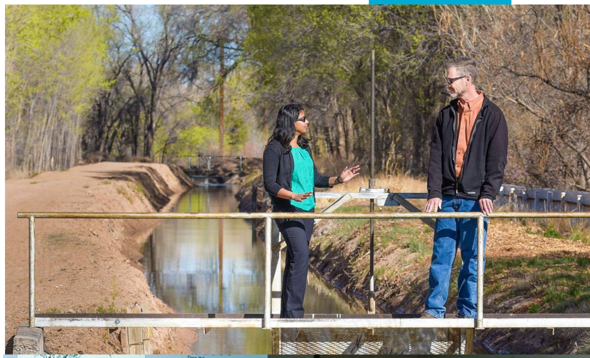
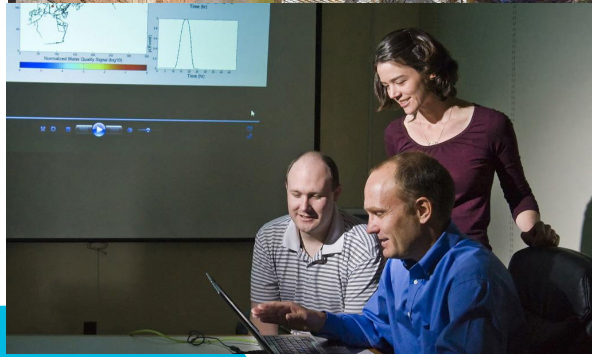
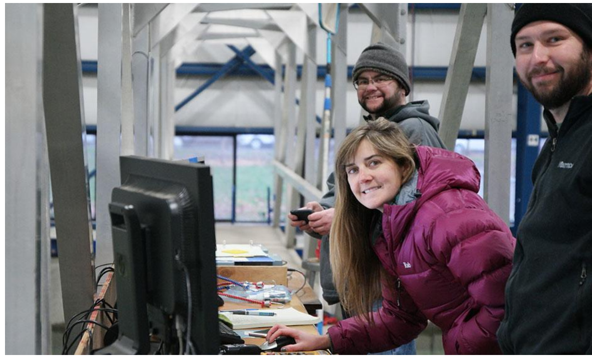
Harnessing AI and ML to Advance Water Management

Thushara Gunda

December 2025







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U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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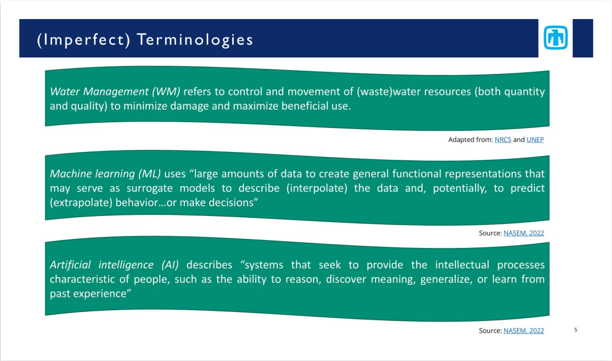
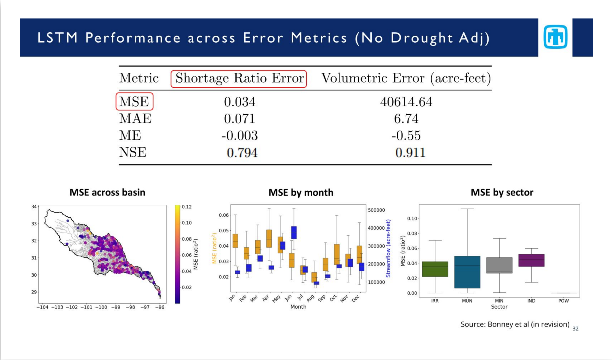
Outline



Background



Project Highlights

Looking Ahead

Background

(Imperfect) Terminologies

Water Management (WM) refers to control and movement of (waste)water resources (both quantity and quality) to minimize damage and maximize beneficial use.

Adapted from: NRCS and UNEP

Machine learning (ML) uses "large amounts of data to create general functional representations that may serve as surrogate models to describe (interpolate) the data and, potentially, to predict (extrapolate) behavior…or make decisions"

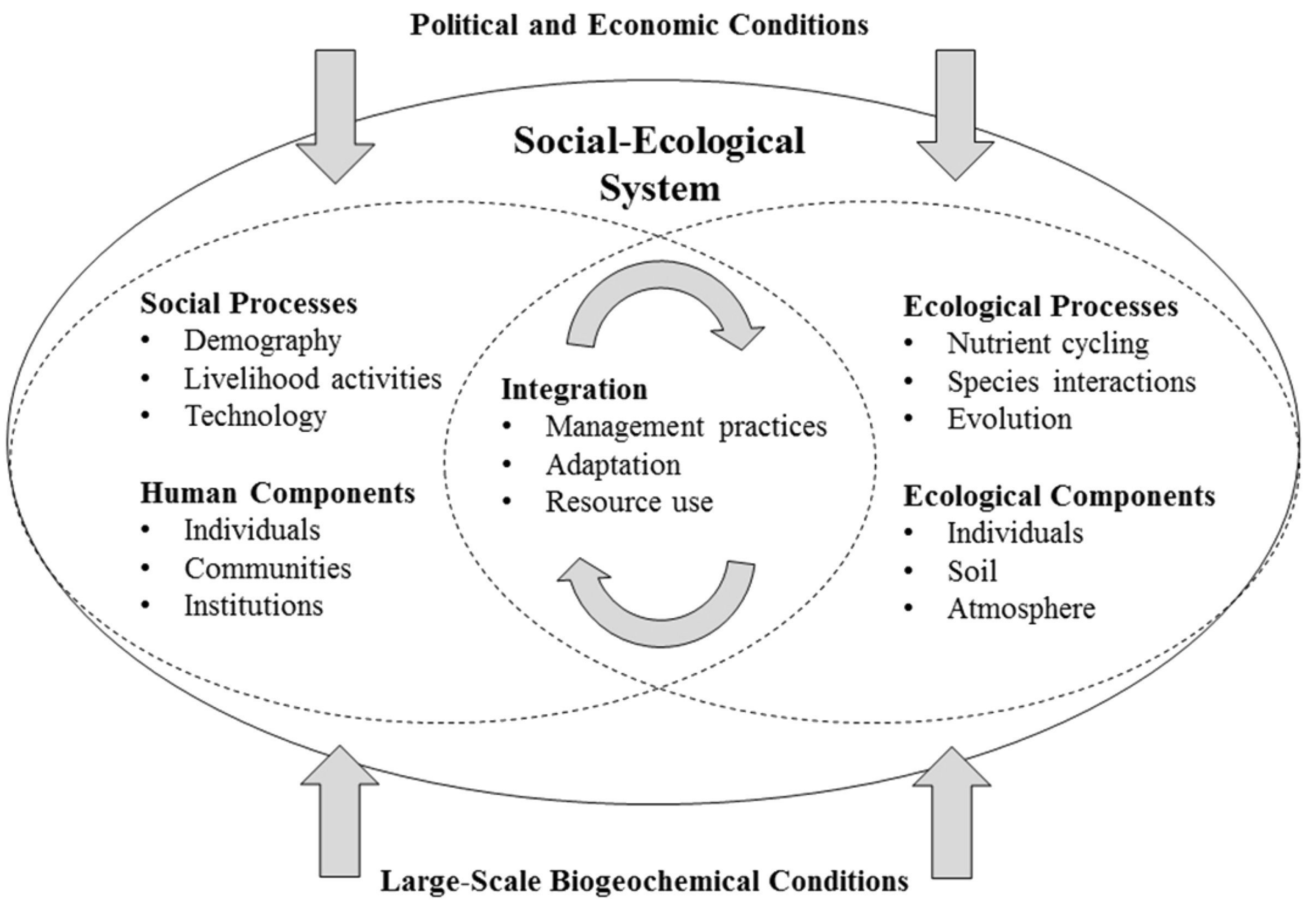
Source: NASEM, 2022

Artificial intelligence (AI) describes "systems that seek to provide the intellectual processes characteristic of people, such as the ability to reason, discover meaning, generalize, or learn from past experience"

Source: NASEM, 2022

Water Interactions with Human Systems

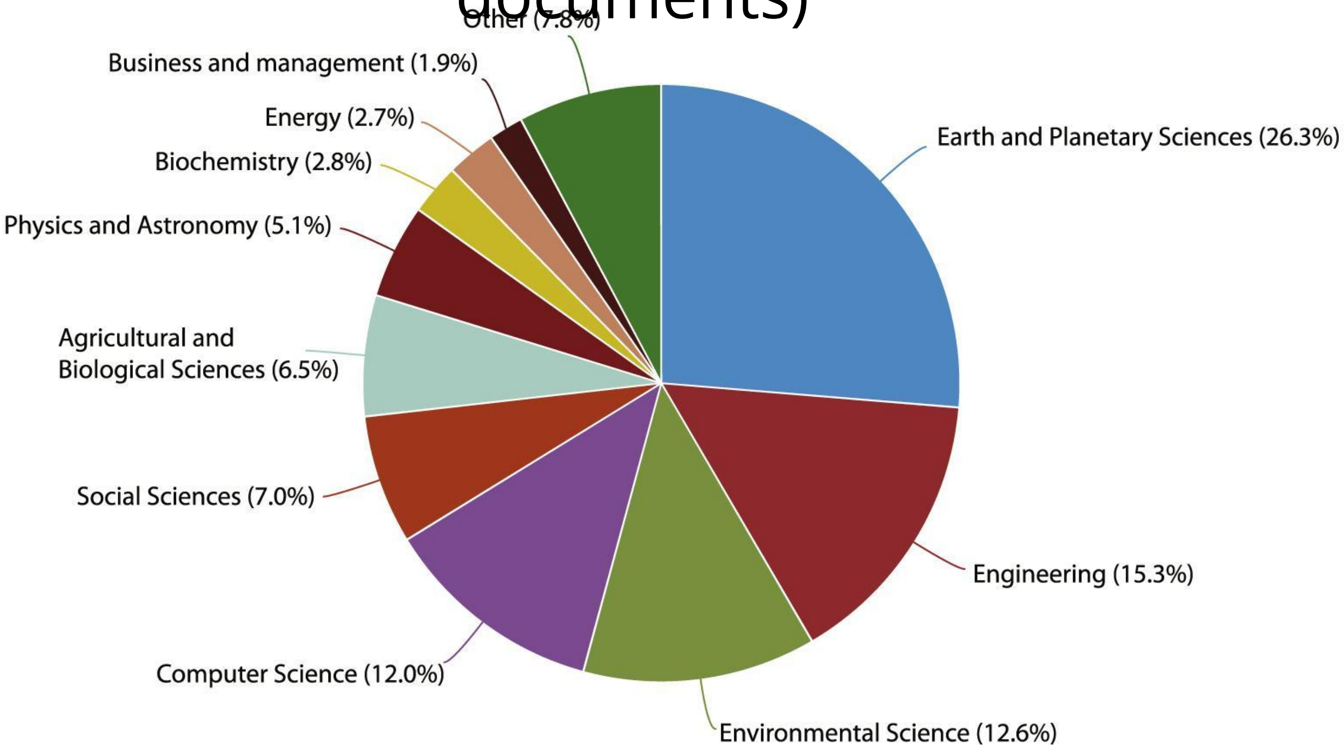
- Water activities are heavily influenced by management activities across sectors and scales
- Numerous scales are of interest, including:
  - International
  - National
  - Regional
  - Local
- Nature of interactions are driven by various factors, including:
  - Existing contracts/agreements
  - Built infrastructure
  - Social capacity and resources
  - Market dynamics
  - Weather risk(s)



Source: Virapongse et al., 2016

AI/ML in Water Management Spans Multiple Domains

Subject Areas (2,227 documents)



Source: Sun & Scanlon, 2019

Water Science and Technology Board Fall Meeting 2025: Frontier Applications of AI and Water Management

AI for Water Infrastructure Management

- *AI is Enabling a New Science of Real-time Hydrology*
  Matt Bartos, University of Texas, Austin
- *From Data to Decisions: Advancing and Adopting Real-Time Digital Twins in Smart Water Networks*
  Luis Montestruque, HydroDigital

AI for Wastewater Treatment and Resource Recovery

- *Emerging Challenges and Research Frontiers for Artificial Intelligence in Water and Wastewater Treatment*
  Kate Newhart, Oregon State University
- *Applied AI at HRSD: Achievements, Challenges, and the Road Ahead*
  Jeff Sparks, Hampton Roads Sanitation District

The Art of the Possible for AI and Water Management

- *Democratizing Knowledge, Automating Work, Expanding What is Possible: Recent Observations and New Directions in AI for Water Resources*
  Marcus Quigley, Environmental Financial Consulting Group

Source: NASEM WTSB, 2025

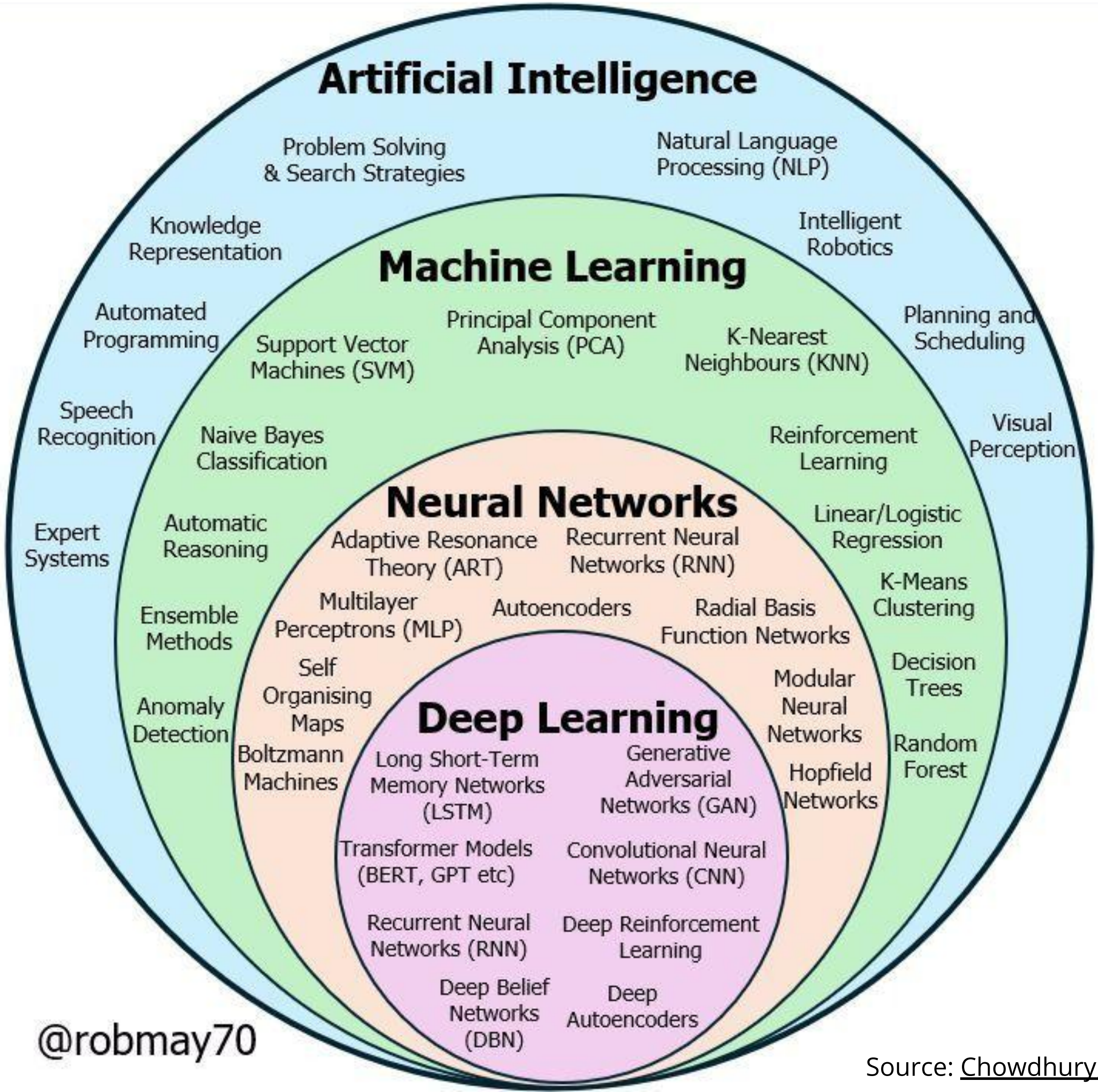
Central Role of Water for Critical Infrastructures

SUPPORTING SECTOR

SECTOR OF INTEREST																
Chemical			●				●	●					●	●	●	●
Commercial Facilities			●				●	●	●	●			●		●	●
Communications				●				●					●		●	●
Critical Manufacturing	●		●					●					●	●	●	●
Dams			●					●					●		●	●
Defense Industrial Base	●		●				●	●					●	●	●	●
Emergency Services			●					●				●	●		●	●
Energy	●		●	●	●								●	●	●	●
Financial Services			●					●					●		●	●
Food and Agriculture	●		●		●			●	●			●	●		●	●
Government Facilities			●				●	●					●		●	●
Healthcare and Public Health	●		●				●	●		●			●	●	●	●
Information Technology			●					●							●	●
Nuclear Reactors, Materials and Waste			●				●	●					●		●	●
Transportation Systems	●		●	●	●		●	●	●				●			●
Water and Wastewater Systems	●		●		●			●					●		●	

Source: DHS CISA

Project Overviews



Source: Chowdhury, 2025

Project #1: NLP, Clustering

Water narratives

Project #2: LSTMs

Water allocations

Project Highlight: Water Narratives

Motivation: Water Narratives

- Understand how we communicate about water as a resource
  - Drinking water, energy production, natural disasters, farming, scarcity, etc.
- Newspapers as a social scientific data source
  - Data is abundant and often free
  - Local, regional, and national
  - Agenda setting effects
  - Reflect community interests
  - Content broadly distributed online

Local

CHANGING LIVES

New pantry chief looks to serve, 2L

SUNDAY, AUGUST 6, 2017 • SECTION L

WATER POLLUTANTS FOUND

Report: 5 North Jersey systems have contaminants

KATIE SOBKO
STAFF WRITER, @KATESOBKO

A report released recently by an environmental group revealed several towns throughout North Jersey – Lyndhurst, Elmwood Park, Garfield, Wallington and Bloomfield – had harmful pollutants in their water supply.

Although all but Elmwood Park and Bloomfield tested within the national guidelines for contaminants, Environmental Working Group reported Lyndhurst, Garfield and Wallington tested higher than the group's suggested health guideline, which could put residents at a higher risk for cancer, developmental issues in children, problems in pregnancy and other serious health conditions.

Elmwood Park tested above the legal limit for trihalomethanes, which are used in industry as solvents or refrigerants. The federal limit for trihalomethane in water is 80 parts per billion, with Environmental Working Group suggesting .8 parts per billion would be the necessary level for healthy water. Elmwood Park's level was 83 ppb.

Tests that look for more than 80 contaminants in drinking water are conducted regularly by the U.S. Environmental Protection Agency. Environmental Working Group used the EPA testing data from 2010 to 2015 for the entire country to compile a database. The American Water Works Association and more than 200 water utilities reviewed the testing and violation data and either verified the accuracy of the data or pro-

See WATER, Page 7L

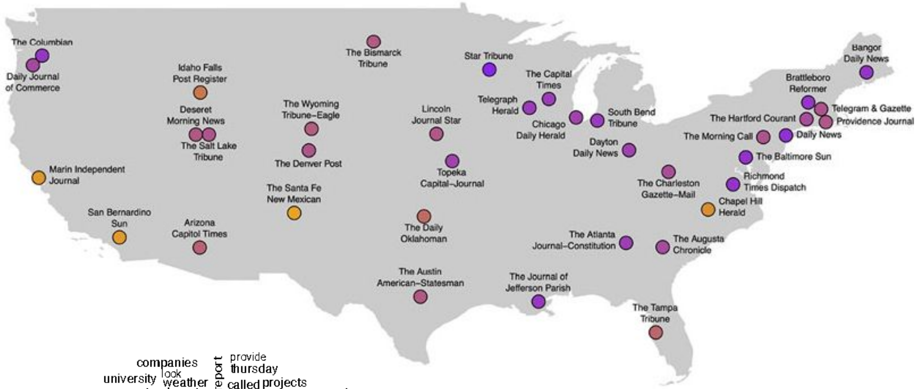
FILE PHOTO

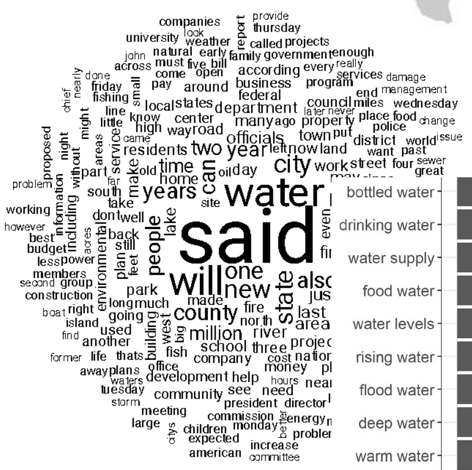
The report named Lyndhurst, Elmwood Park, Garfield, Wallington and Bloomfield.

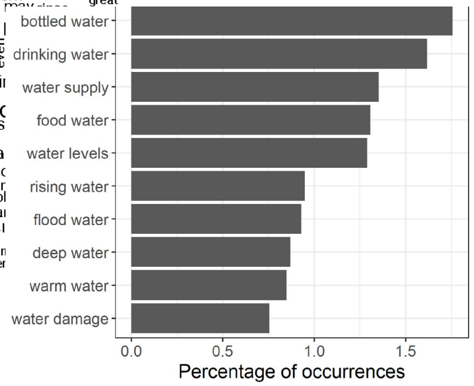
Source: North Jersey

Analysis Workflow

Data Collection → Pre-Processin g → Analysis







- U.S. Newspaper corpus scraped from LexisNexis databases using the keyword ”water”
- N = 1.8 million articles published between September 11th, 1990 and December 15th, 2017 (37 local/regional newspapers from 34 different states represented
- Metadata: Title, author, date published, source, section

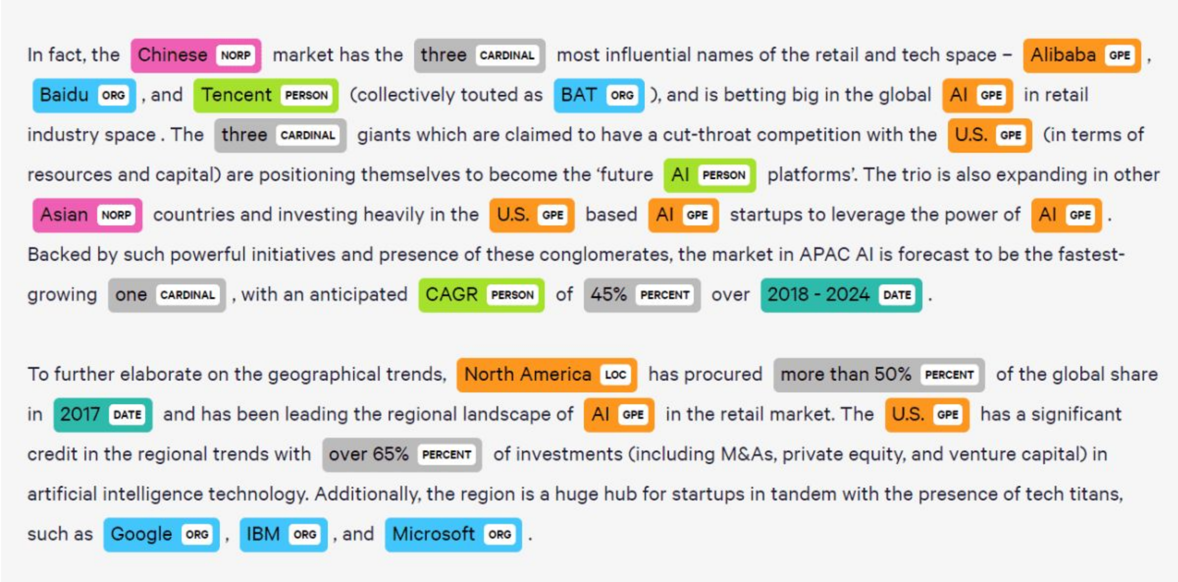
- Parsed html content, removed punctuation, lower cased, etc.
- Reviewed content for relevance for water resources (e.g., “troubled waters in congress”, “body found in the water”)
- Filtered corpus to relevant content using a combination of structural topic modeling (STM) and cluster analysis prior to pattern analysis
- Implemented STM using R-package (Roberts et al., 2019)

Source: Sweitzer et al., 2023

Natural Language Processing

- Leverages computers' ability to process human language
  - Derived from content analytic methods in the social sciences
  - Describe and make inferences about the characteristics of communication
- Underlying algorithms can be rule-based or machine/deep learning based (e.g., transformer models)

Example of Entity Extraction

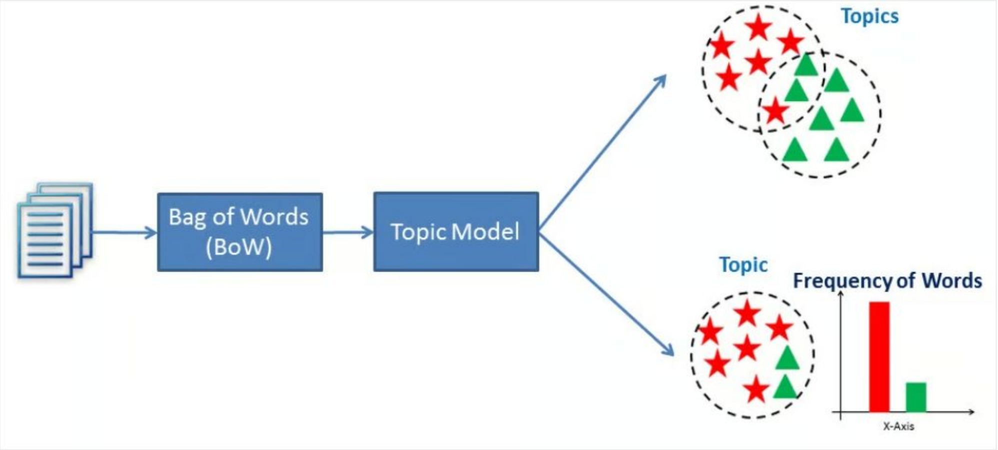


Source: Meena Vyas

Project objective: leverage NLP computational tools for analyzing a large body (corpus) of text data

Topic Modeling

- Topic models are used to describe the content of groups of documents from a larger corpus. Two common approaches:
  - Latent Dirichlet Allocation (Chauhan & Shah, 2021)
  - Structural Topic Model (Roberts et al. 2014)
- STMs enable specification of topic covariates in the form of document metadata
  - Documents which have similar covariates will tend to talk about the same topics
  - Documents which have similar covariates will tend to talk about topics in the same way
- Groups documents together into topics based on FREX words: FRequently occur in a group of documents that are EXclusive to that group of documents



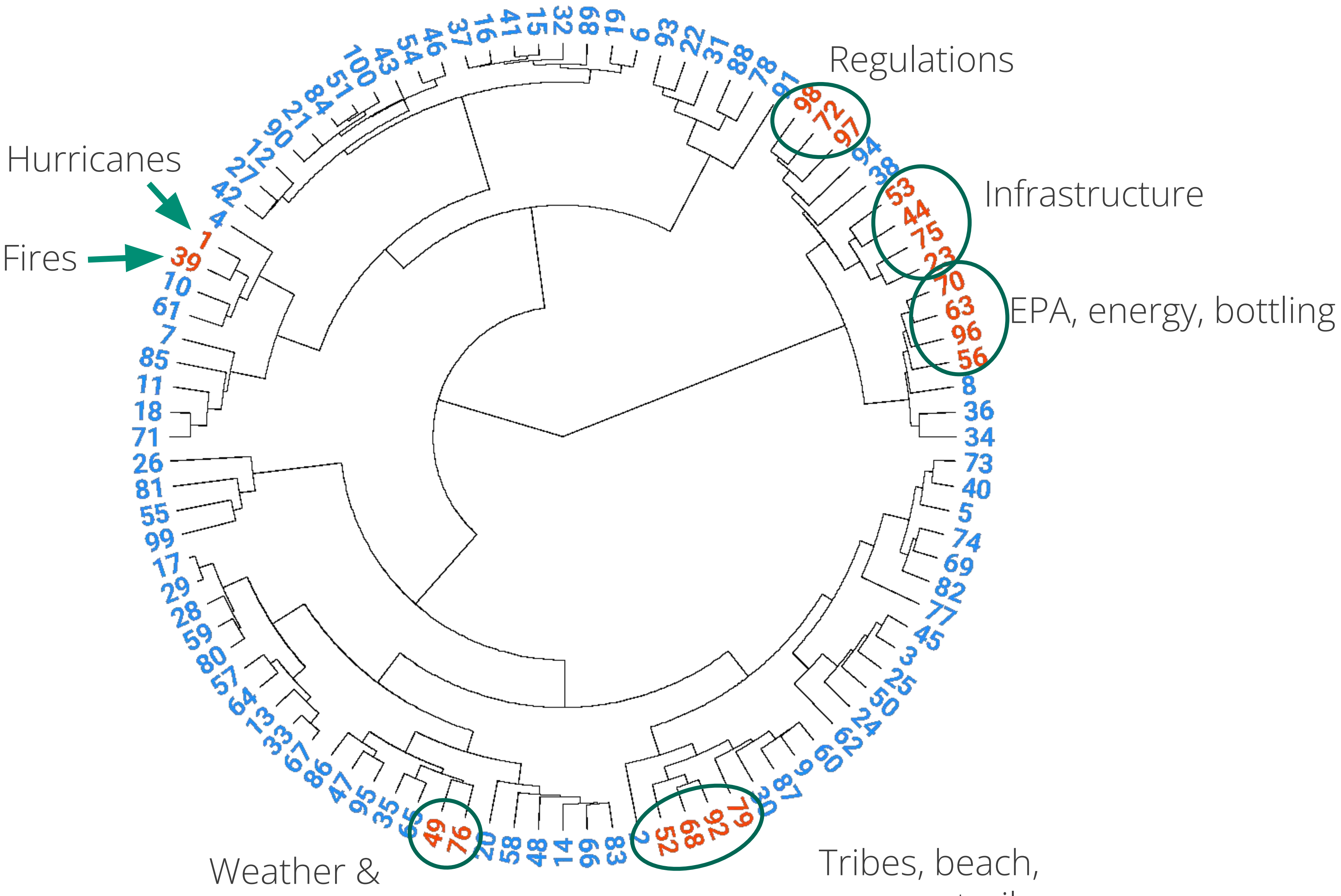
Source: Datacamp

Topic Labeling: Analyst-Driven

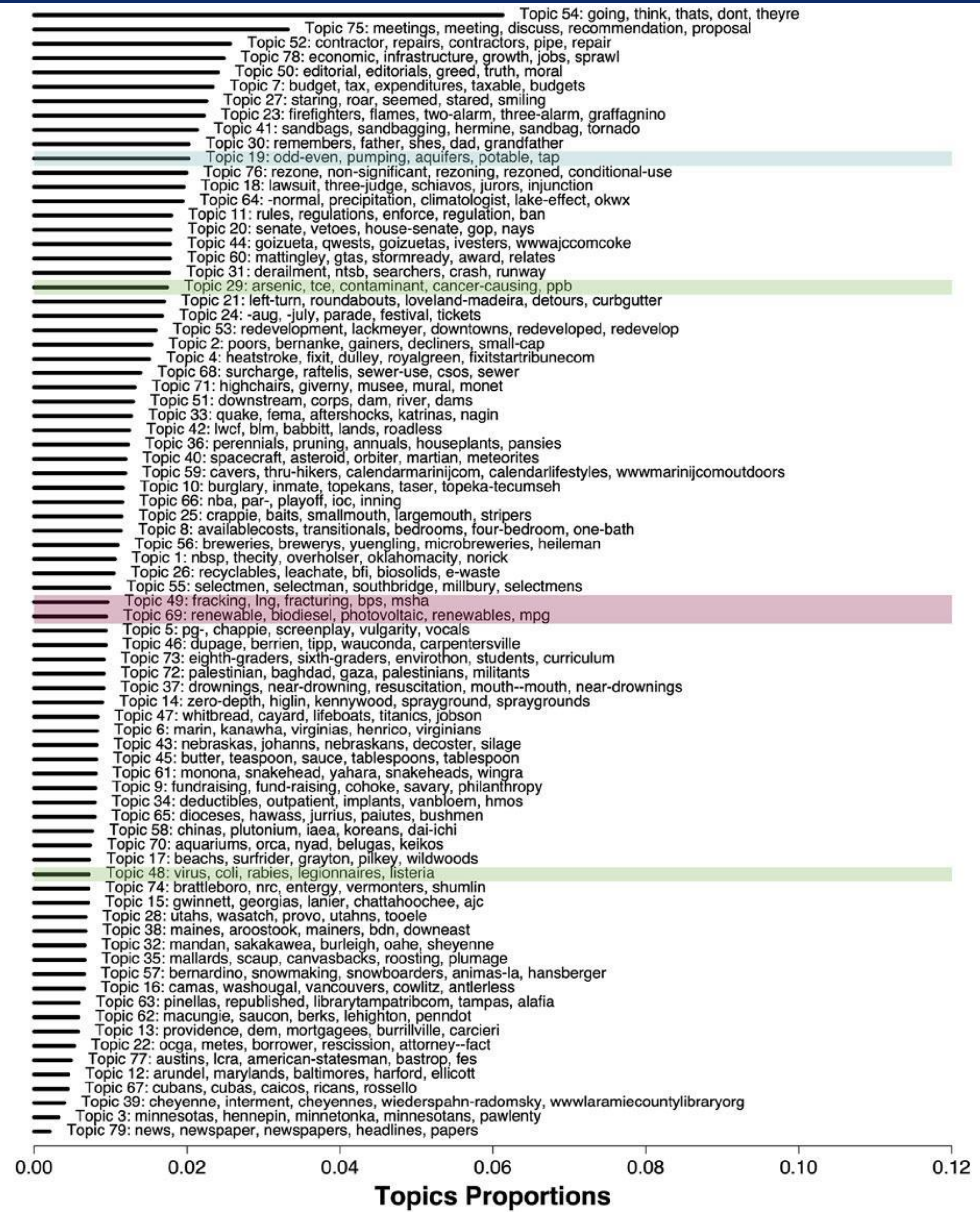
- Analysts interpret FREX words to derive meaning from the document classifications
- Manual process that benefits from domain knowledge

Topic Number	Highest Probability	FREX	Analyst Label
Topic 1	storm, flood, people, hurricane, emergency, damage, flooding	fema, katrinas, nagin, femas, storm-related, tacloban, west-northwest	Hurricanes
Topic 39	fire, said, firefighters, department, smoke, building, chief	firefighters, two-alarm, water-dropping, lightning-caused, fireworks-related, flashover, six-alarm	Fires

Initial STM: Identify Relevant Topics for Filtering



Water Resources Topics



Drinking water

pumping
aquifers
potable
tap

Contaminants

arsenic
tce
Cancer-causing
PPB

Energy Production

Fracking
Fracturing
Biodiesel
Photovoltaic

Infrastructure

pumping
dams
septic
budget

Extreme Weather

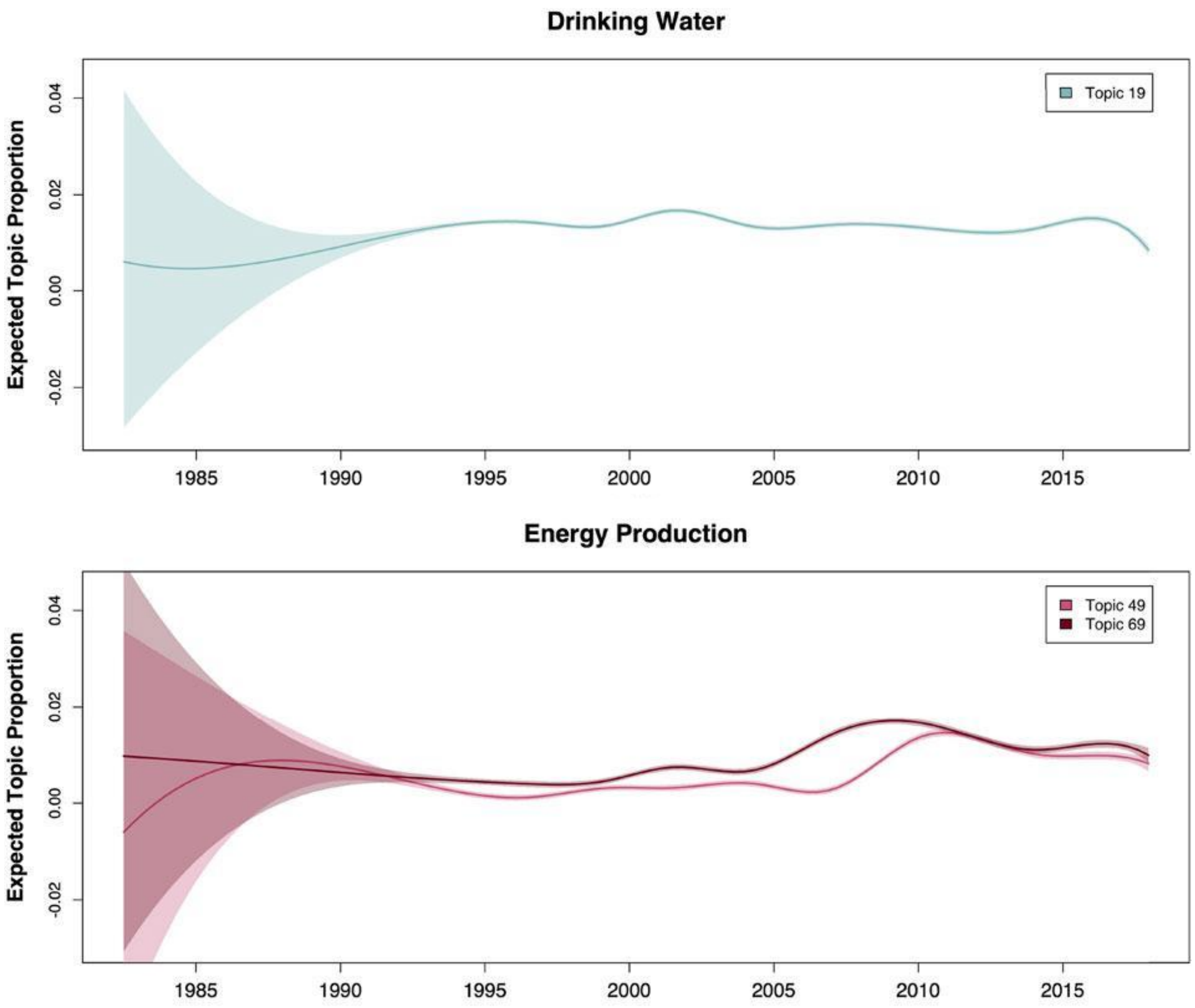
ice
snow
firefighting
tornado

…

aquariums
beach
snowmaking
garden

Source: Sweitzer et al., 2023

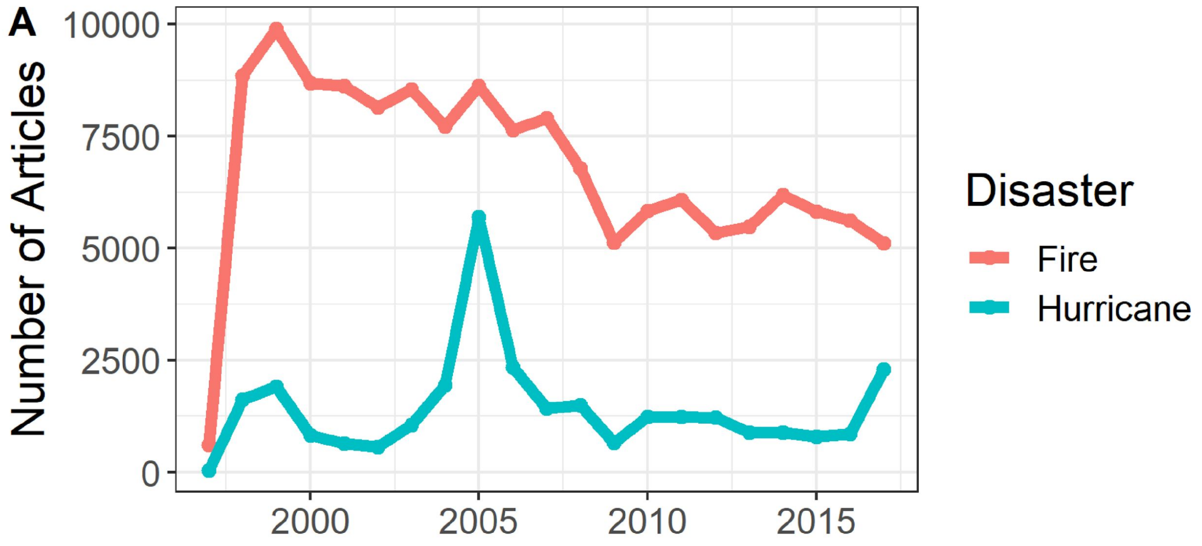
Conversations Vary over Time



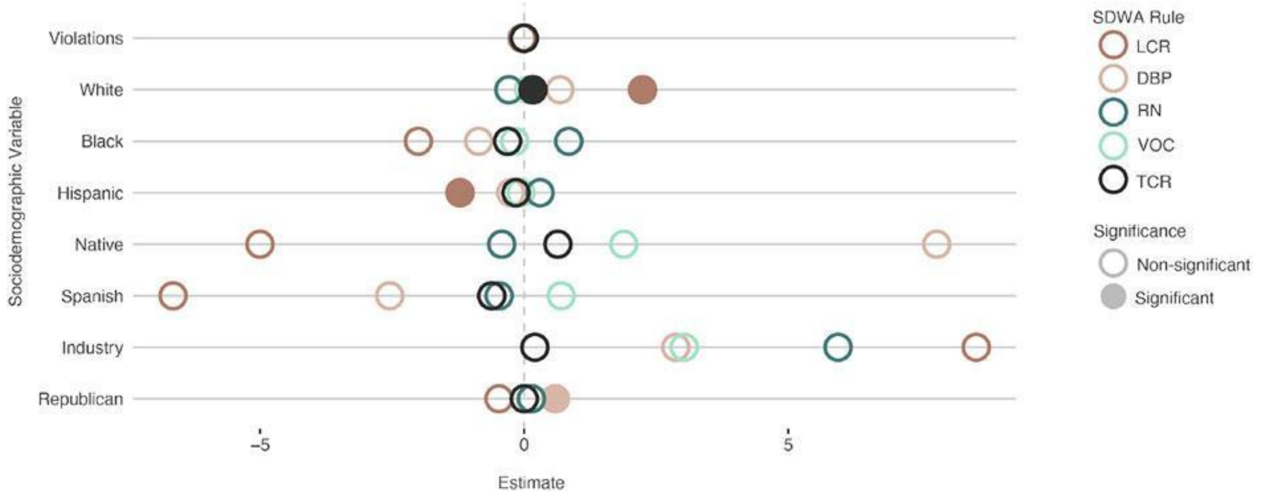
Source: Sweitzer et al., 2023

Narrative Differences

- Extreme weather events do not have similar coverage patterns
  - Diversity of drivers for "fires" vs. hurricanes
  - Population density varies in regions with prevalence
- Contaminant discussions did not correlate with observed violations
  - Generally, less discussion occurred in underserved regions
  - Associations with cultural, economic, and political factors varied



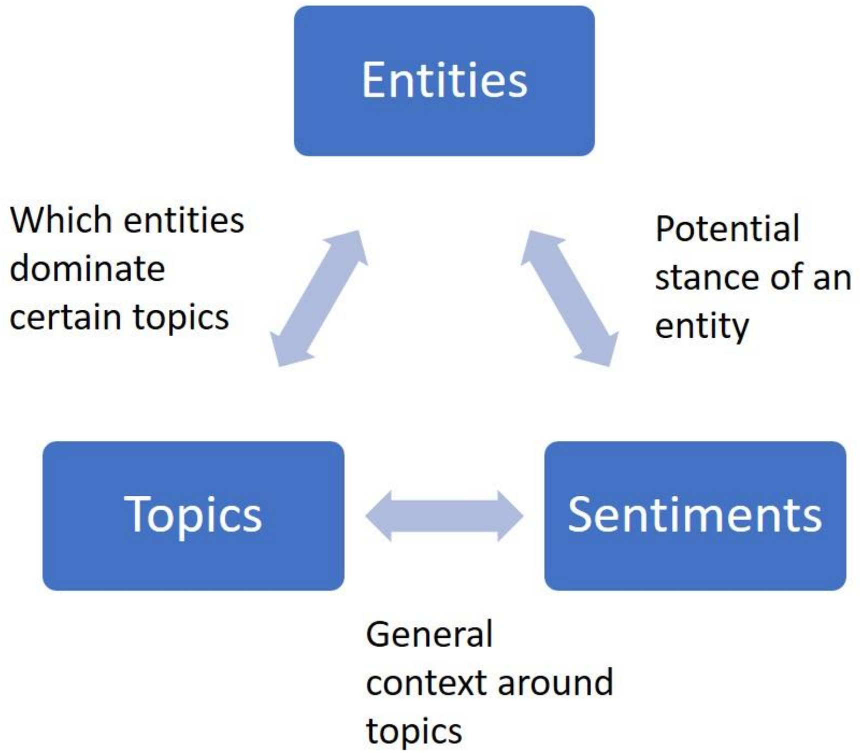
Sanchez et al., 2021



Caballero et al., 2022

NLP Reflections

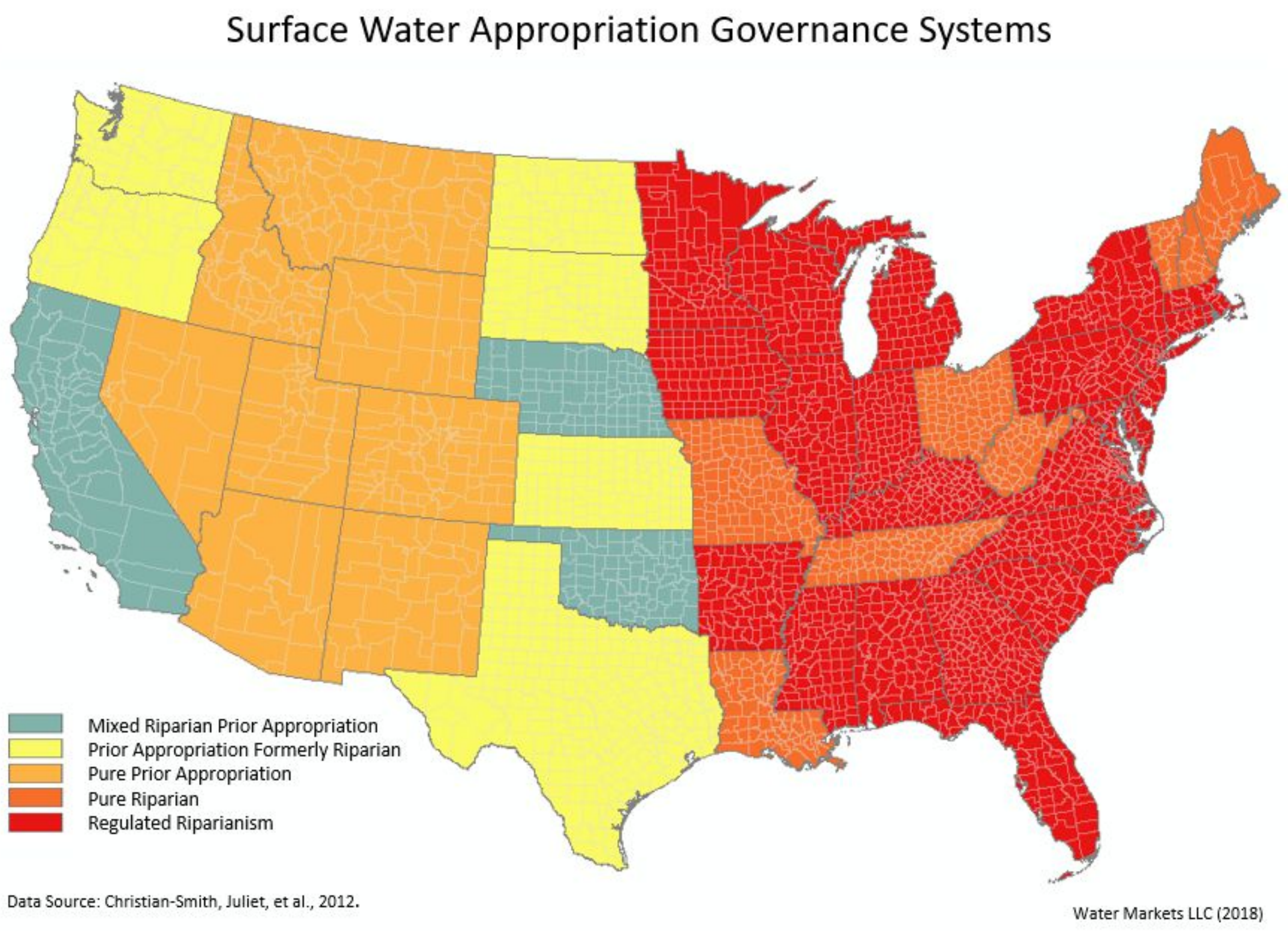
- Broadly applicable to text data in a variety of domains
  - Leverage computation to process large datasets
  - When linked to metadata (e.g., geospatial or temporal data), important associations can be found
  - Can also extract additional insights (entities, sentiments) as needed
- Multiple opportunities exist to integrate domain insights (e.g., qualitative methods) into analytical workflows
- Is impacted by data availability (i.e., sampling biases) that can make generalization tricky



Project Highlight: Water Allocations

Motivation: Water Rights

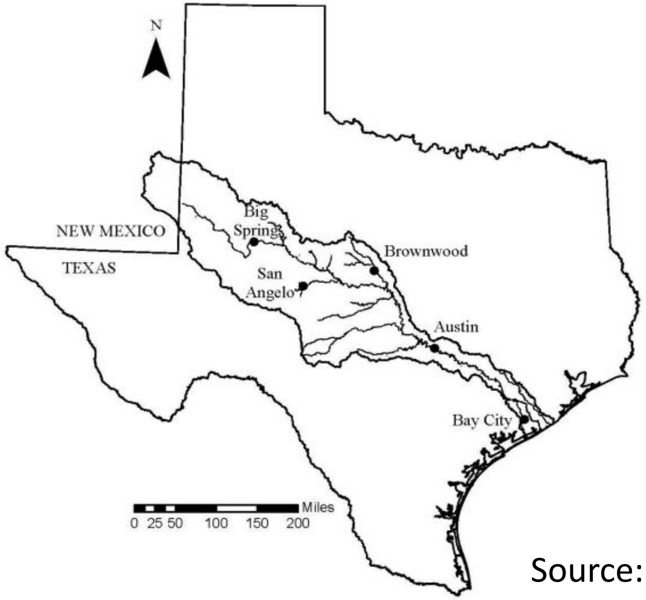
- Two dominant governance systems
  - Riparian Rights – Water rights align with land rights; if your land touches the water resources, then you have rights to it
  - Prior Appropriation – "first in time, first in right"
- Most states have either one or a mixed variation of these governance systems
- Focus is on surface water for this effort



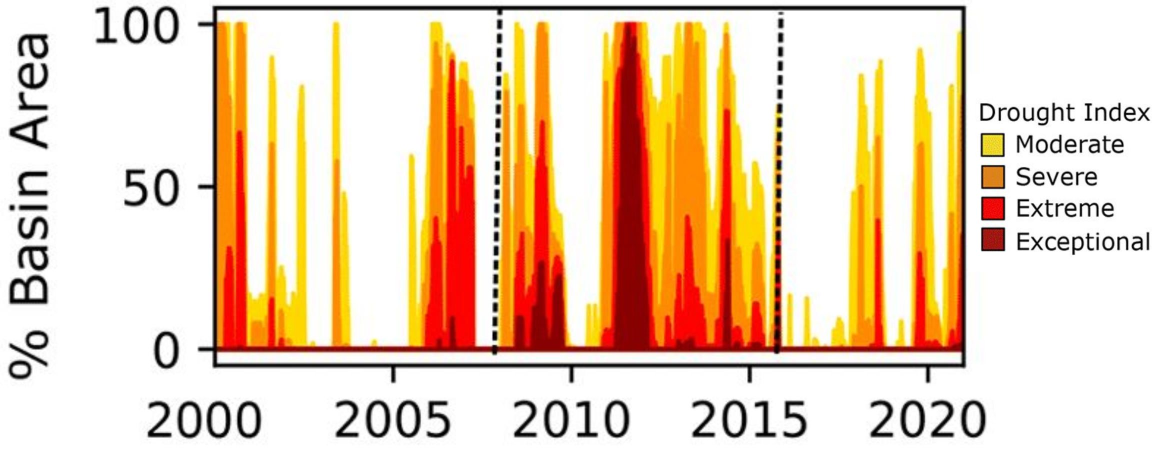
Source: Water Rights LLC

Case study: Colorado River Basin of Texas

- Single river basin within Texas
  - Second longest river within the state
  - Third largest basin by area
  - Sixth largest by average annual flow volumes
- Large portion of basin located in relatively arid regions
  - Downward trends in annual streamflow, mostly in the upper and middle basin regions
  - Multiple periods of drought in recent years

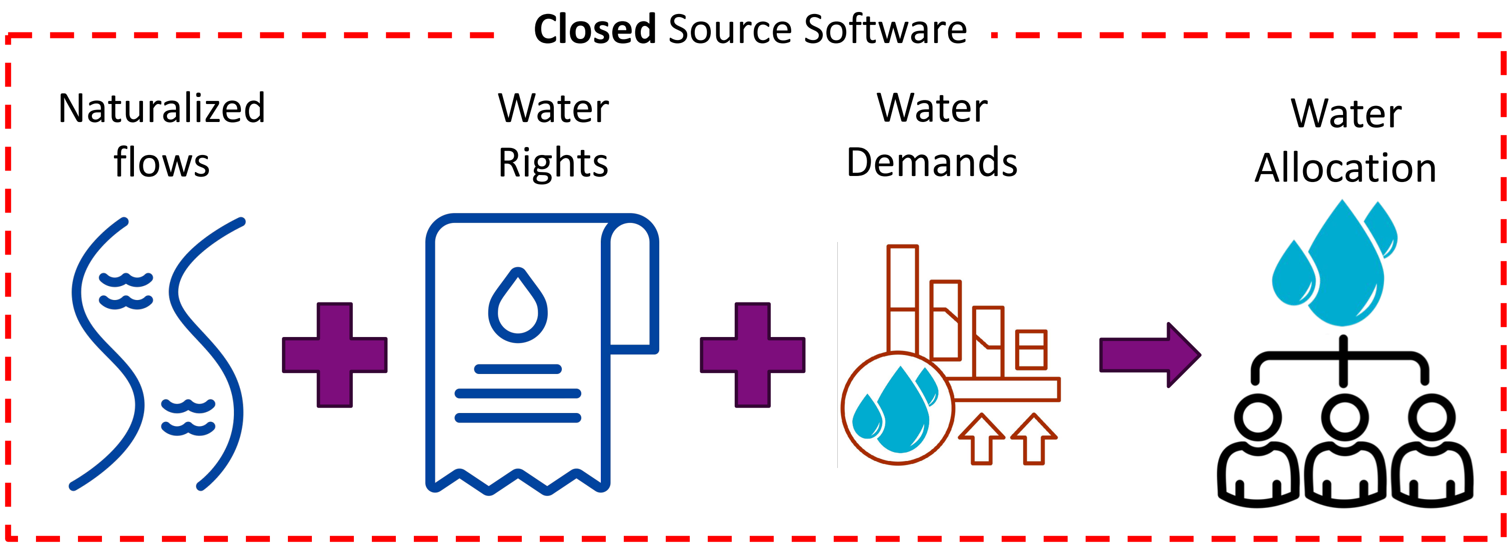


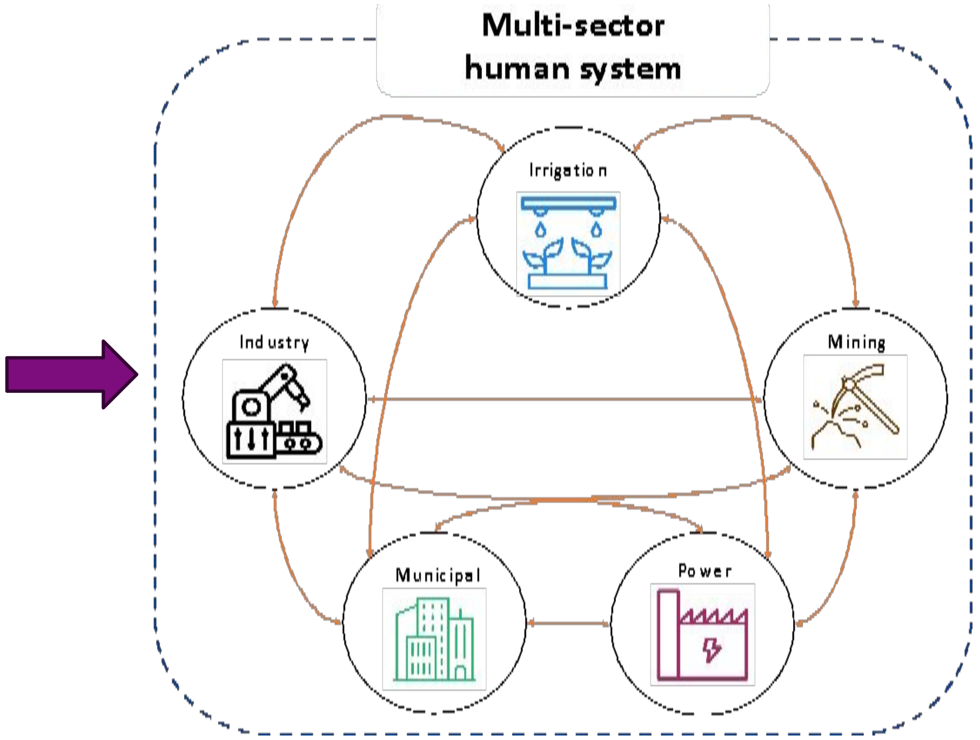
Source: WRAP



Source: Ferencz et al. (2024)

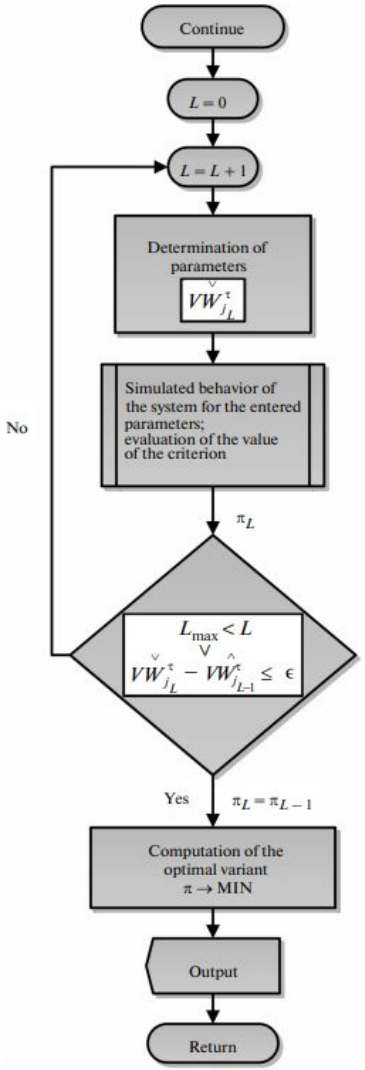
Current Water Allocations

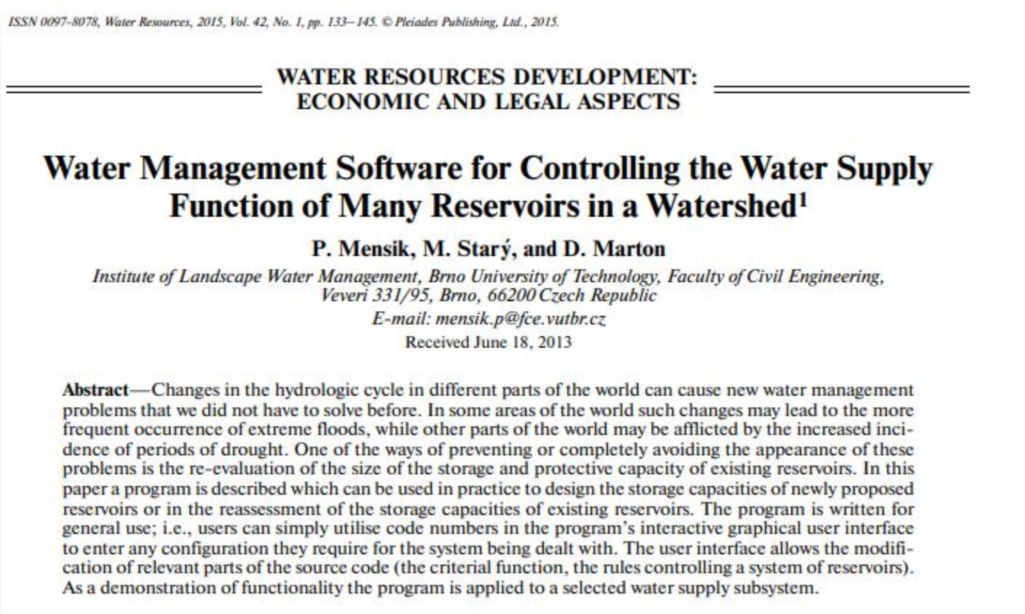




- Texas uses the closed source Water Rights Analysis Package (WRAP) for water management modeling
- WRAP is a closed source software since it's used to inform permitting activities
- Project objective: Implement an open source AI/ML-driven approach to develop insights into water allocations within the region

Water Allocation Algorithms





ISSN 0097-8078, Water Resources, 2015, Vol. 42, No. 1, pp. 133–145. © Pleiades Publishing, Ltd., 2015.

WATER RESOURCES DEVELOPMENT:
ECONOMIC AND LEGAL ASPECTS

Water Management Software for Controlling the Water Supply Function of Many Reservoirs in a Watershed[1]

P. Mensik, M. Starý, and D. Marton

Institute of Landscape Water Management, Brno University of Technology, Faculty of Civil Engineering, Veveri 331/95, Brno, 66200 Czech Republic
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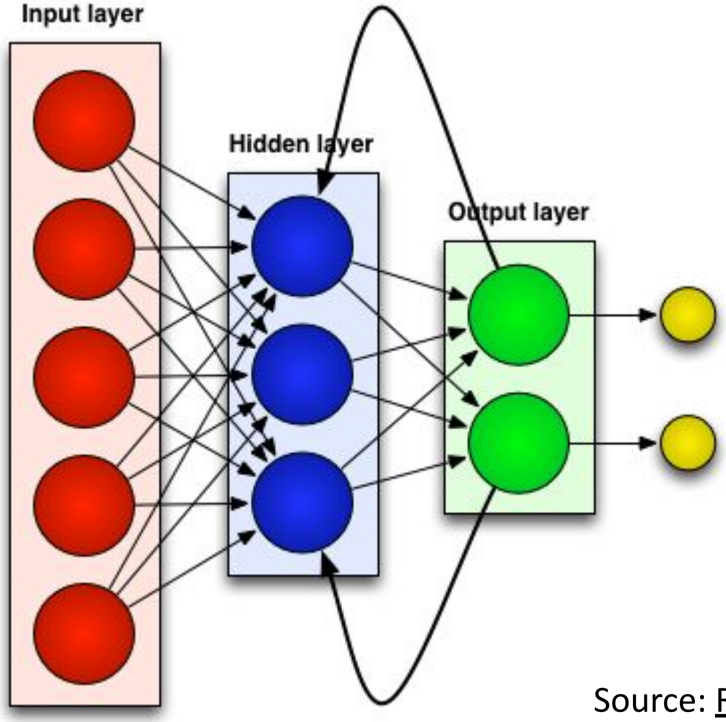
Received June 18, 2013

Abstract—Changes in the hydrologic cycle in different parts of the world can cause new water management problems that we did not have to solve before. In some areas of the world such changes may lead to the more frequent occurrence of extreme floods, while other parts of the world may be afflicted by the increased incidence of periods of drought. One of the ways of preventing or completely avoiding the appearance of these problems is the re-evaluation of the size of the storage and protective capacity of existing reservoirs. In this paper a program is described which can be used in practice to design the storage capacities of newly proposed reservoirs or in the reassessment of the storage capacities of existing reservoirs. The program is written for general use; i.e., users can simply utilise code numbers in the program's interactive graphical user interface to enter any configuration they require for the system being dealt with. The user interface allows the modification of relevant parts of the source code (the criterial function, the rules controlling a system of reservoirs). As a demonstration of functionality the program is applied to a selected water supply subsystem.

Source: Mensik et al., 2015



Source: Roell

Current methods for approaching water management largely rely on network optimization techniques

See opportunities for re-envisioning use of neutral network type approach

Numerous questions remain:

- How do we effectively train the model?
- What are our "metrics of success"?

Analytical Workflow

Synthetic Streamflow Generation → WRAP Executions → LSTM Development → Performance Assessment

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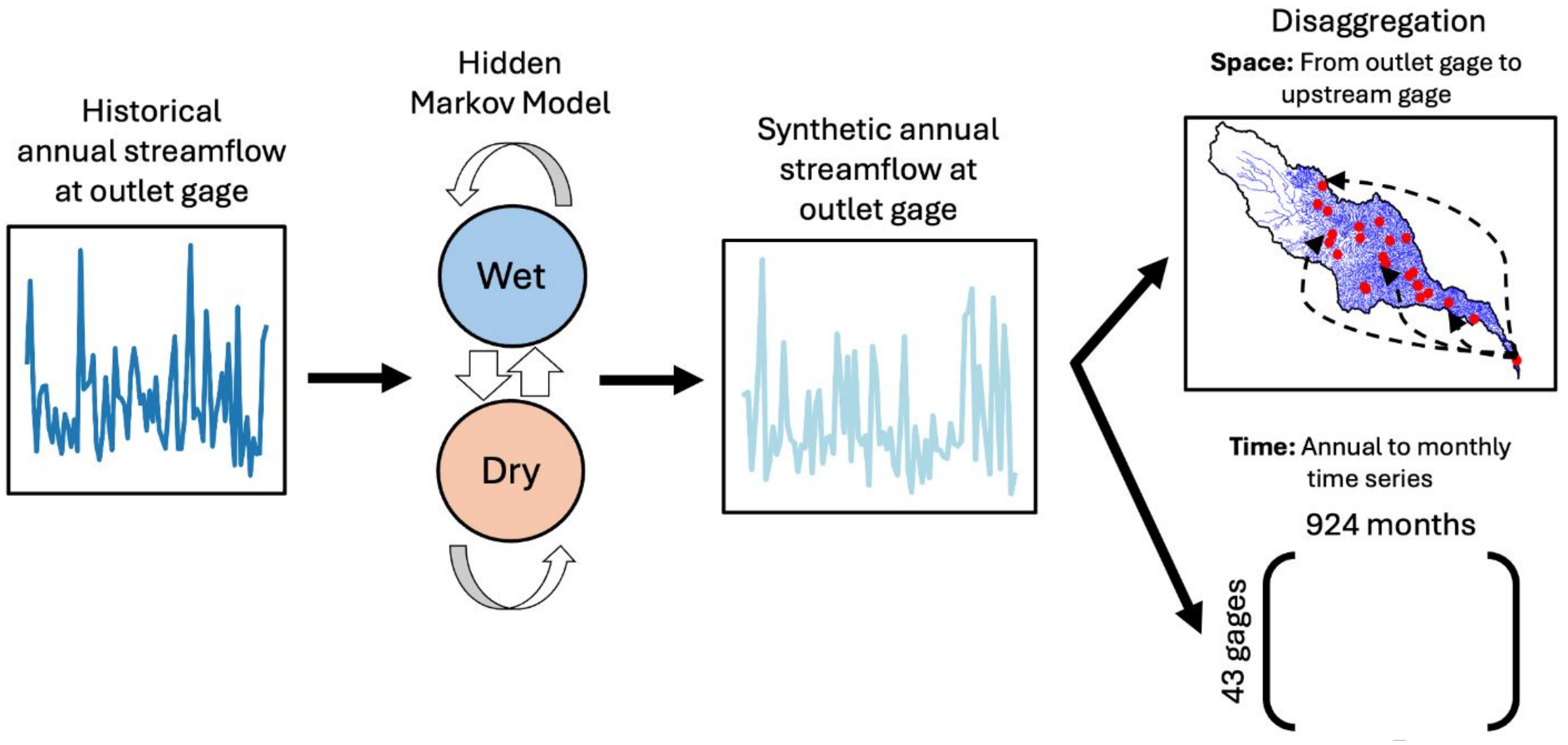
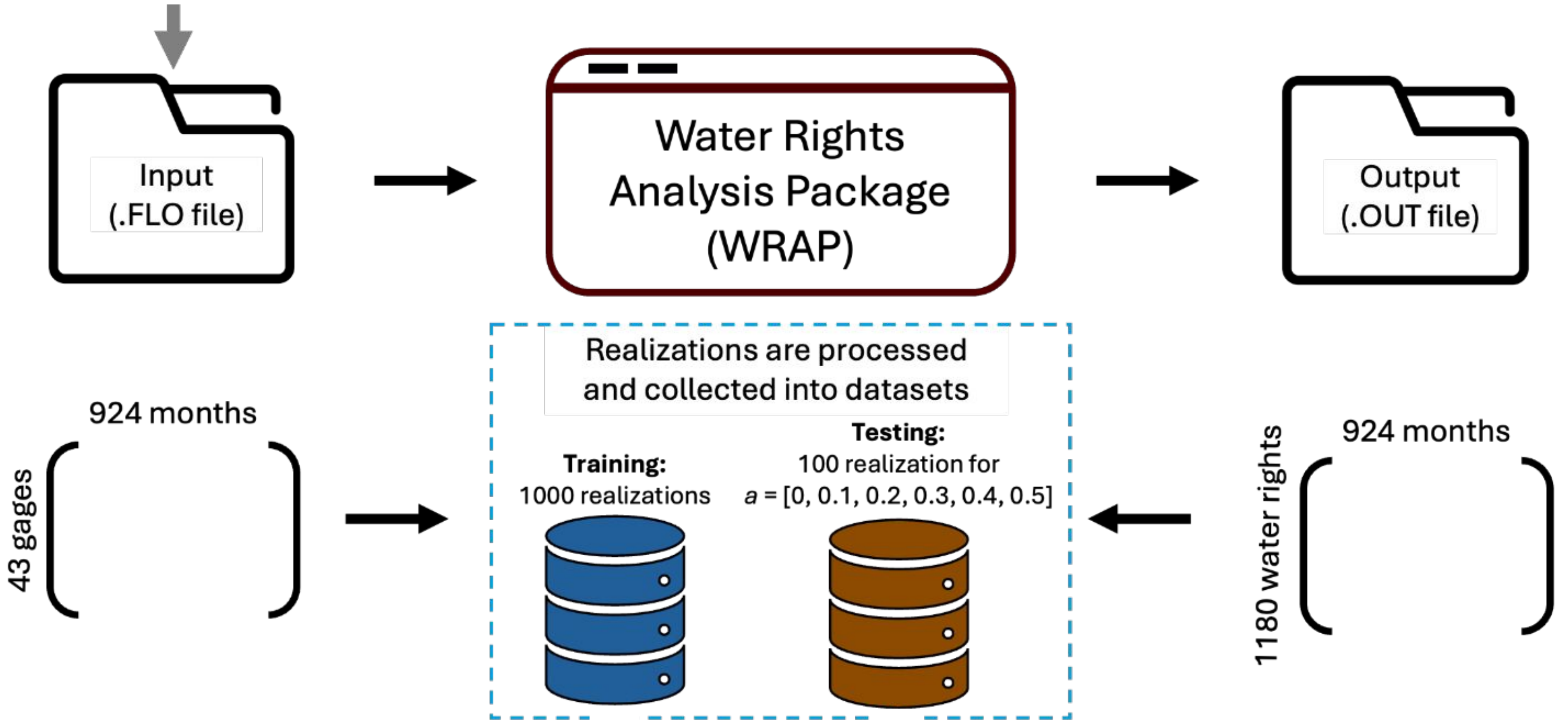


Source: Bonney et al (in review)

- Require multiple realizations of streamflow to effectively train and assess AI/ML approach
- Leverage Hidden Markov Models to generate synthetic streamflows at outlet gage
  - Characterize transitional probabilities (wet/dry) for historical streamflow
  - Generate additional streamflows with increased drought probabilities (0.1-0.5) for additional weather conditions

Analytical Workflow

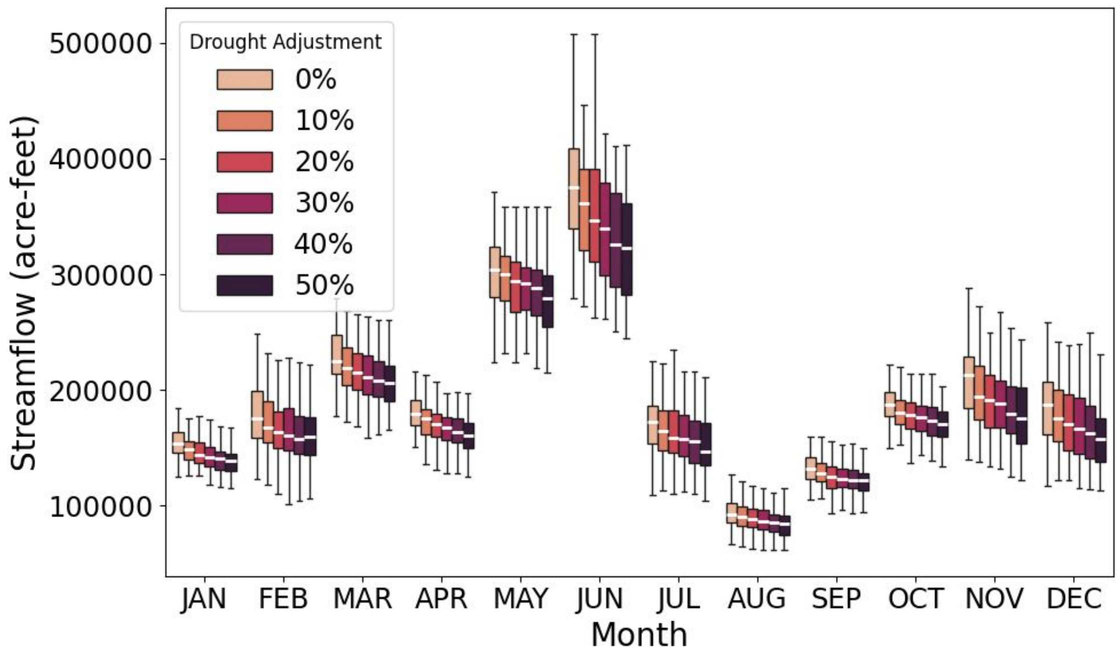
Synthetic Streamflow Generation → WRAP Executions → LSTM Development → Performance Assessment

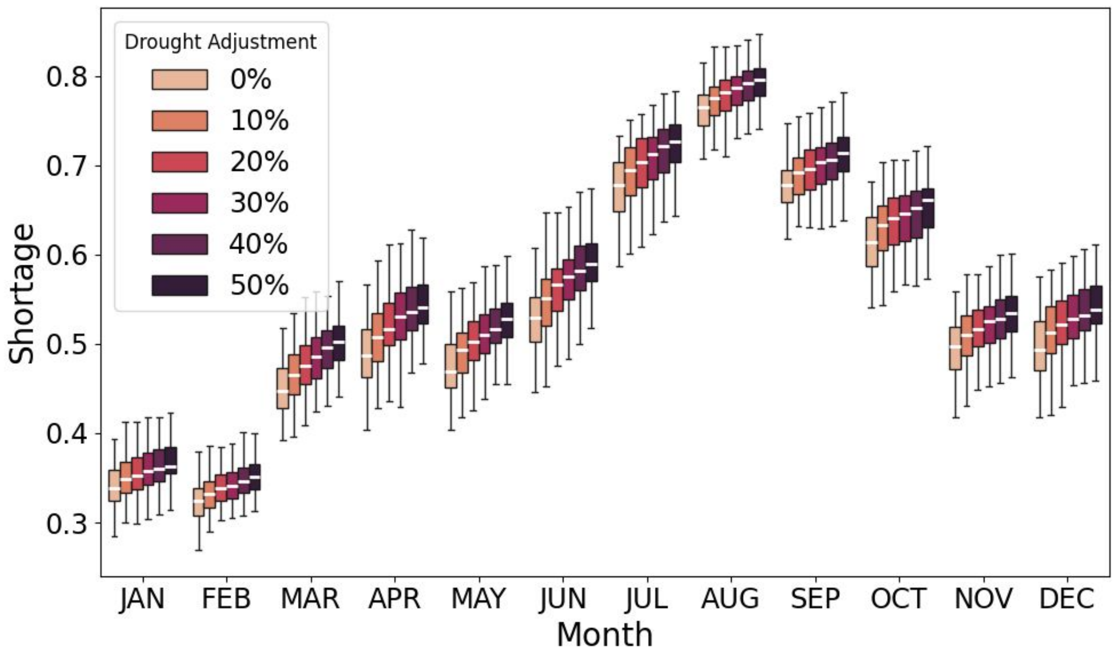


Source: Bonney et al (in review)

- Input synthetic streamflows into WRAP software
- Process output files from WRAP
- Parse data into training & testing splits
  - Training: only conducted on non-drought adjusted data
  - Testing: conducted on all drought variations

Synthetic Streamflow & Shortage Ratio Generation





$$shortage\ ratio = \frac{allocation\ shortage}{allocation\ target}$$

- Training data: 1000 synthetic streamflow values WRAP allocation shortages
- Allocation shortages converted to shortage ratios using allocation targets (0 = all water allocated to right was received)

Final distribution of water rights across sectors

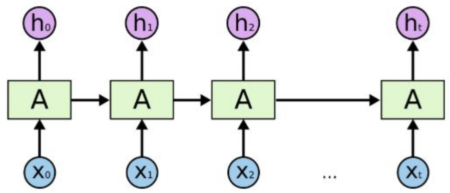
Sector Name	Number of Rights
Irrigation	1,097
Municipal	53
Industry	18
Mining	11
Power	1
Total	1180

Source: Bonney et al (in review)

Analytical Workflow

Synthetic Streamflow Generation → WRAP Executions → **LSTM Development** → Performance Assessment

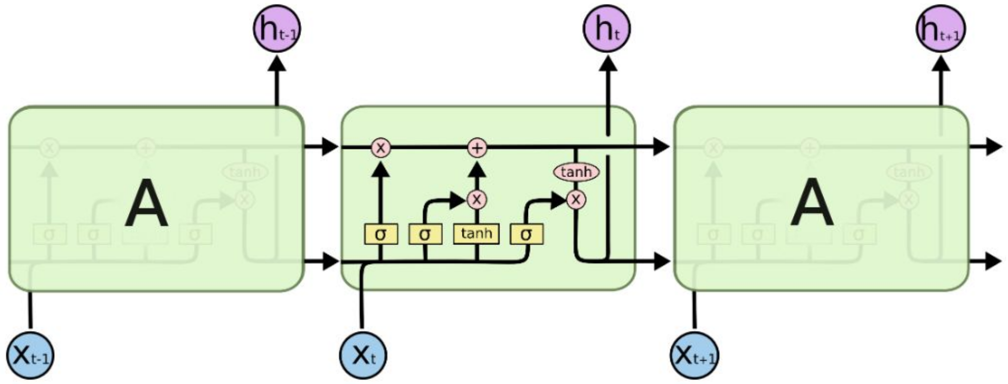
RNN



A. Dataset shape	
Input Size (# of streamflow gauges)	43
Output Size (# of water rights)	1180
Timesteps (# of months)	924
B. Optimized parameters	
LSTM Layer Size	256
Number of LSTM Layers	3
Dropout	0.1
Learning Rate	2e-4
Optimizer	Adam
Loss Function	Mean Squared Error
Epochs	500
Batch Size	5

Source: Bonney et al (in review)

LSTM

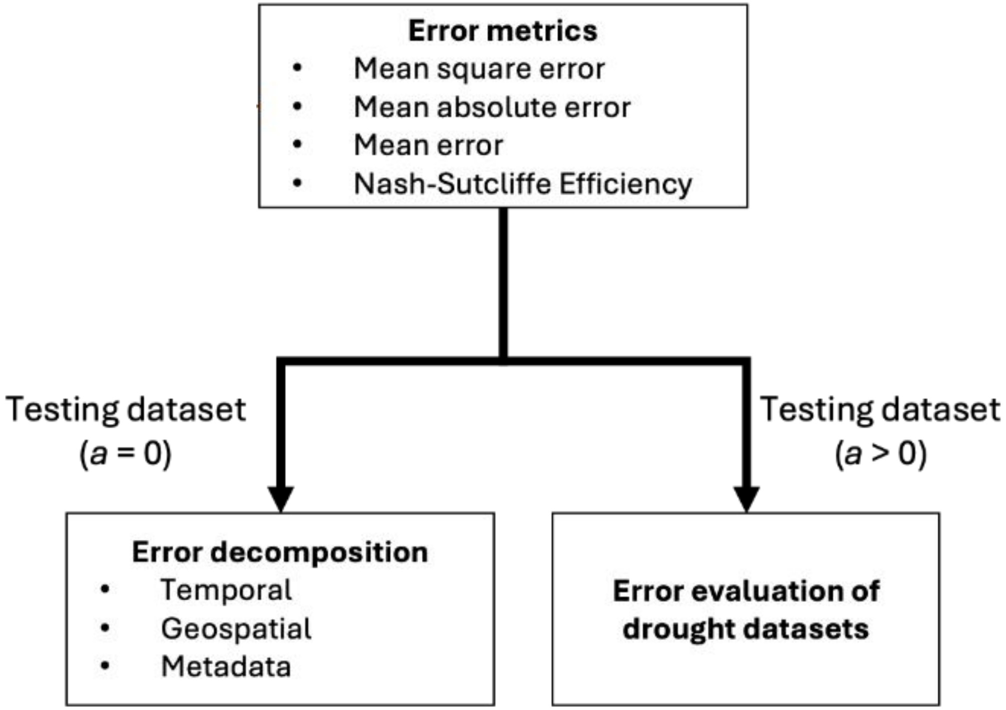


Source: colah

- Long-short term memory (LSTM) networks
  - Type of recurrent neural networks (RNN), which build in persistence
  - LSTM balance long-term information (through cell state) with shorter term updates
- Selected due to successful implementations in various hydrological applications
- Multi-layer network with batch normalization, linear transformation, and sigmoid activation function

Analytical Workflow

Synthetic Streamflow Generation → WRAP Executions → LSTM Development → **Performance Assessment**



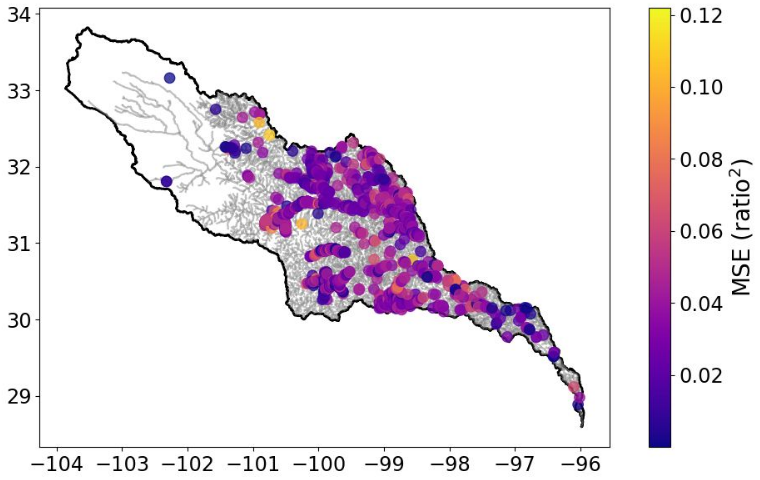
Source: Bonney et al (in review)

- Used multiple error metrics to characterize model performance
  - MSE: used as loss function in LSTM training
  - MAE: same units as variable
  - ME: over/under prediction
  - NSE: predictive power assessment in hydrology
- Temporal and geospatial patterns in error(s)

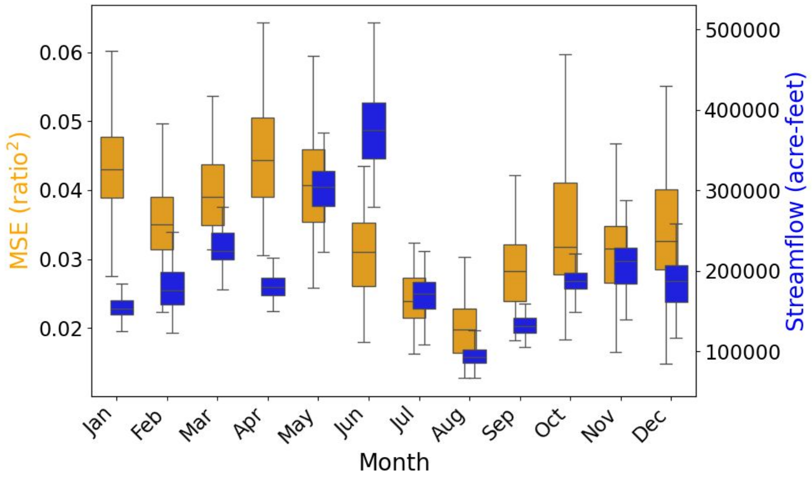
LSTM Performance across Error Metrics (No Drought Adj)

Metric	Shortage Ratio Error	Volumetric Error (acre-feet)
MSE	0.034	40614.64
MAE	0.071	6.74
ME	-0.003	-0.55
NSE	0.794	0.911

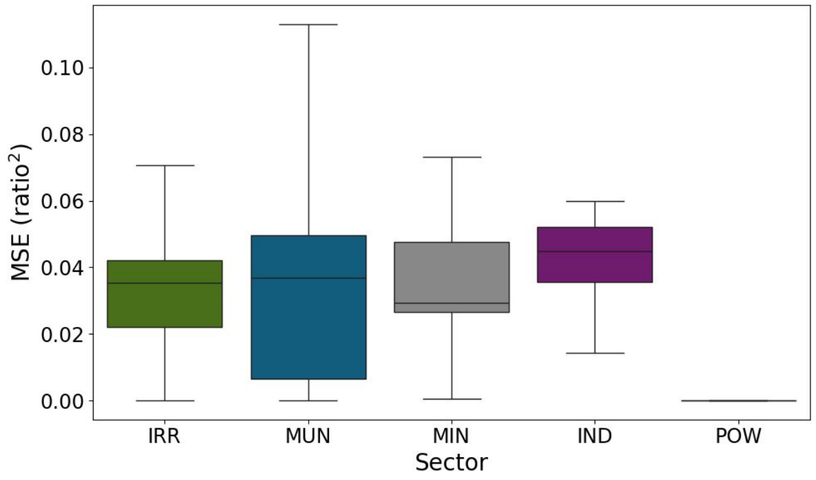
MSE across basin



MSE by month



MSE by sector

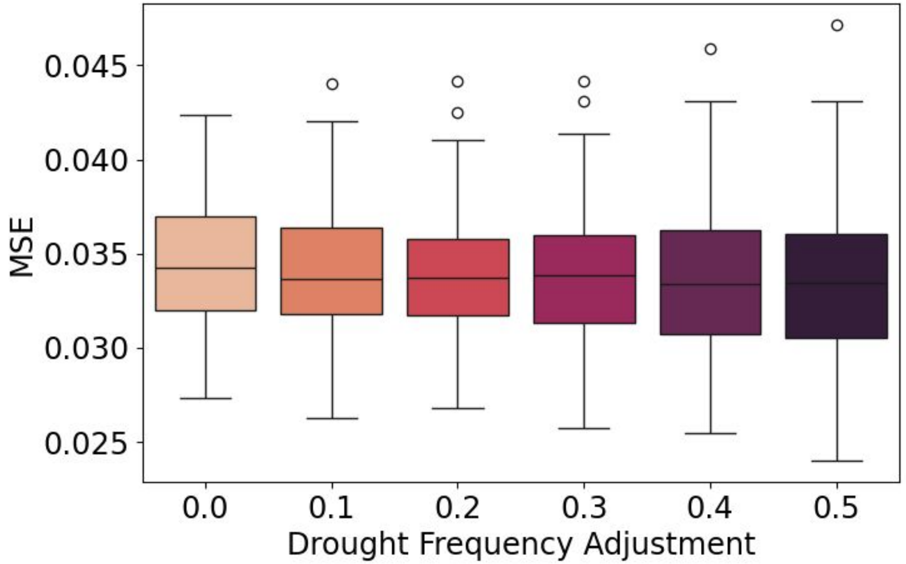


Source: Bonney et al (in review)

LSTM Performance across Error Metrics (Drought Adjusted)

- Overall, model performance across the drought datasets is similar to the historically-grounded (i.e., no drought adjustment) dataset
  - 0-0.003 differences across metrics
  - Subtle decreasing monotonic trends in MAE, ME, and NSE but magnitude of is very small
- Demonstrates model's capability to perform well on data with higher drought signatures than those in the training data
  - Counters traditional thinking of need information about infrastructure, operational rules, etc.
  - Ongoing work: model explainability approaches

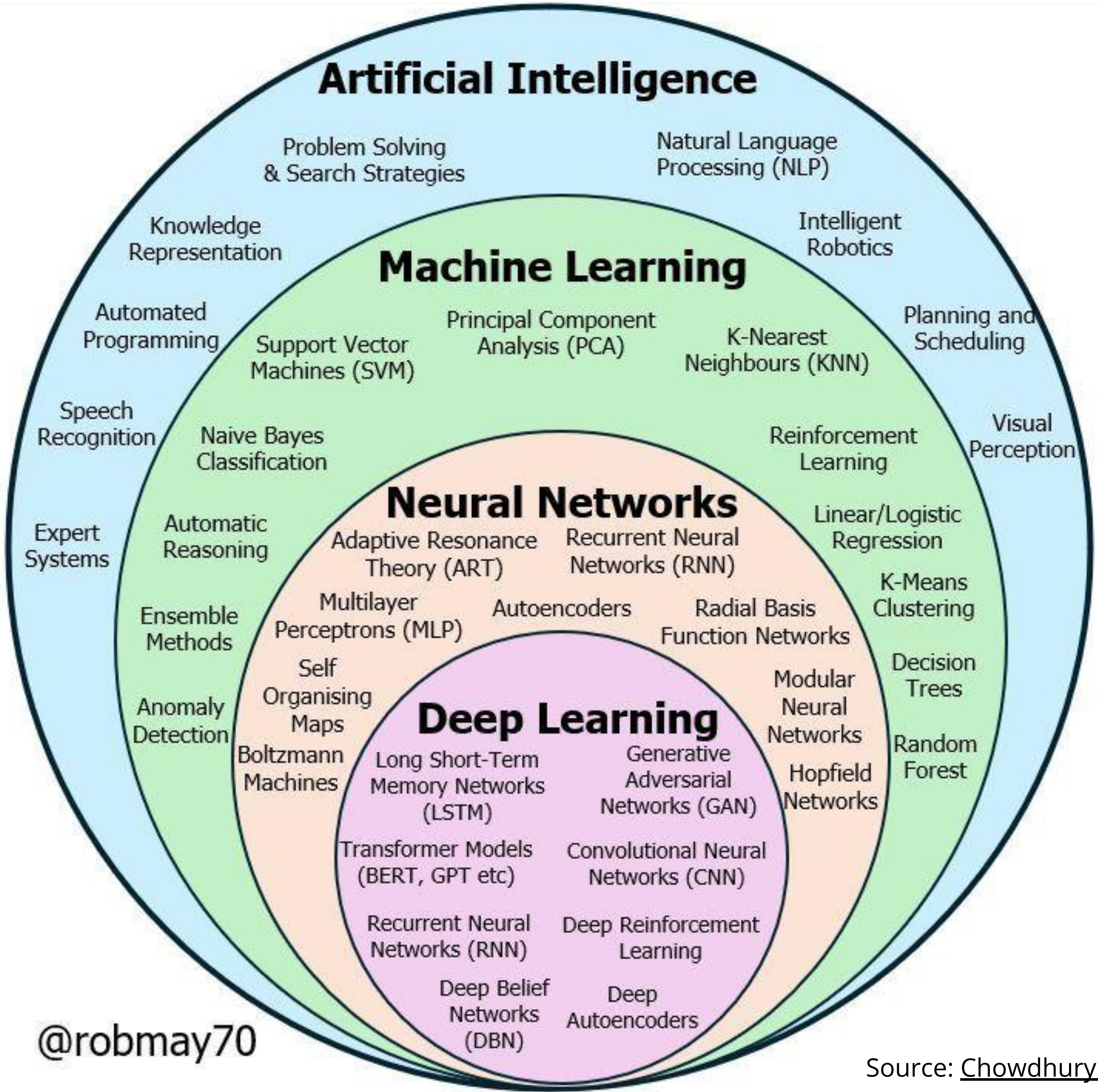
Drought adjustment	MSE	MAE	ME	NSE
0.0	0.034	0.071	-0.003	0.794
0.1	0.034	0.070	-0.002	0.794
0.2	0.034	0.070	-0.002	0.794
0.3	0.034	0.069	-0.001	0.793
0.4	0.034	0.069	-0.001	0.793
0.5	0.033	0.068	-0.000	0.791



Source: Bonney et al (in review)

Looking Ahead

Recap



Source: Chowdhury, 2025

Water Management (WM) refers to control and movement of (waste)water resources (both quantity and quality) to minimize damage and maximize beneficial use.

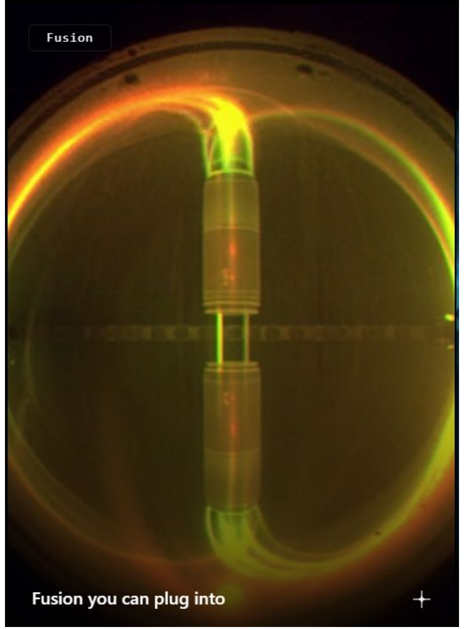
Adapted from: NRCS and UNEP

National Initiative to Build Powerful Science Platforms

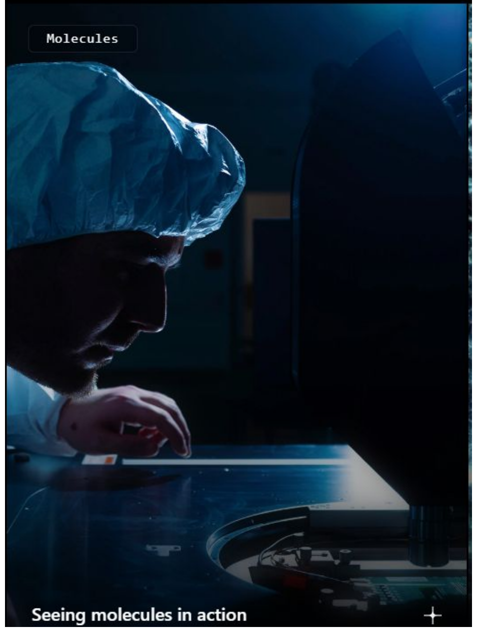
Genesis Mission

A National Mission to Accelerate Science Through Artificial Intelligence

Energy



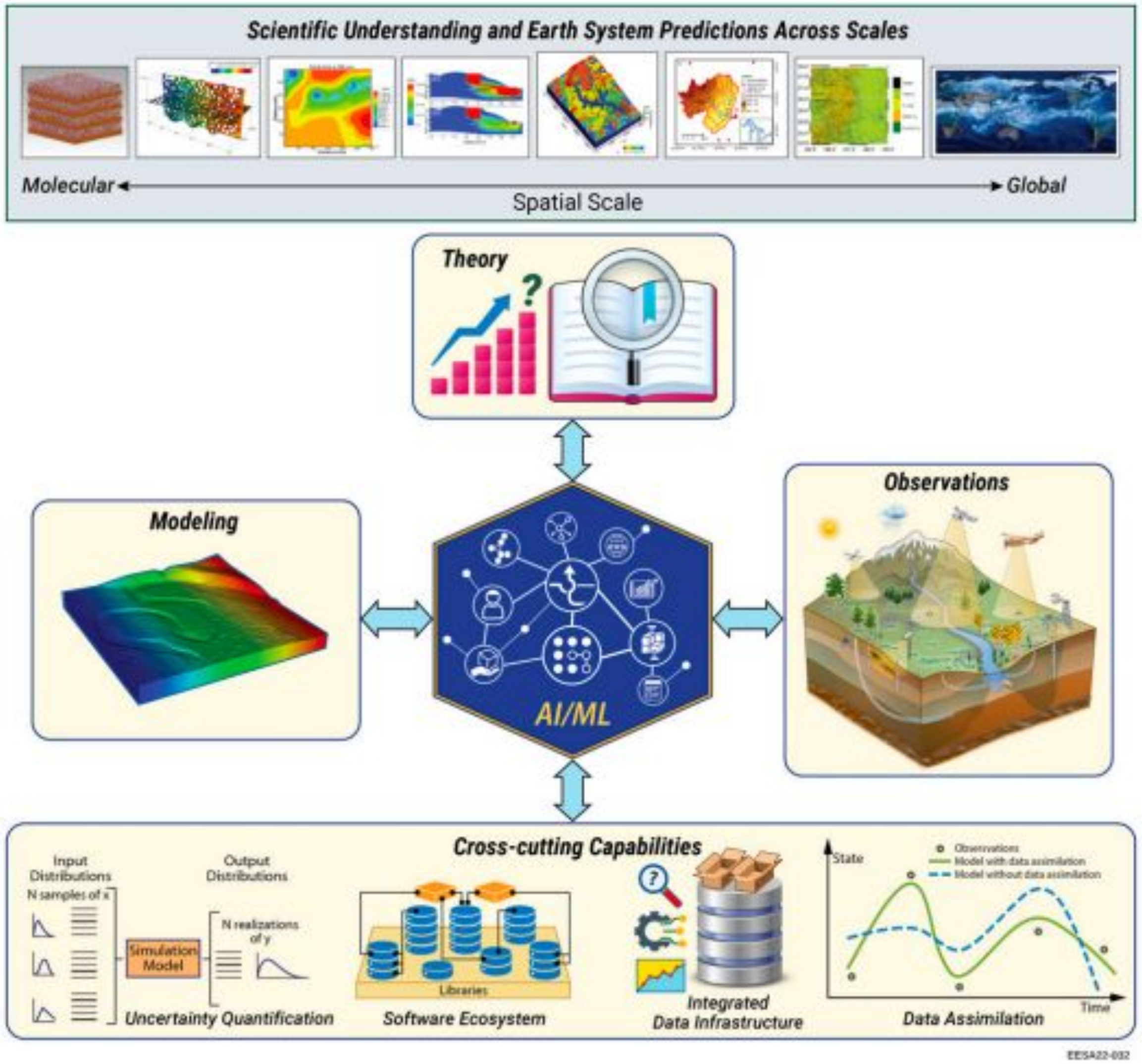
Discovery Science



National Security

Source: DOE, 2025

Many Outstanding Questions Still Persist



Source: AI4ESP, 2022

Develop Better Data of Human Systems

Improve Fusion of Information

Advance Management of Knowledge

Multiple Worldviews of Water

What aspects of the natural system are changing (precipitation patterns, changing ice floes, animal migration, …)?

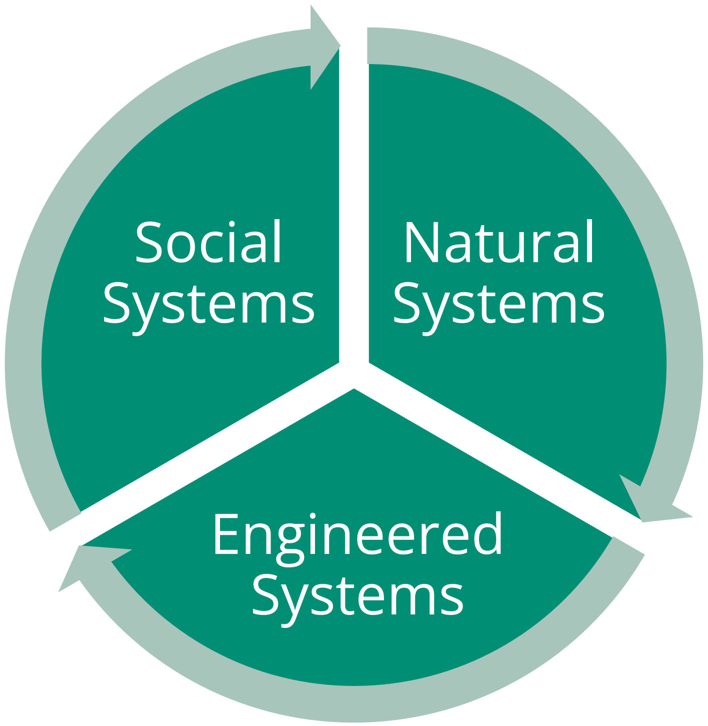
How are social dynamics influencing system states (supply chains, tensions between users, adaptation behaviors, …)?

How are the current and planned systems able to withstand or recover from changing system states (drinking water, energy production, manufacturing, …)?

Multi-disciplinary, Systems Approach

Multi-disciplinary, systems approach will be required to evaluate intersections and interactions between natural, engineered, and social systems.

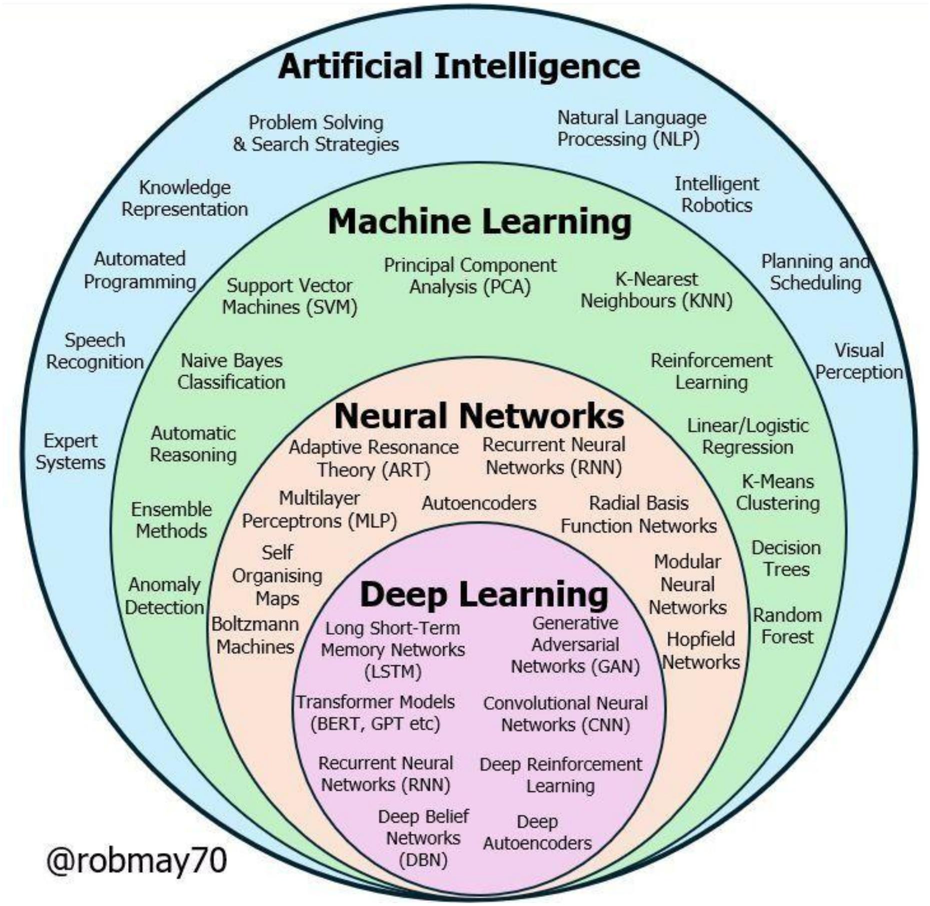
Disciplines	Methods
- Hydrologists - Atmospheric scientists - Civil, mechanical, chemical, environmental engineers - Data scientists - Applied mathematicians - Economists - Political scientists - Software developers	- Artificial Intelligence - Machine learning - Simulation - Optimization - Uncertainty quantification - Multi-scale analysis - Network analytics - Trust evaluations - Visualization



Summary

Management of water resources can be accelerated by harnessing AI/ML algorithms to develop insights into current system states, vulnerabilities, and opportunities.

Multiple Algorithms across AI/ML



Source: Chowdhury, 2025

Scientific Advancements in Water Management with AI/ML

- Ingestion of large (“big”) datasets capturing real-world behavior
- Improved understanding of water narratives (across multiple topic areas) in local newspapers
- Development of parsimonious neural network models characterizing water allocations

Multiple Challenges Persist

- Data gaps across physical, human systems
- Fusion of information across domains, disciplines
- Management of knowledge to support timely decision-making

Thank you for your time!

Happy to answer any questions!

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