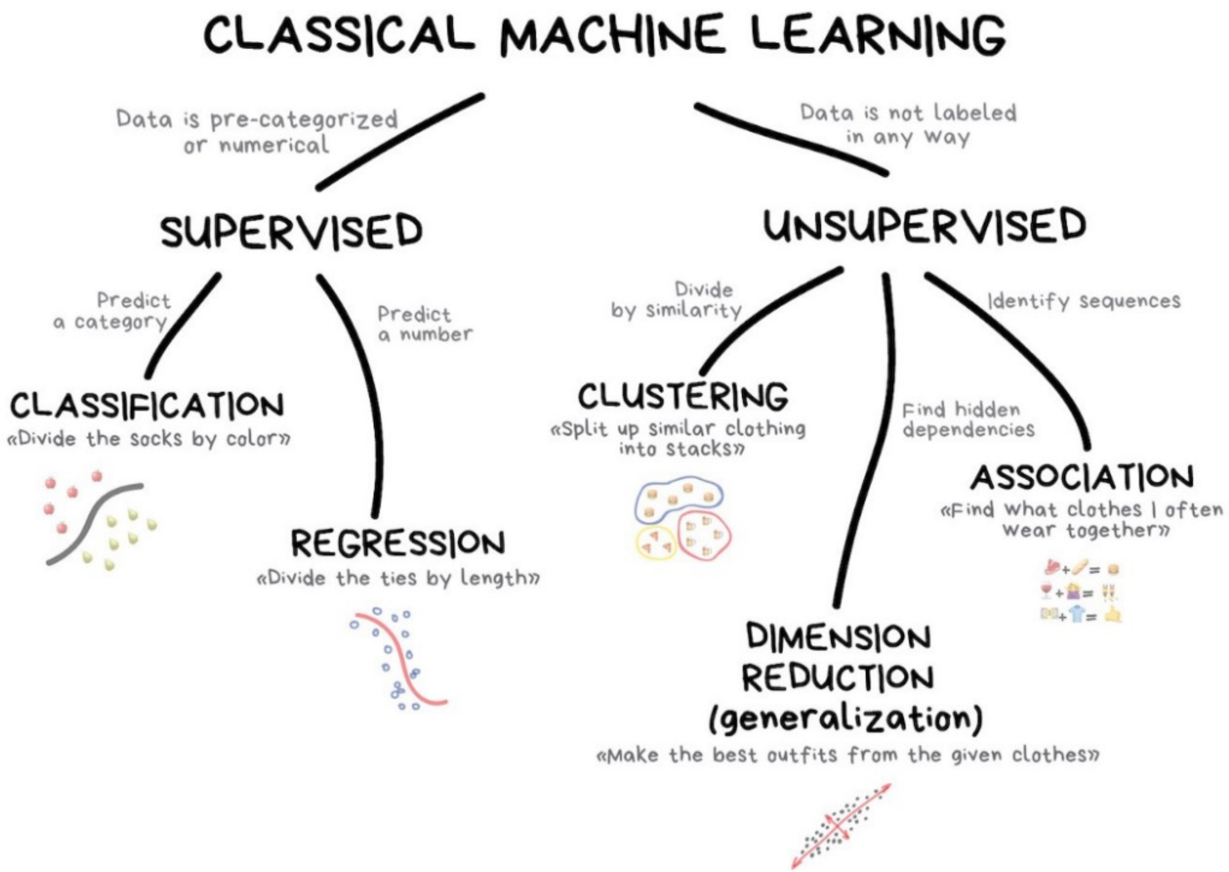


target node →
source node ↓

	A	B	C	D	E
A	0	0	0	1	0
B	1	0	1	0	0
C	0	1	0	0	1
D	0	0	1	0	0
E	0	0	0	0	0

Machine Learning

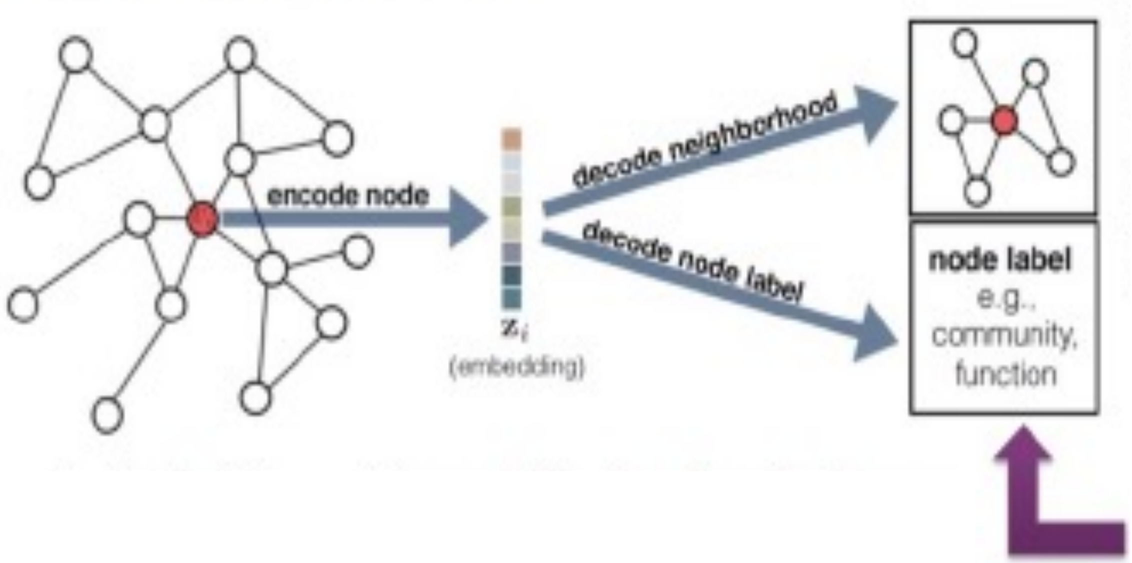
Algorithms that use statistics to learn patterns **and** hidden insights **in data** without being explicitly programmed for it.



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.



Captures graph Attributes.

Recent Research at UMD, 2021

Frame Graph Learning as a Binary Classification Problem

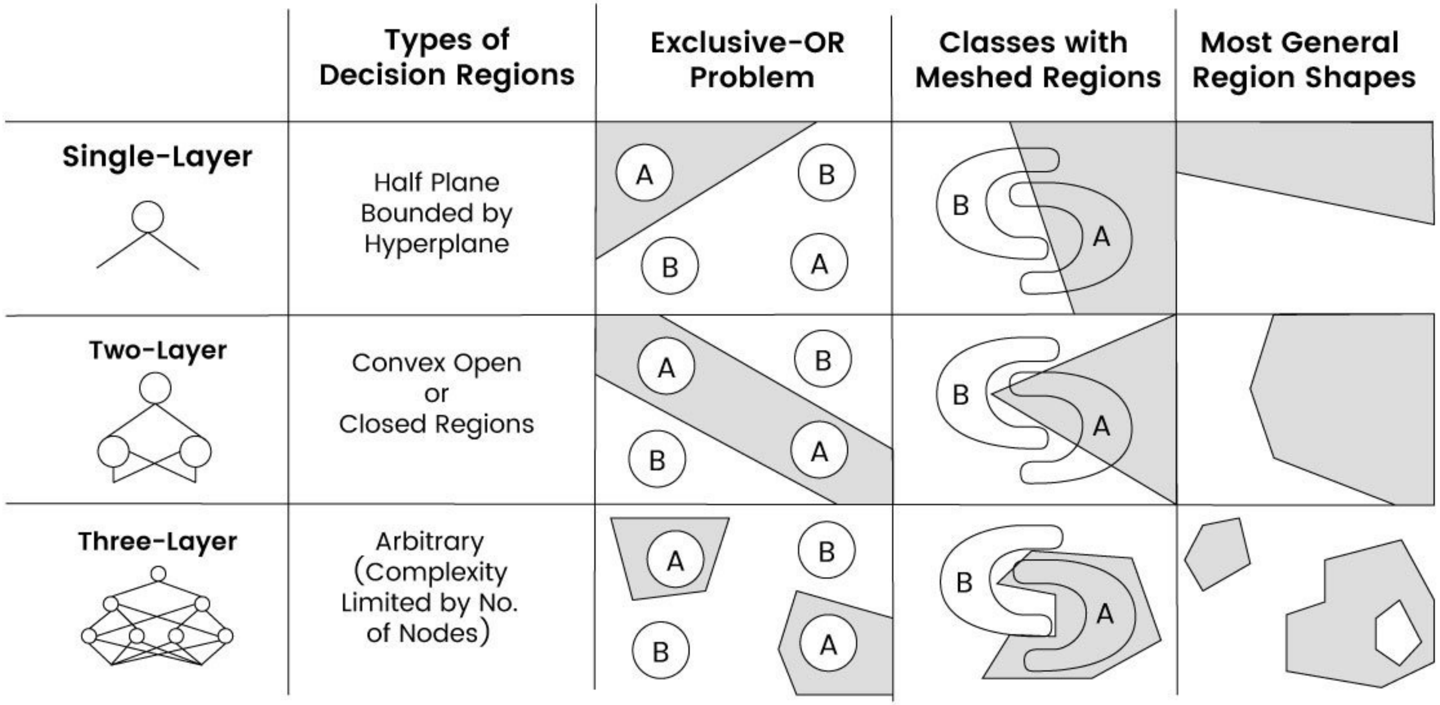
Network Architecture for Classification

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

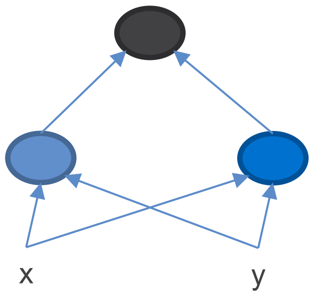
Key Observation: Input-output relations (logic) can be framed in terms of node-to-node connectivity in a graph. It's only a question of interpretation!

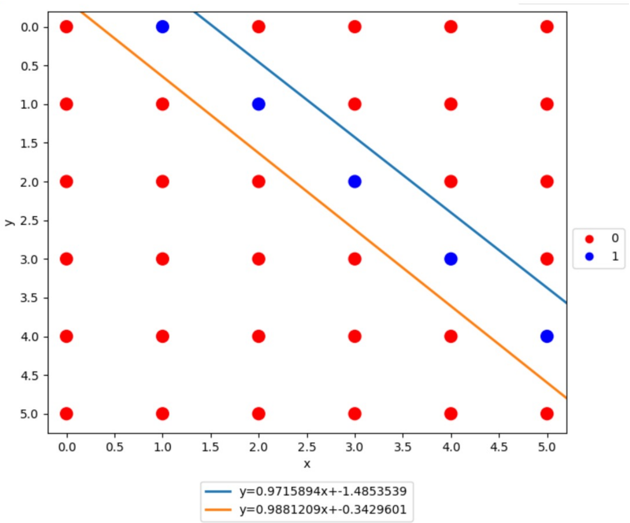
Directed Line Problem (One Region)

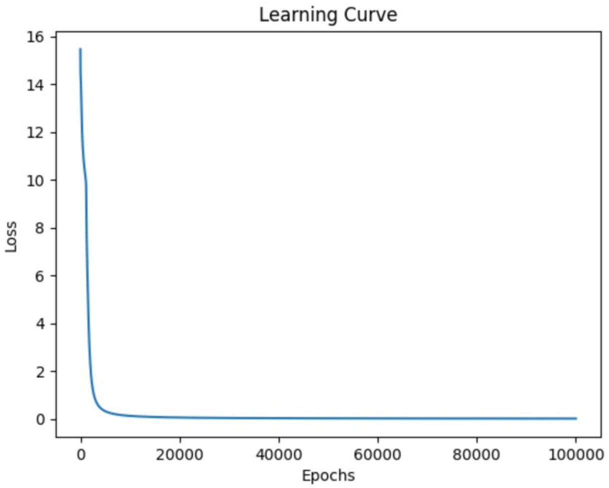
Topology:

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Architecture:



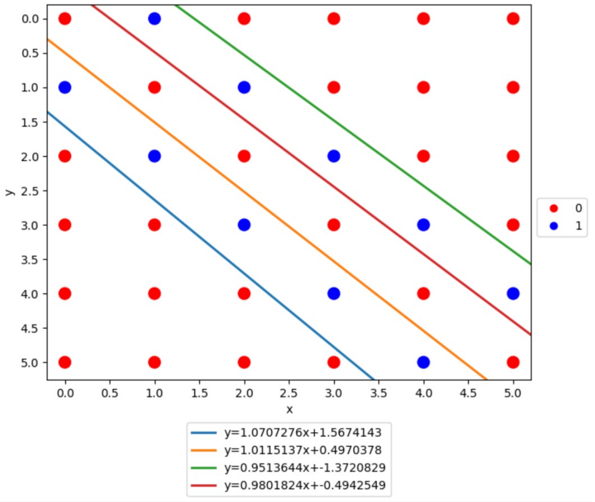


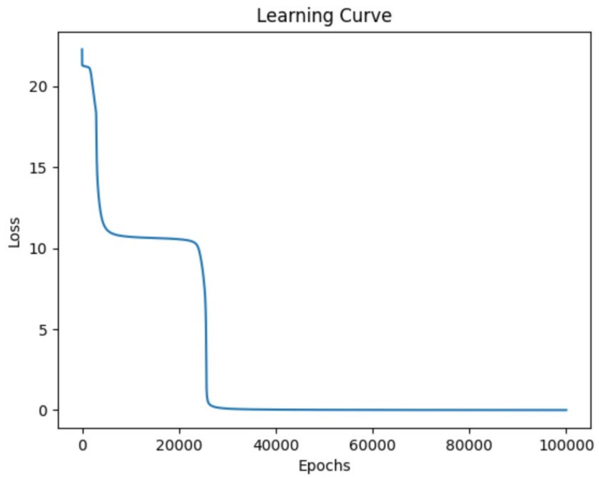


Line Problem (Multiple Regions)

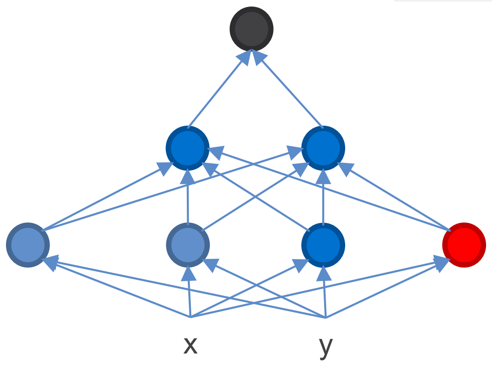
Topology:

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$





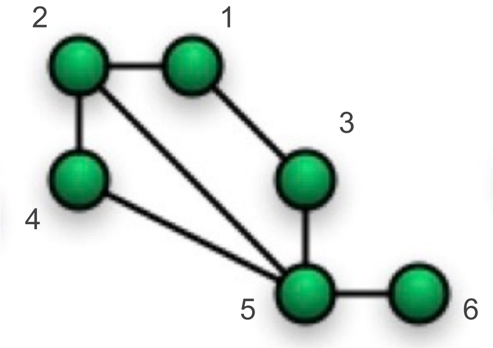
Architecture:



Graph Mesh Problem

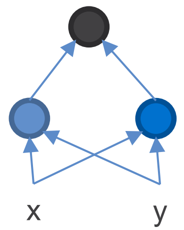
Topology:

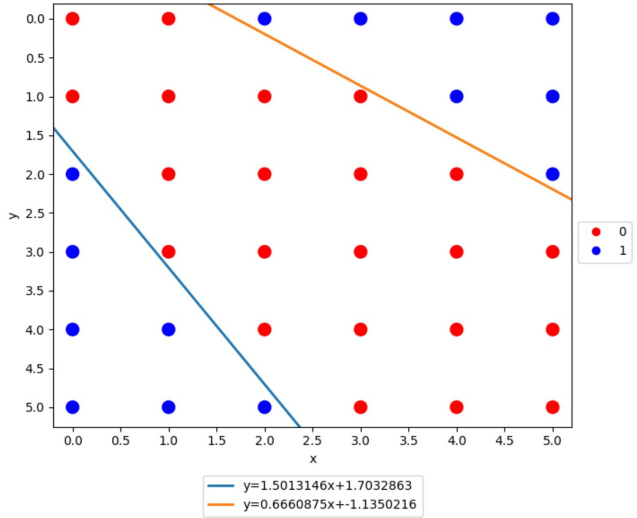
$$A = \begin{bmatrix} 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \end{bmatrix}$$

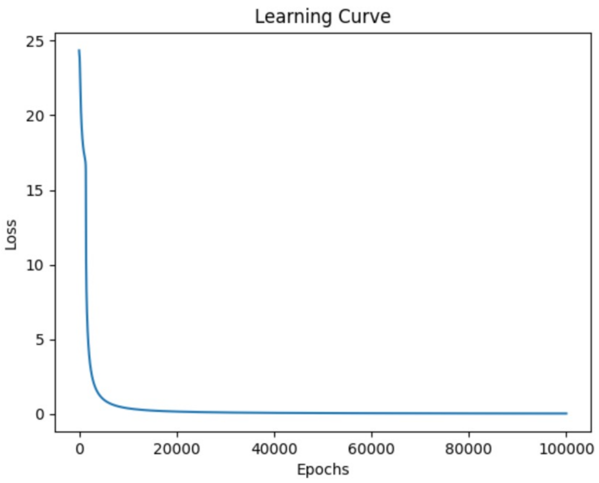


Key Benefit:
Good physical intuition.

Architecture:



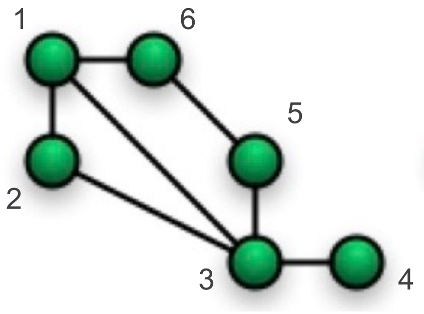




Graph Mesh Problem

Topology:

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

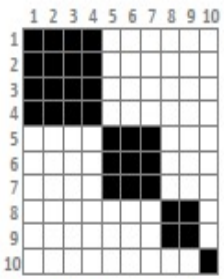


Intuition: Failing.

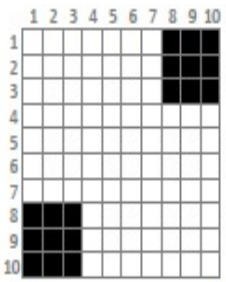
Architecture:

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

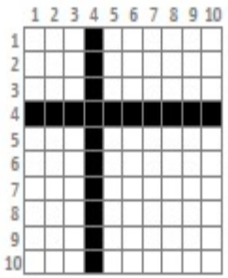
Matrix Reordering: Automation to Reveal Visual Patterns



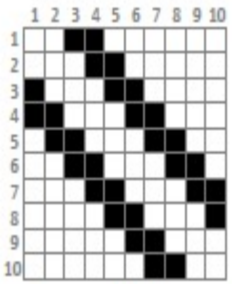
Block Pattern



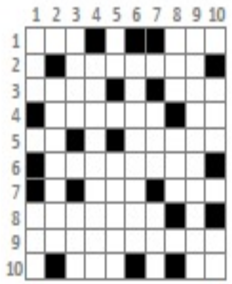
Off-diagonal Block Pattern



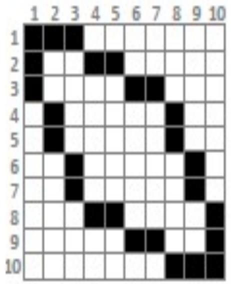
Line/Star Pattern



Bands Pattern



Noise Anti-Pattern



Bandwidth Anti-Pattern

Matrix Reordering for Graph Learning

Example: Water Distribution Network

Topology:

$$A = \begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
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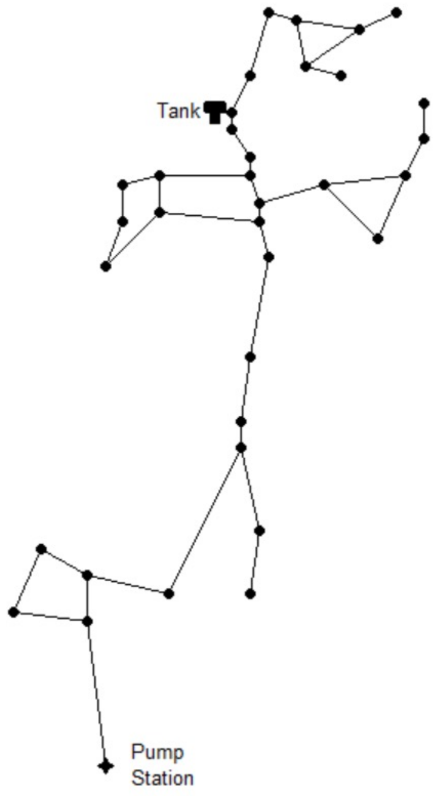
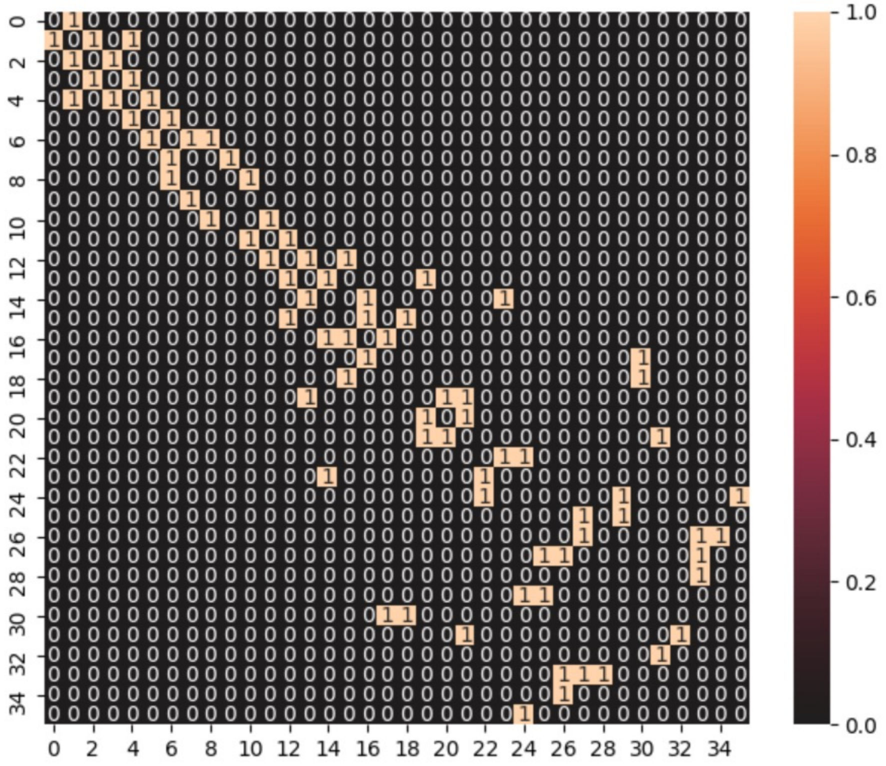
\end{bmatrix}$$

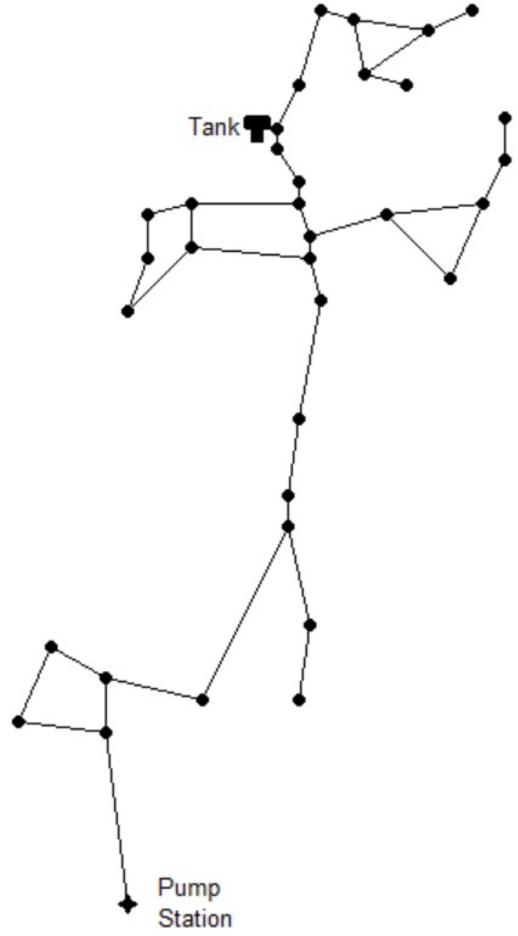


Matrix Reordering for Graph Learning

Water Distribution Network

Heatmap:



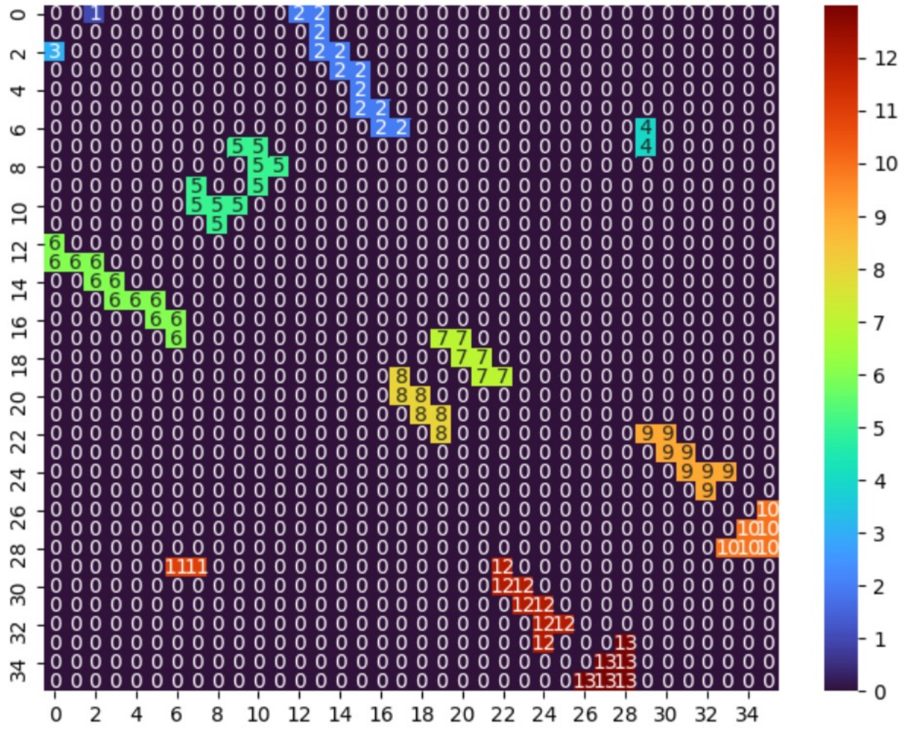


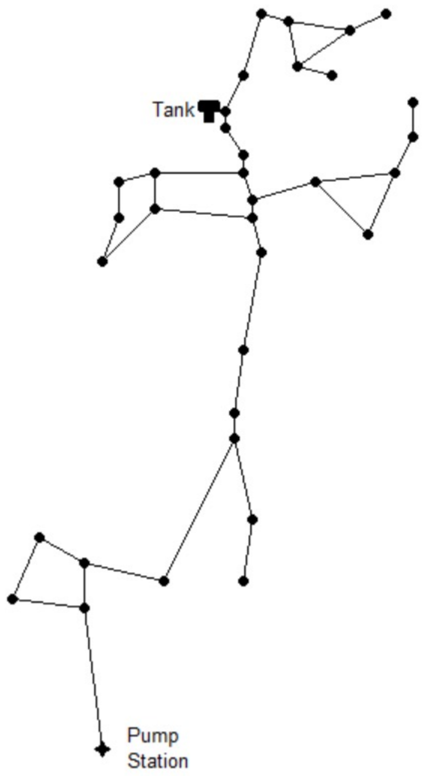
Matrix Reordering for Graph Learning

Matrix Reordered Water Distribution Network

Traveling Salesman:

runtime of
~2 secs.





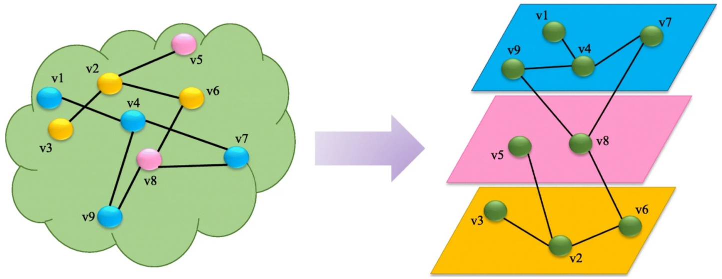
Current Research, 2021-2022.

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

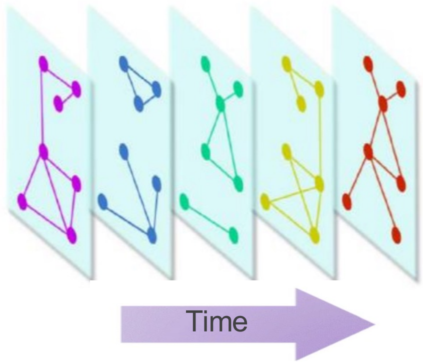
Transition to Networked Decomposition

Attribute-Driven Decomposition of System Graphs

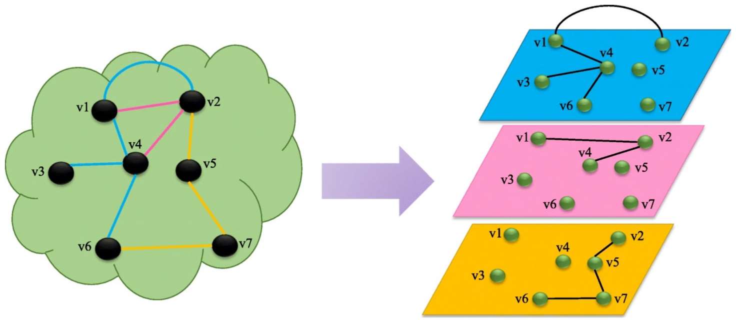
Component Characteristics



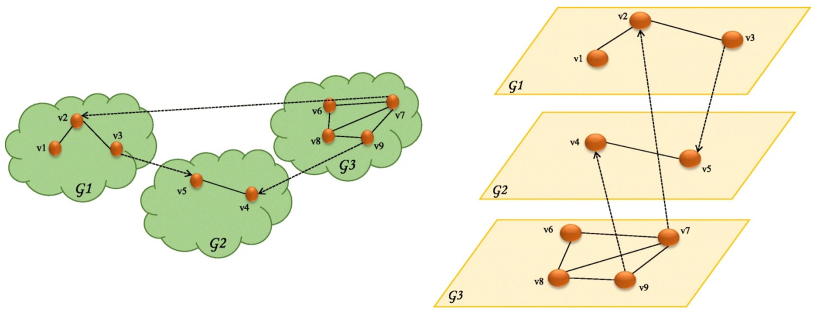
Temporal Characteristics



Connection Characteristics

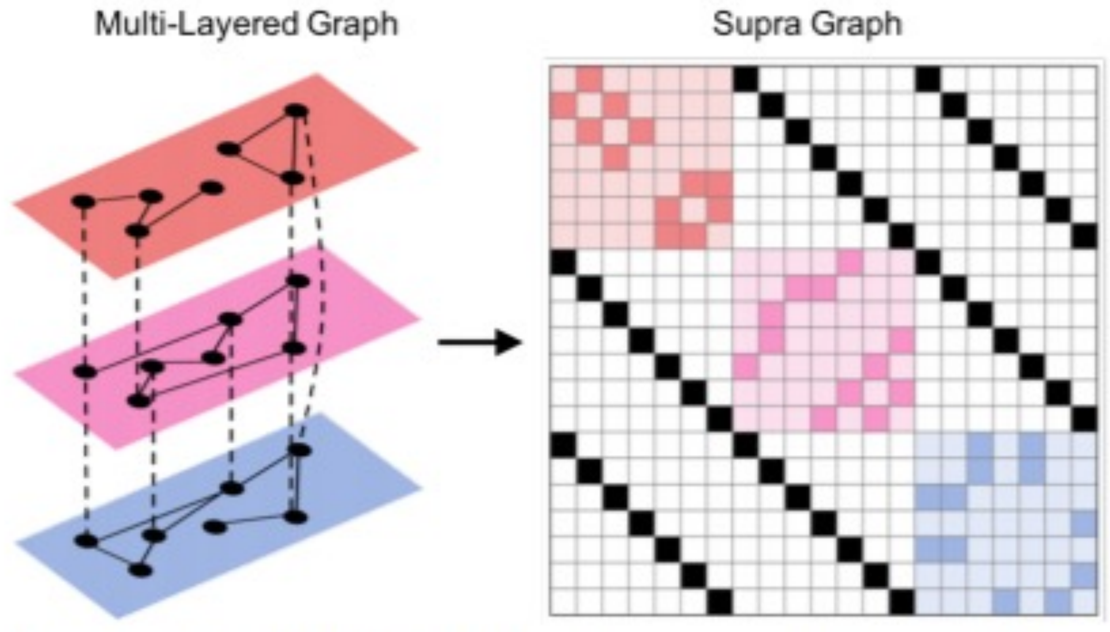


Spatial Characteristics



Transition to Networked Decomposition

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

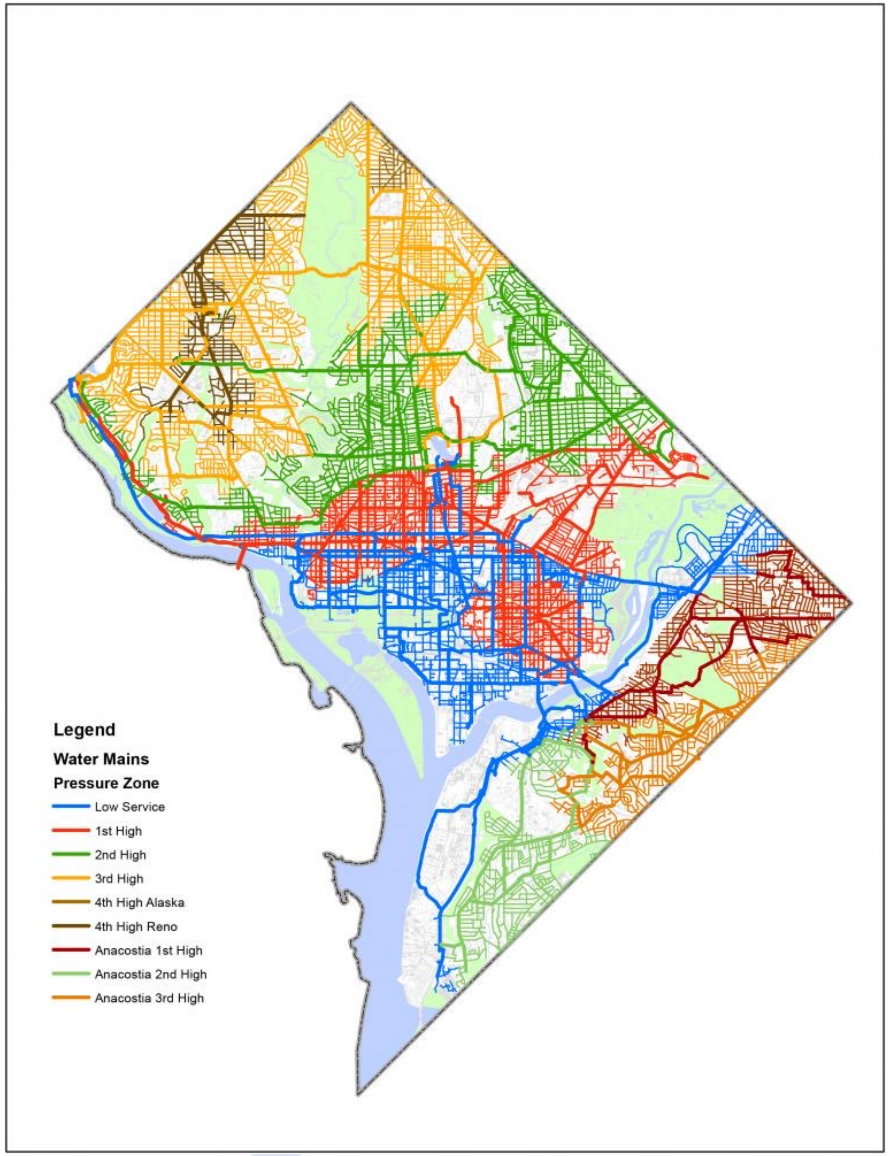


Shanthamallu et al., 2019

Transition to Networked Decomposition

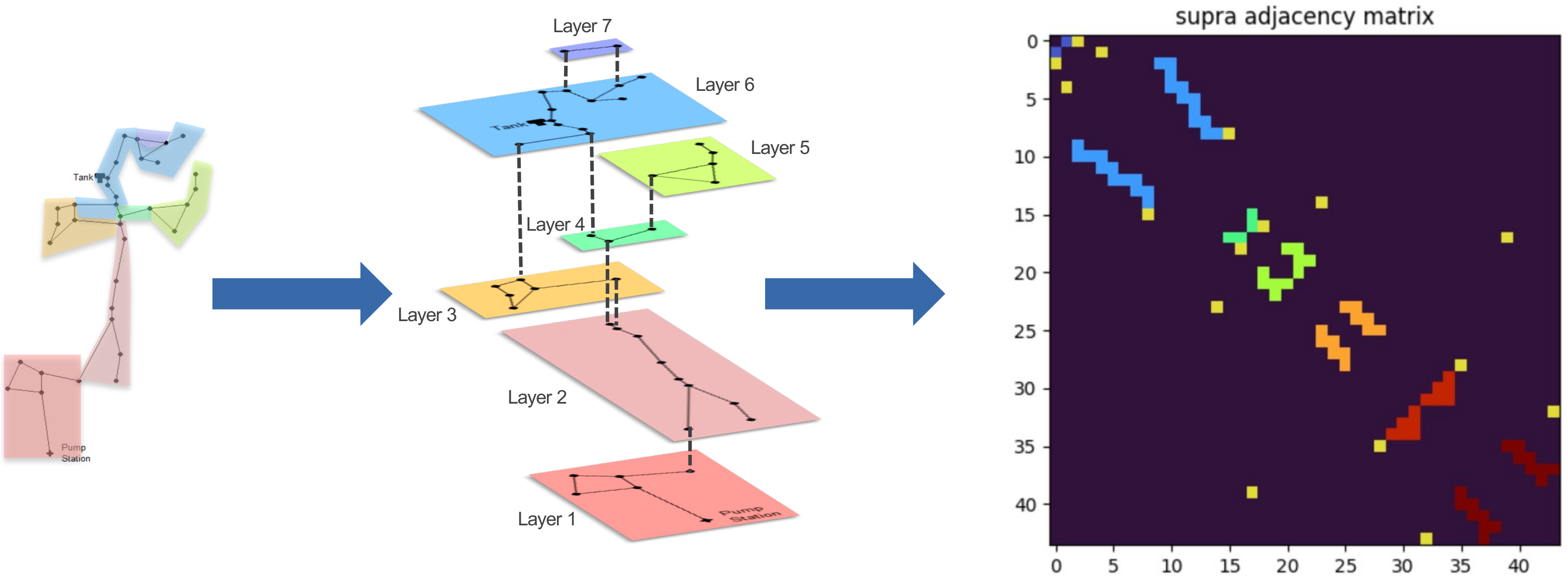
Example: Washington DC Water Network

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



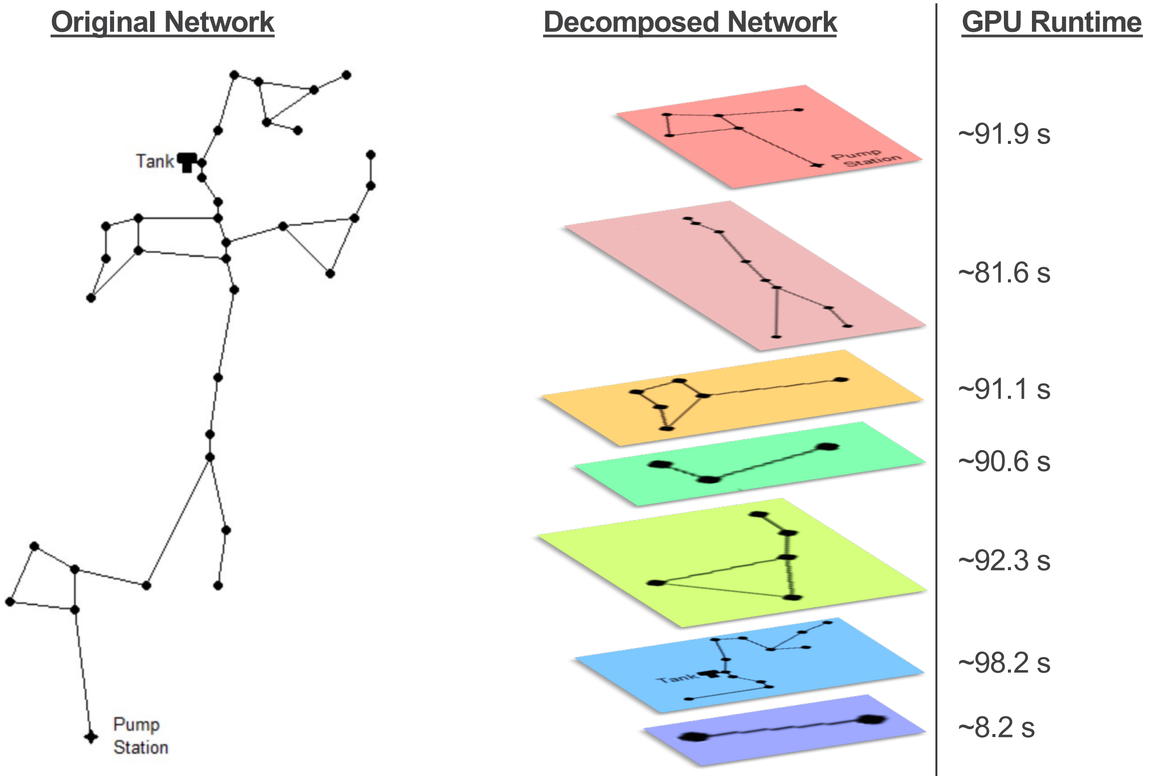
Transition to Networked Decomposition

Water Network Decomposition into Graph Layers



Transition to Networked Decomposition

Incremental Learning of Network / Graph Zones

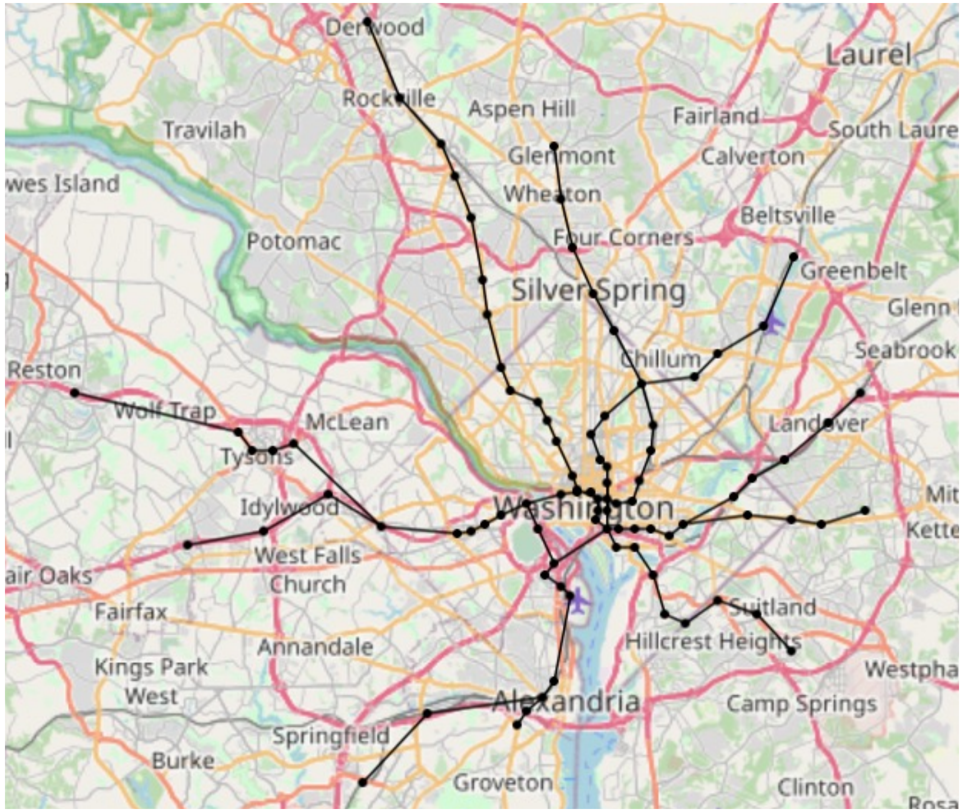


Accelerated Learning

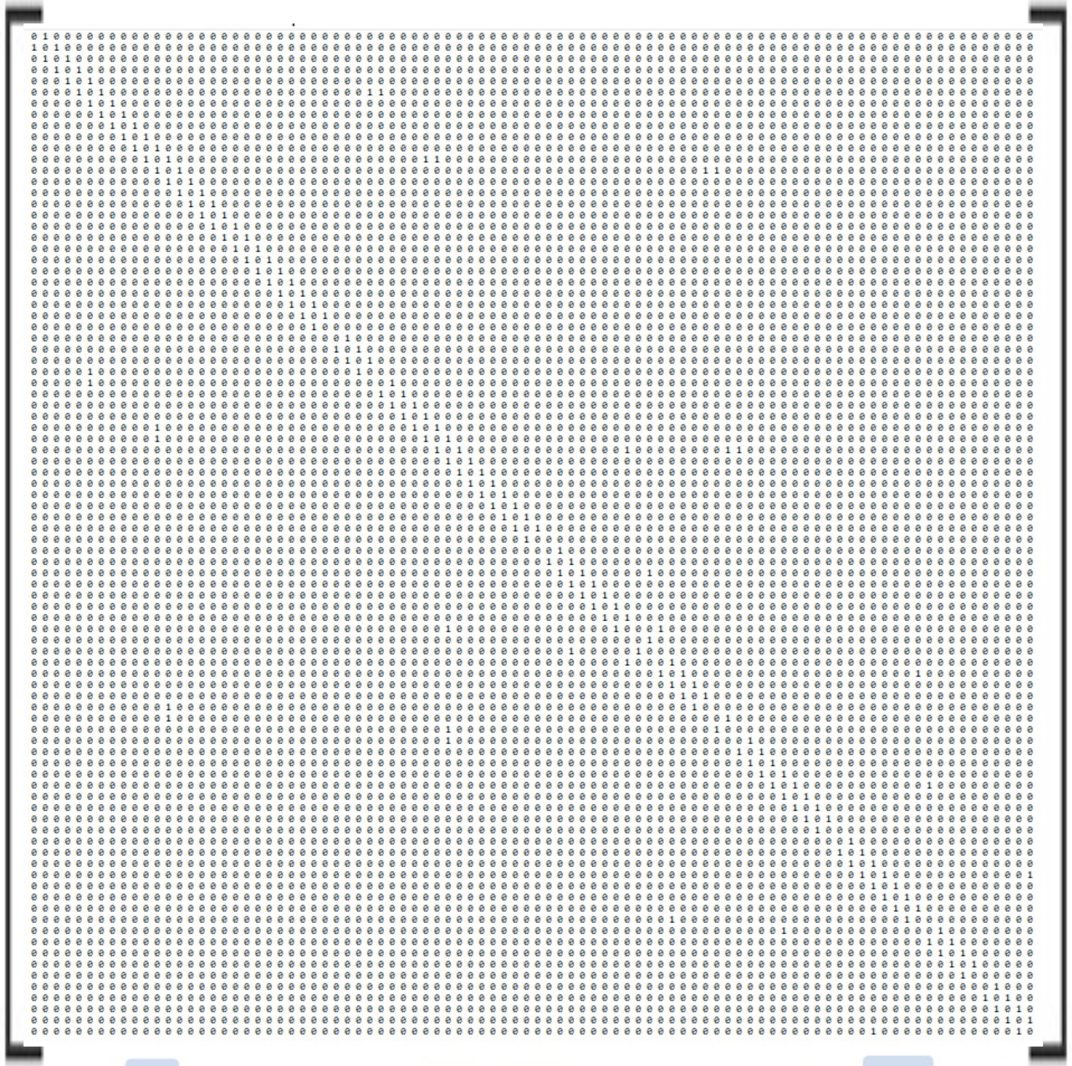
Total GPU Runtime = 2935.4 s **Total GPU Runtime = 553.9 s**

Transition to Networked Decomposition

Washington DC Metro System Network

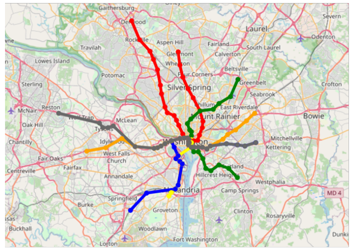


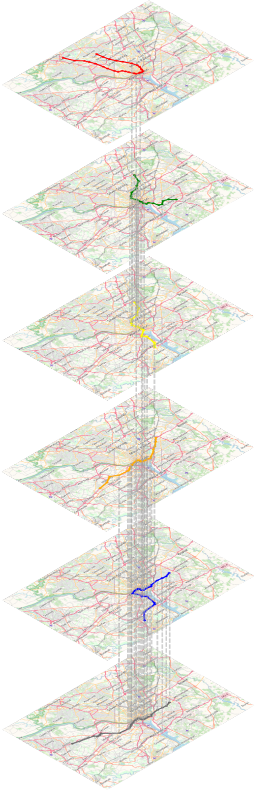
A =

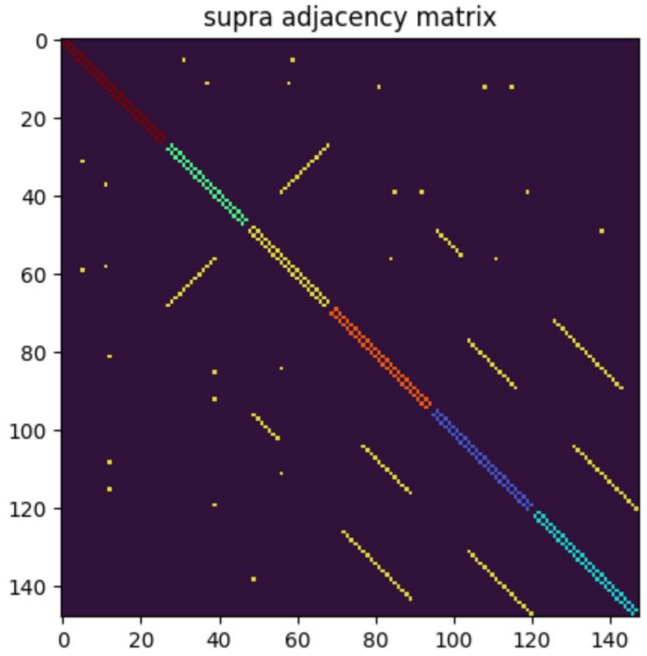


Transition to Networked Decomposition

Washington DC Metro System Network



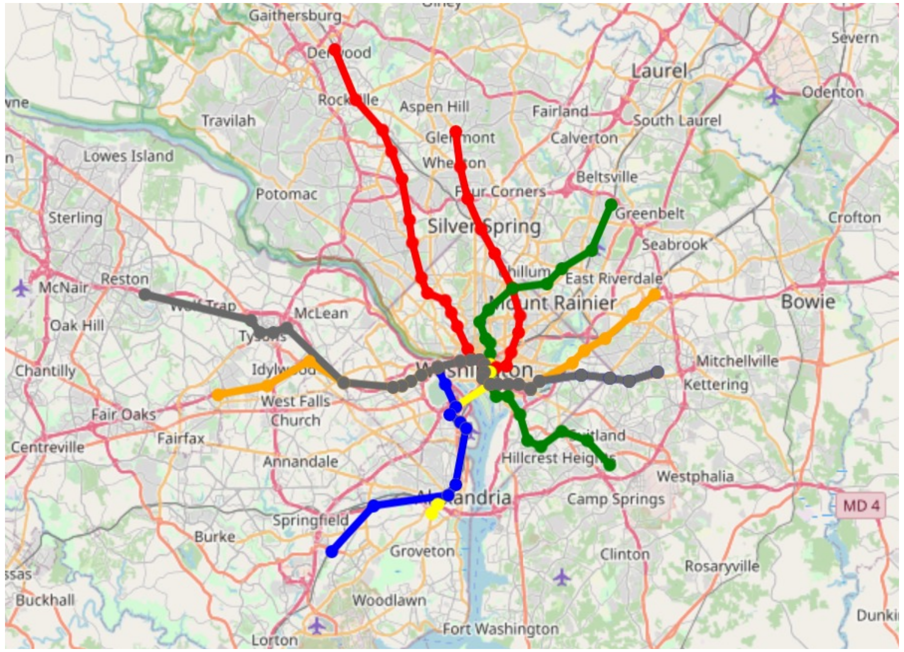




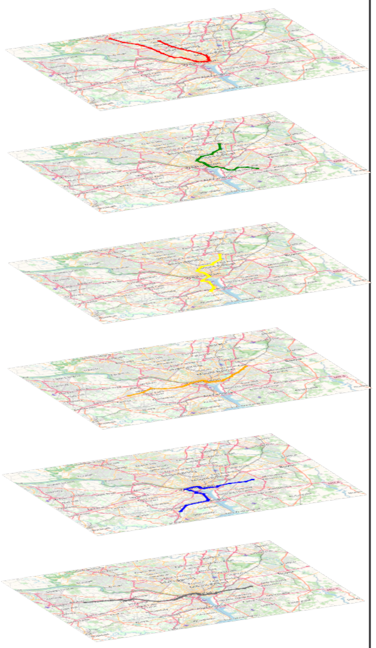
Transition to Networked Decomposition

Accelerated Learning of Network / Graph Zones

Original Network



Decomposed Network



GPU Runtime

~115.03 s

~97.26 s

~98.33 s

~102.95 s

~102.86 s

~101.12 s

Total GPU Runtime = 25582.10 s

Total GPU Runtime = 617.55 s

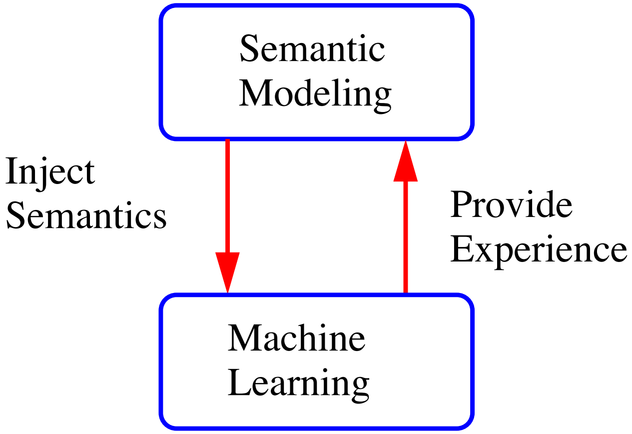
Results and Future Work

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.



Thank You

Questions?

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