

Welcome to the June Edition of the 2023 M&R Seminar Series



- Remote attendees' audio lines have been muted to minimize background noise. For attendees in the auditorium, please silence your phones.
- A question and answer session will follow the presentation.
- For remote attendees, Please use the "<u>Chat</u>" feature to ask a question via text to "Host". For attendees in the auditorium, please raise your hand and wait for the microphone to ask a verbal question.
- The presentation slides will be posted on the MWRD website after the seminar.
- This seminar has been approval by the ISPE for one PDH and has been approved by the IEPA for one TCH. Certificates will only be issued to participants who attend the entire presentation.

Dr. Kathryn (Kate) B. Newhart Assistant Professor of Environmental Engineering United States Military Academy West Point, New York



Dr. Kate Newhart is an Assistant Professor of Environmental Engineering with a specialization in data-driven monitoring and control for the water sector. Dr. Newhart holds a Ph.D. in Civil and Environmental Engineering from the Colorado School of Mines and previously worked at Metro Water Recovery, the largest wastewater utility in the Rocky Mountains, as an engineer in their Technology and Innovation Division, where she led data handling and data-driven modeling efforts. Dr. Newhart's current work includes soft-sensor development for disinfection, resource recovery, and disinfection by-product mitigation in collaboration with utilities and universities across North America.



Understanding and Embracing Machine Learning and Predictive Analytics

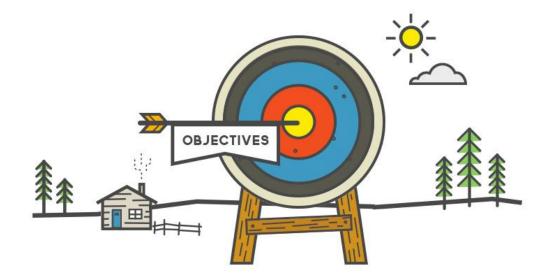
Dr. Kate Newhart

Assistant Professor of Environmental Engineering
United States Military Academy



Objectives

- Define artificial intelligence (AI), machine learning (ML), digital twin, and soft sensor
- Explain the process of developing an ML model
- Understand how a machine learning model can be deployed, used, and maintained at a water utility





WHAT IS ARTIFICIAL INTELLIGENCE?

WEST POINT. What is Artificial Intelligence?

Slide credit: Branko Kerkez

A Proposal for the

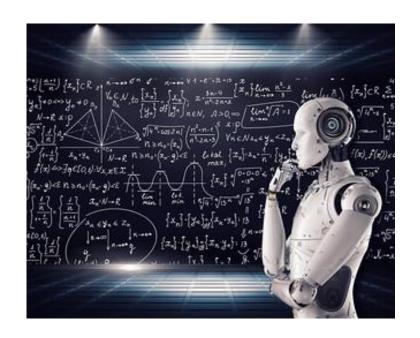
DARTMOUTH SUMMER RESEARCH PROJECT ON ARTIFICIAL INTELLIGENCE June 17 - aug. 16

We propose that a 2 month, 10 man study of artificial intelligence be carried out during the summer of 1956 at Dartmouth College in Hanover, New Hampshire. The study is to proceed on the basis of the conjecture that every aspect of learning or any other feature of intelligence can in principle be so precisely described that a machine can be made to simulate it. An attempt will be made to find how to make machines use language, form abstractions and concepts, solve kinds of problems now reserved for humans, and improve themselves. We

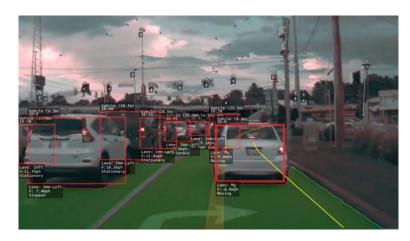


WEST POINT. What is Artificial Intelligence?

"AI" is a computer system that can perform tasks that typically require human intelligence (e.g., learning, reasoning, perception, decision-making)





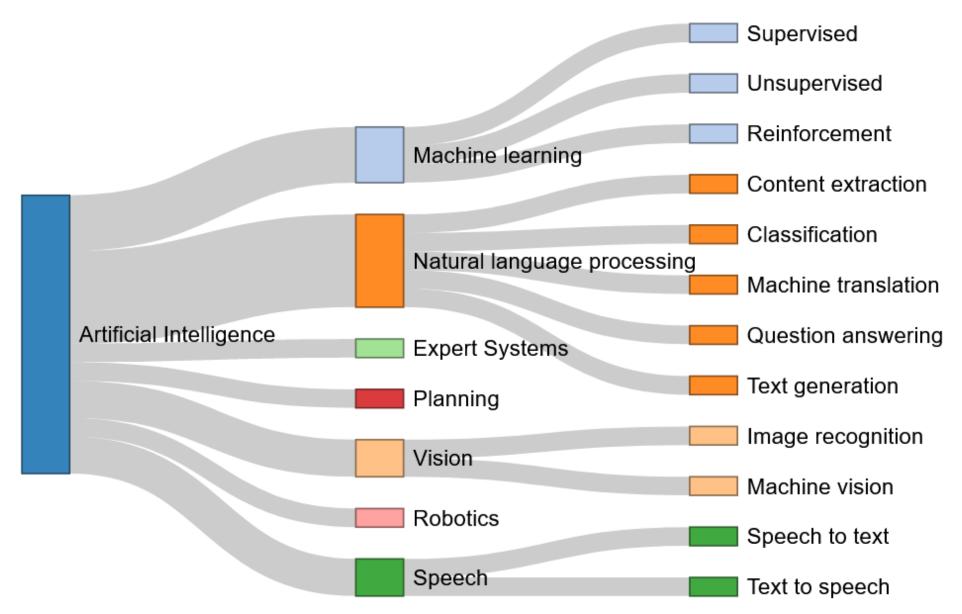








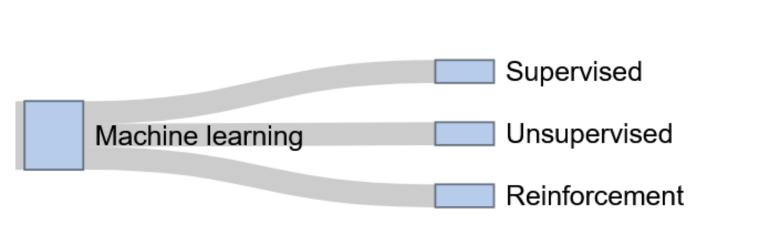
WEST POINT. What is Artificial Intelligence?

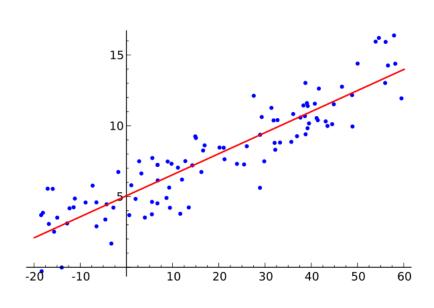




What is Machine Learning (ML)?

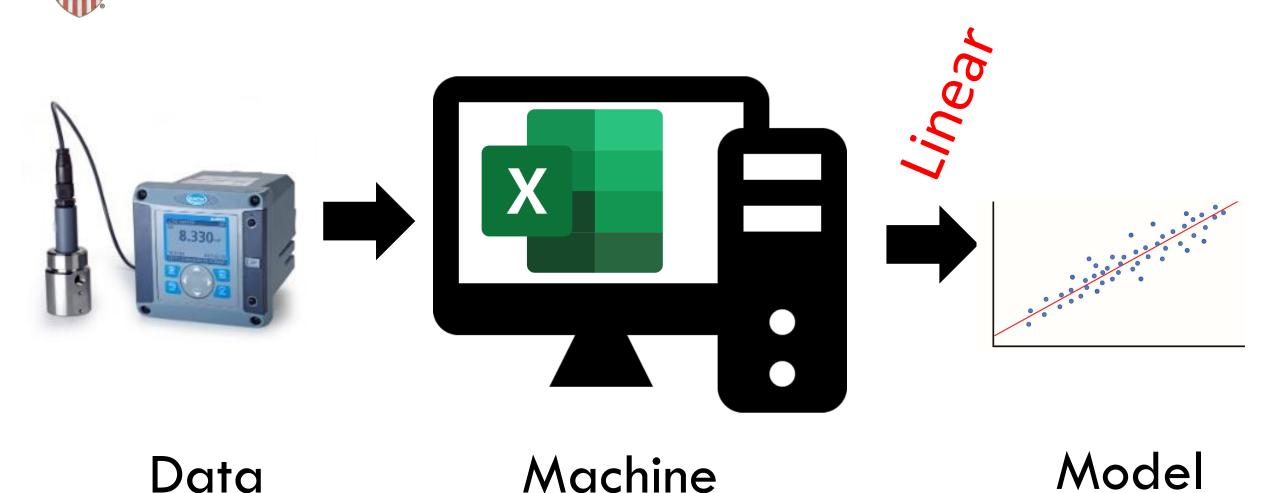
- "ML" involves an algorithm that can infer how to do a specific task without explicit instruction from data
- Supervised → Explicit examples of results







Model Training Process



Slide credit: Branko Kerkez11



Model Training Process



Data

Machine

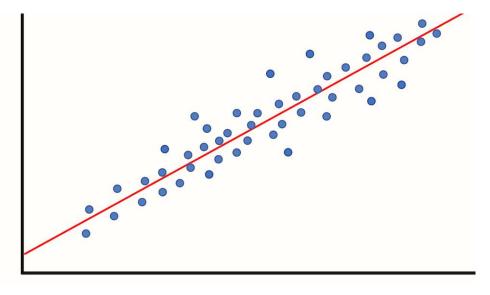
Model



Let's determine the treatment dose to remove chemical X, for real-time dose control.

Relationship between dose and removal appears linear → fit linear regression → statistical

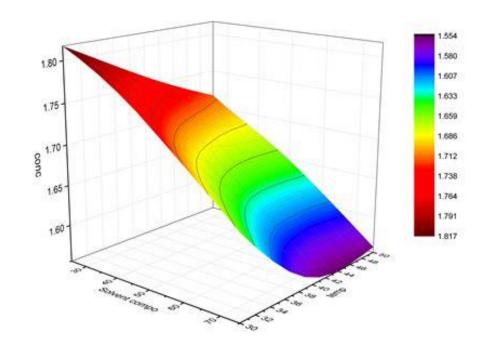
Removal



Dose

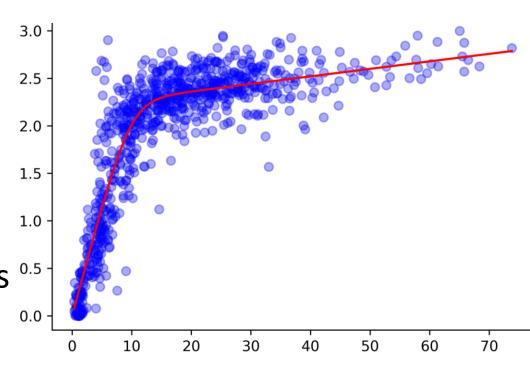
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 → mechanistic



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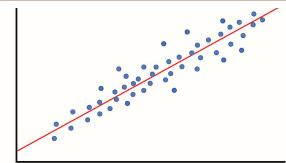
- Relationship between dose and removal appears linear → fit linear regression → statistical
- 2. Known relationship between dose,
 removal, and pH → fit equilibrium model
 → mechanistic
- 3. Error in statistical and mechanistic models is too great for the application...
 Dose + removal + 10 other WQ variables
 → fit incredibly flexible model → ML

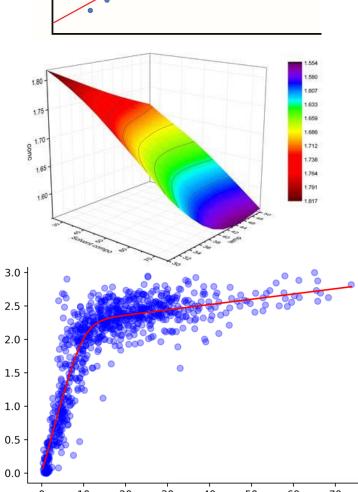




Let's determine the treatment dose to remove chemical X, for real-time dose control.

- 1. <u>Statistical models</u> = define relationship between variables, **analytical uncertainty estimates**
- 2. <u>Mechanistic models</u> = define relationship between variables, can **infer meaning** in coefficients
- 3. <u>ML models</u> = **no known relationship** between variables, experimental uncertainty estimates
 - More complex model building process
 - Answers different types of questions
 - Great flexibility requires great data!



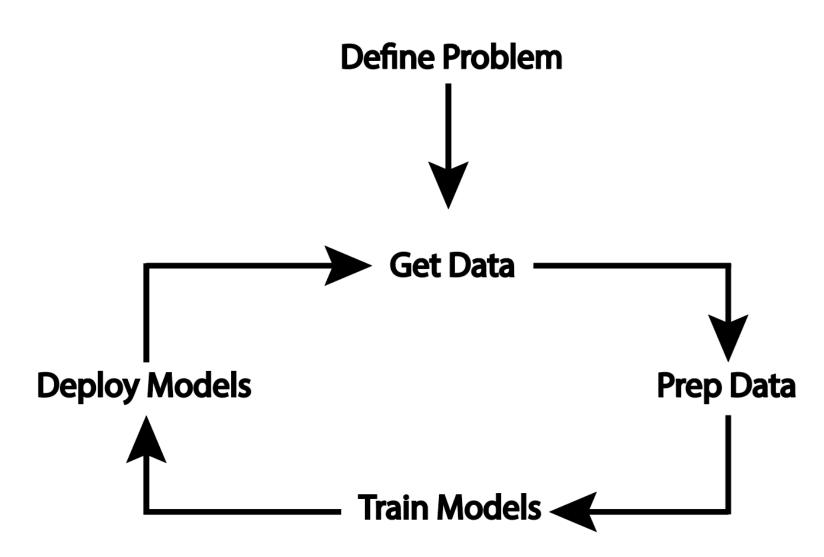




MACHINE LEARNING WORKFLOW

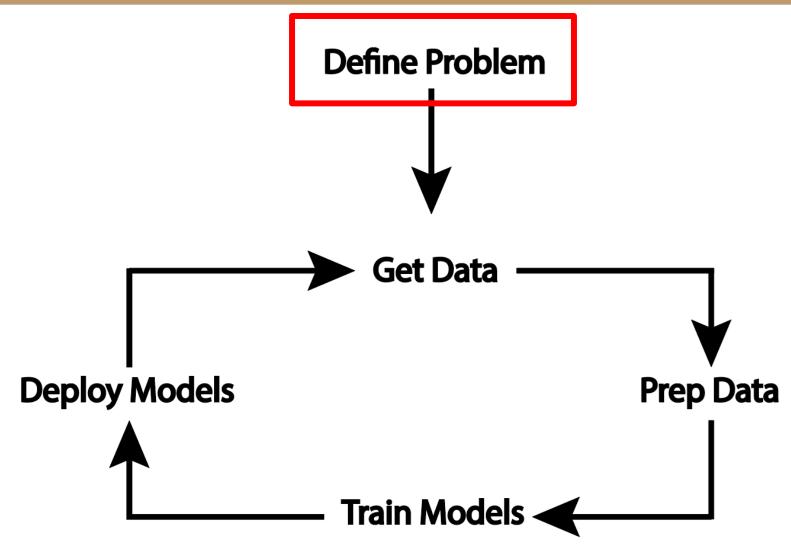


ML Workflow





ML Workflow





What types of problems?

- Water Quality and Flow Monitoring
 - "Soft sensor" uses an ML model to predict a constituent based on other online data. Often used for time-consuming laboratory measurements.
 - Early warning systems can detect faults in processes or changes in water quality, often before operator-set limits are exceeded.
 - Flow or load forecasting for early response
- Optimization
 - "Digital Twins"



What is a digital twin?

"Digital twin" is a model of a physical entity with an automated, bidirectional live data connection ... that allows for dynamic updating to maintain an accurate description ... as it evolves over time

—Peter Vanrolleghem + Torfs et al., 2022

Real Blower



Live data

Setpoints

Blower Model







A "good" ML problem



<u>Yishi Zuo</u>, 2021



A "good" ML problem

- Problem statement is specific to an objective
 - Example: Objective may be to minimize chemical dose, not to understand chemical kinetics



<u>Yishi Zuo</u>, 2021

The biggest problem is keeping the original problem the problem!



A "good" ML problem

- Problem statement is specific to an objective
 - Example: Objective may be to minimize chemical dose, not to understand chemical kinetics
- Simpler models cannot capture the observed trends (with sufficient accuracy for a given application)
- Sufficient, quality historical data is available for model development and will continue to be available

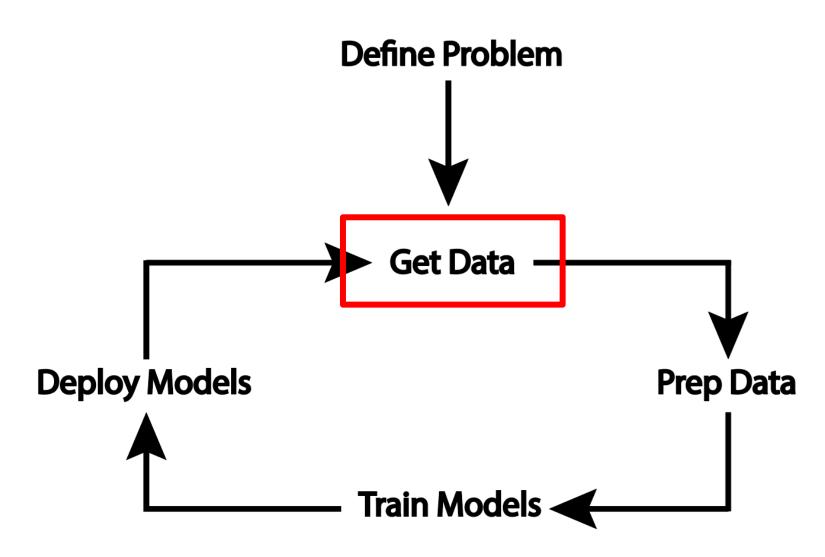


<u>Yishi Zuo</u>, 2021

The biggest problem is keeping the original problem the problem!

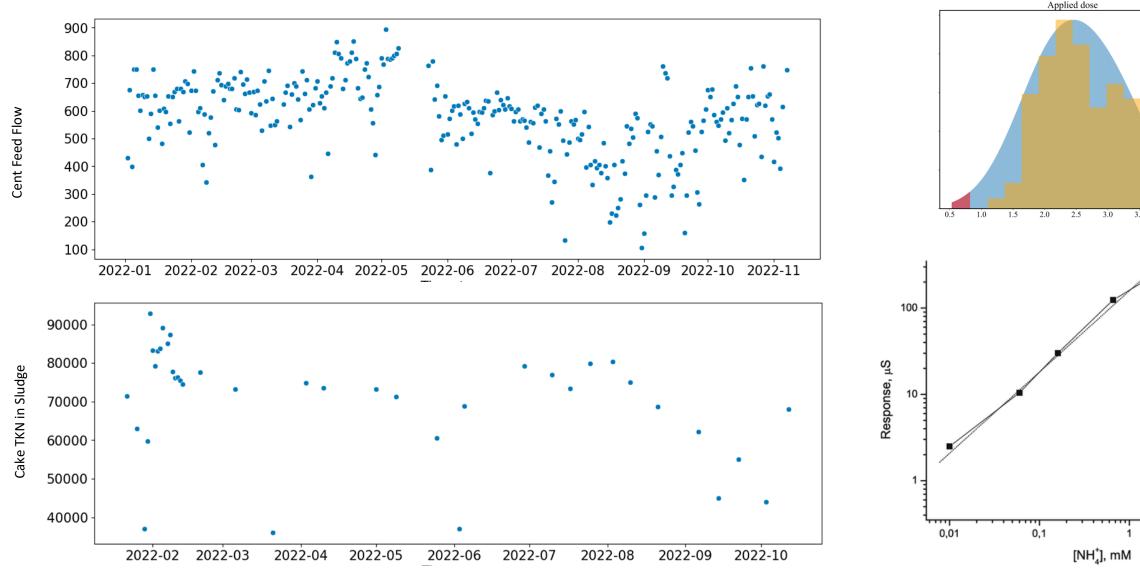


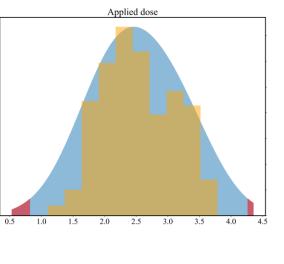
ML Workflow

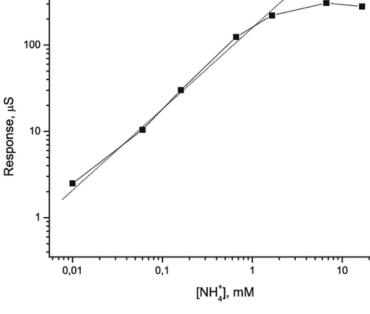




"I have SO much data"

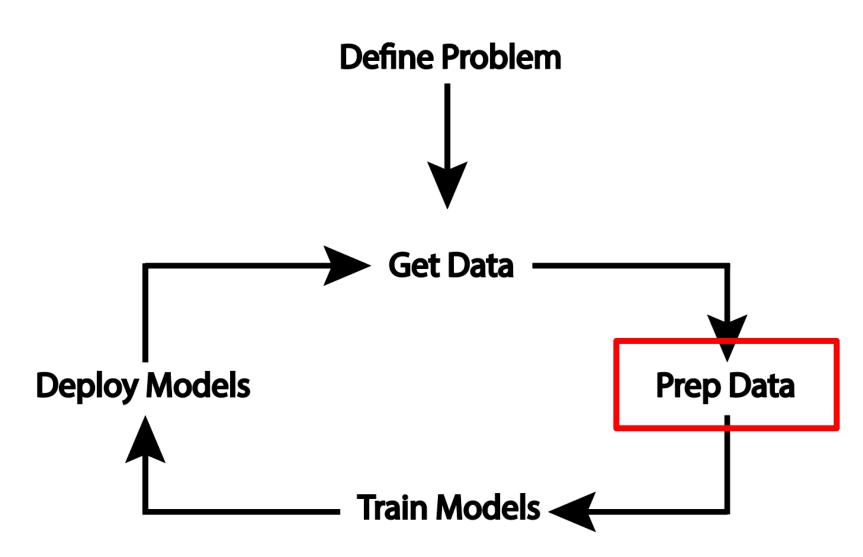






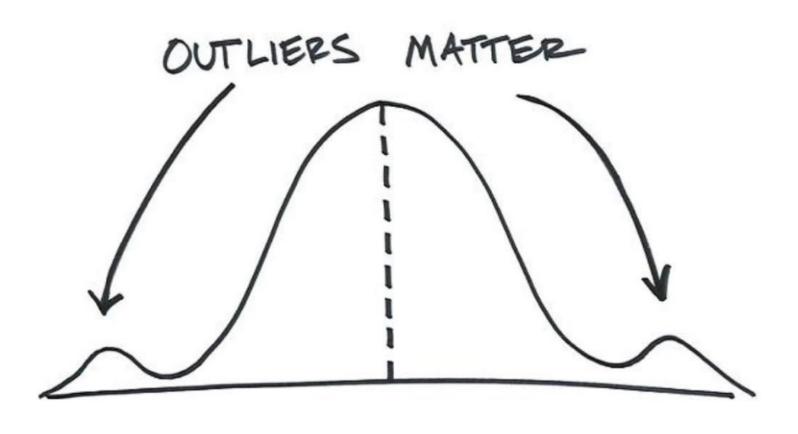


ML Workflow



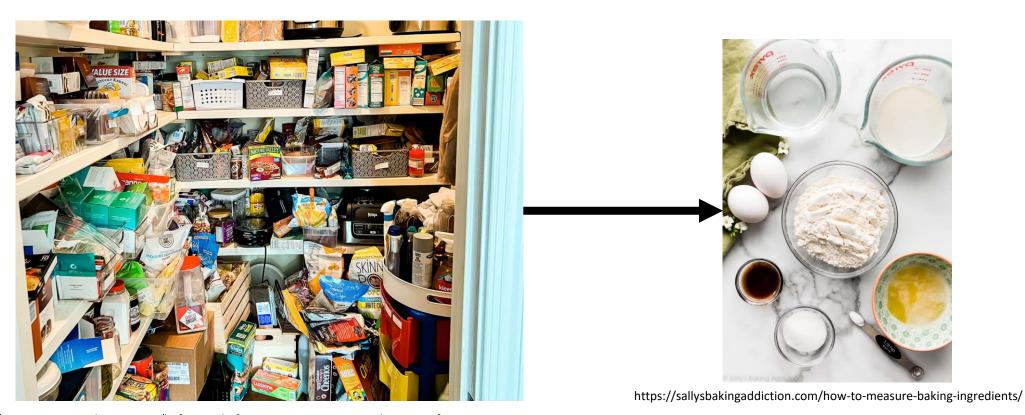


Remove Outliers (?)





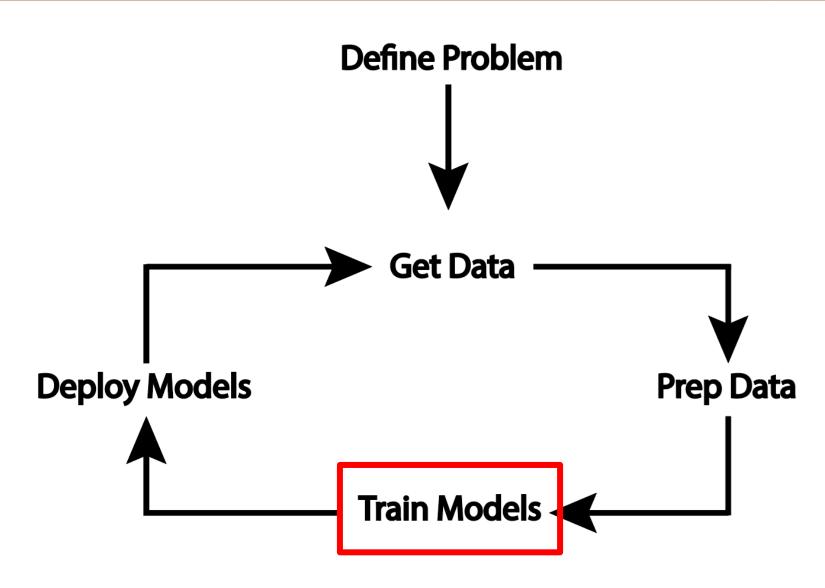
WEST POINT. Remove Irrelevant "Features"



https://www.apartmenttherapy.com/before-and-after-messy-pantry-gets-realistic-transformation-37200882



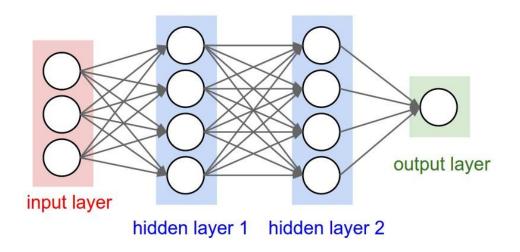
ML Workflow





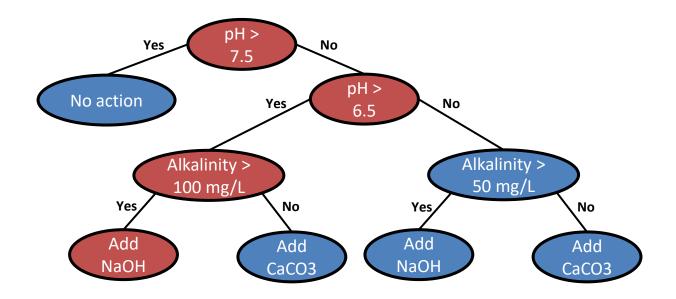
Common Supervised ML Models

Neural Networks ANN, RNN, LSTM



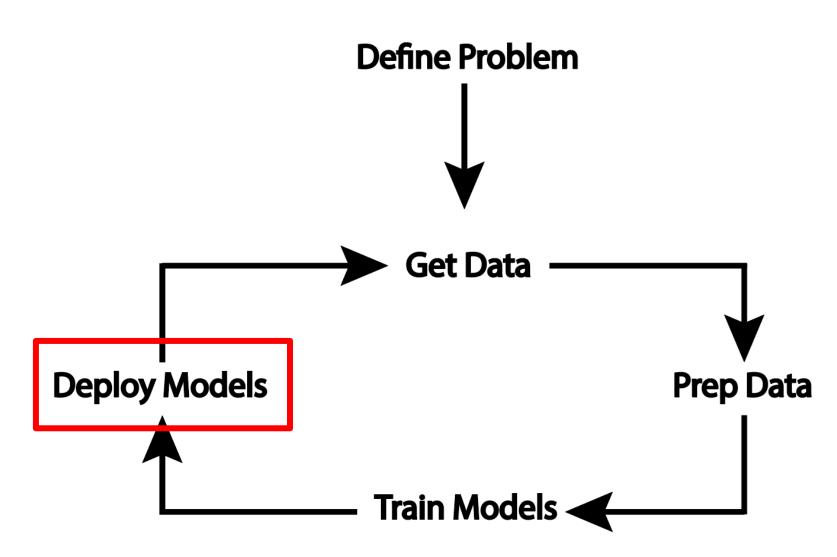
Decision Trees

RF, AdaBoost, XGBoost



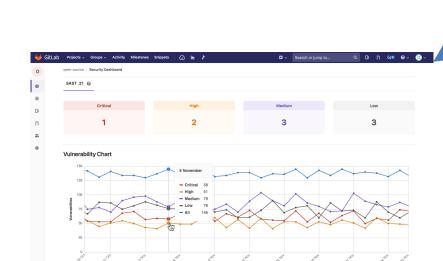


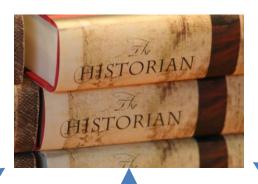
ML Workflow



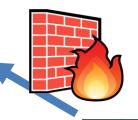


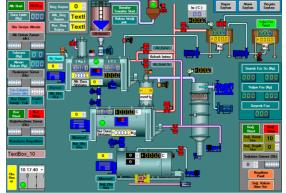
How do I use the model?









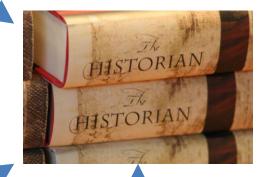


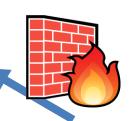


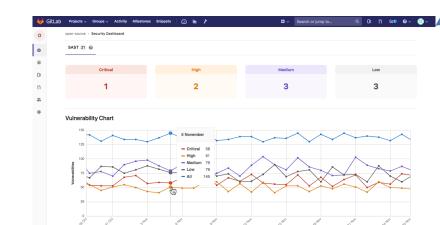
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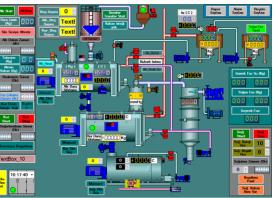










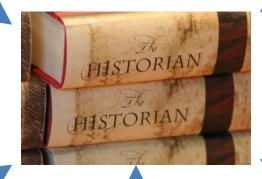


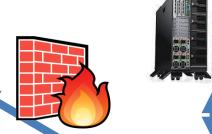


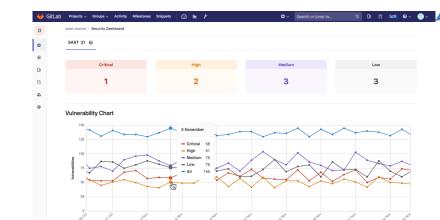
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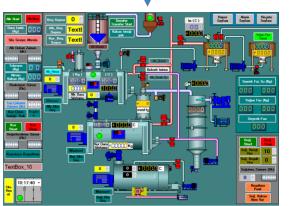














MACHINE LEARNING EXAMPLES



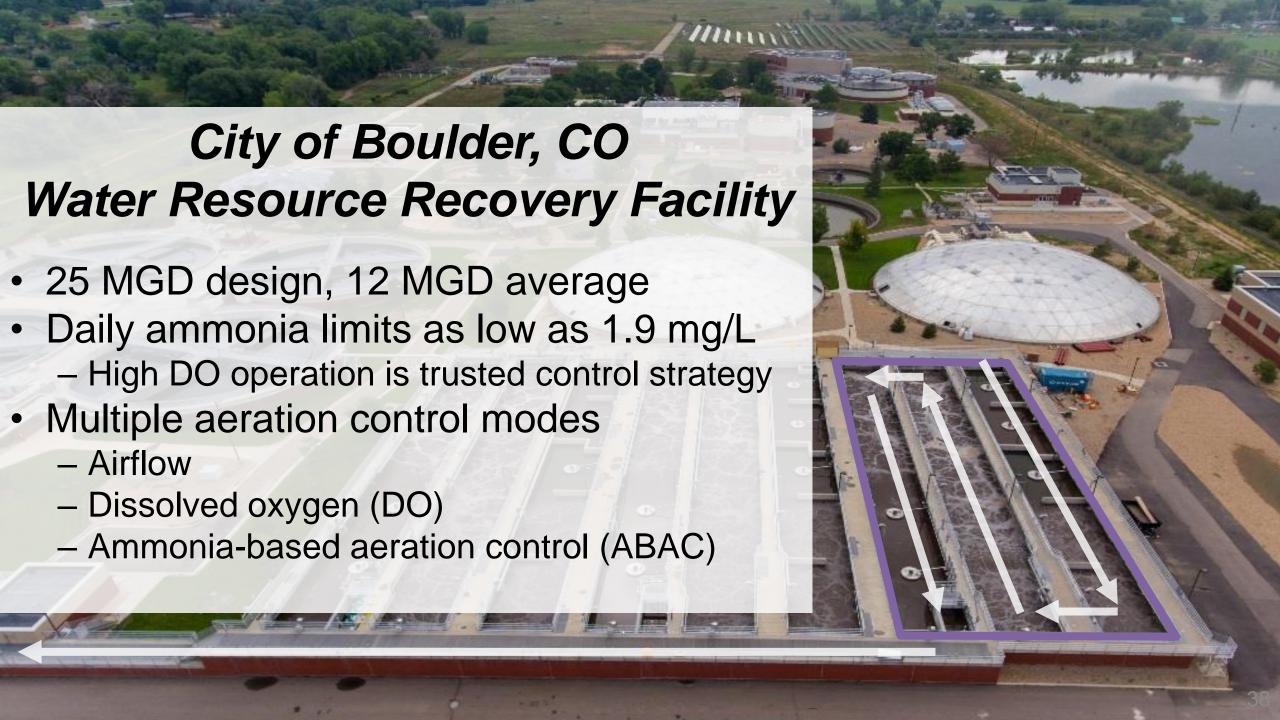








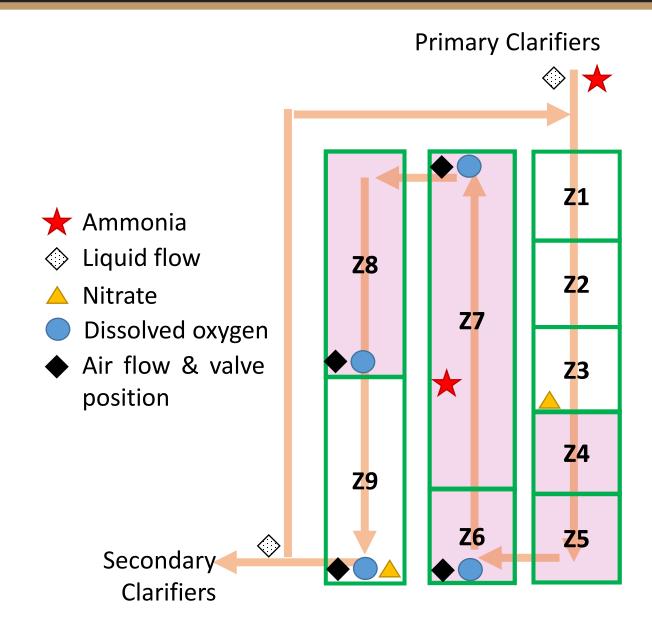
FORECASTING





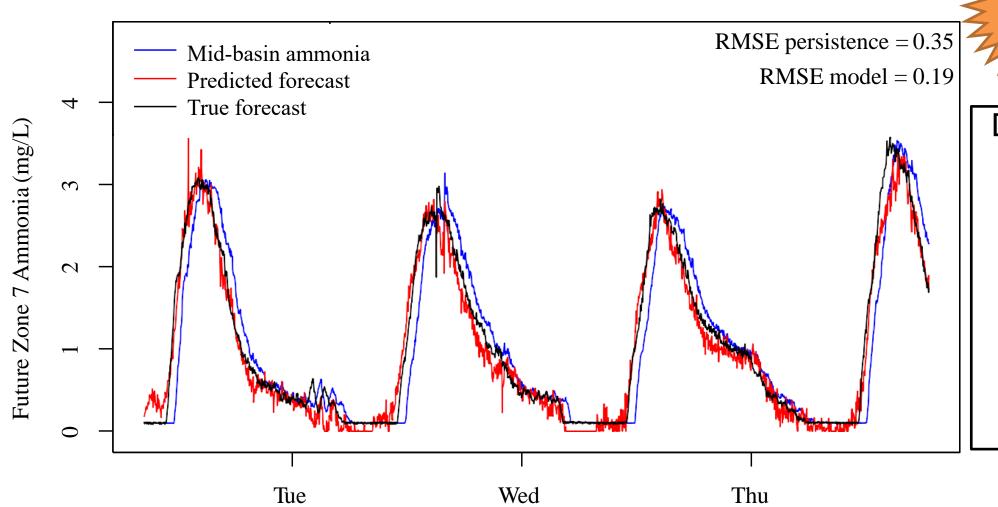
WEST POINT. Forecasting Aeration Demand

- Influent ammonia sensor was difficult to maintain
- Mid-basin ammonia was stable, but led to a delayed response
- Replace ammonia in control strategy with a "forecasting" soft sensor





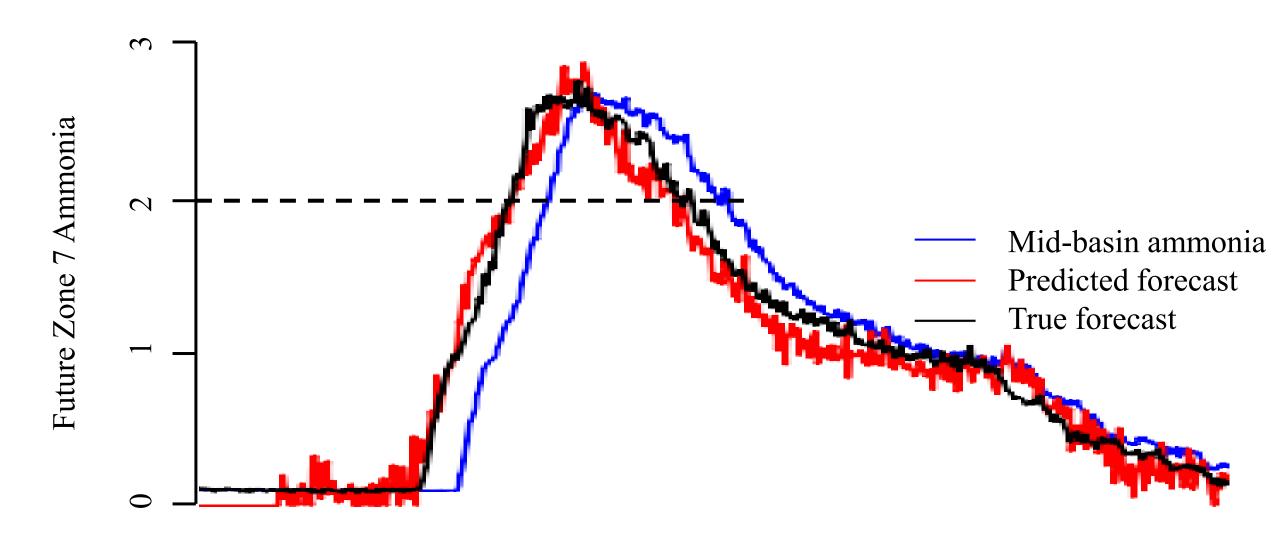
WEST POINT. Forecasting Aeration Demand

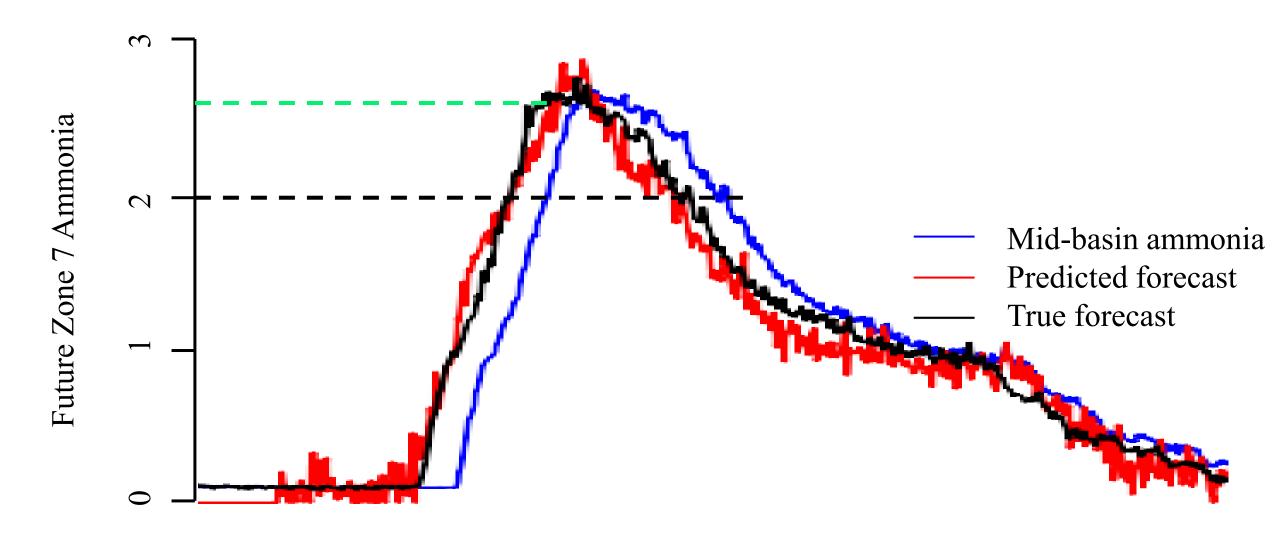




Diurnal, linear, and artificial neural network hybrid model.

> 2-min data frequency, 3-day training window.





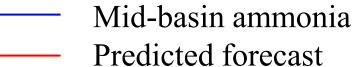
Ammonia



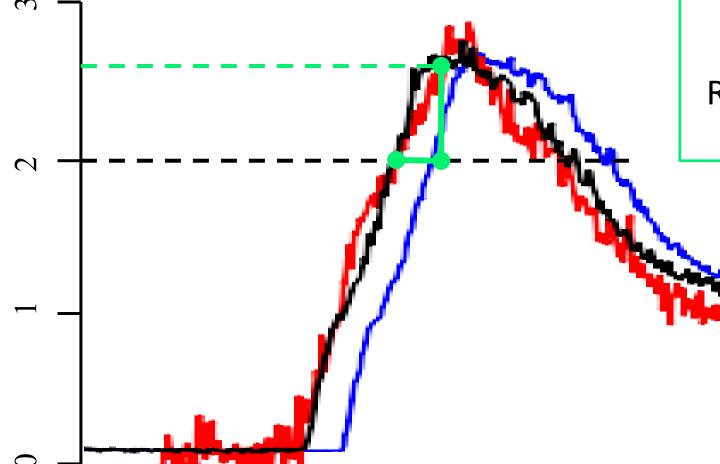
Increase air output prior to exceeding setpoint

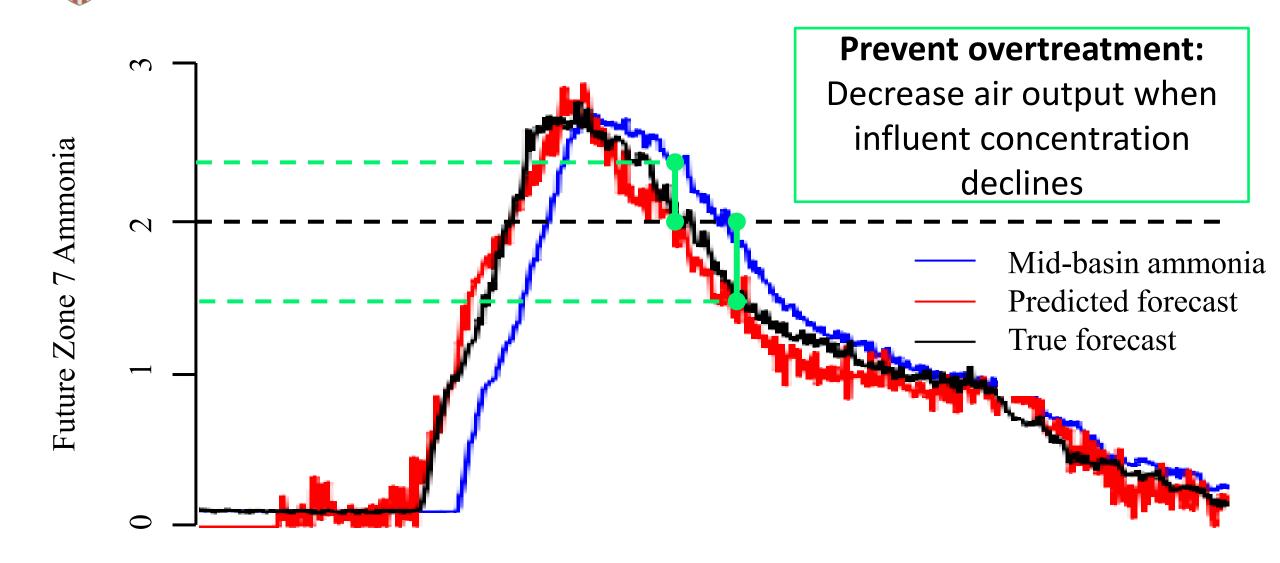
Easy on the blowers:

Reduce sudden changes in air blower speed



True forecast



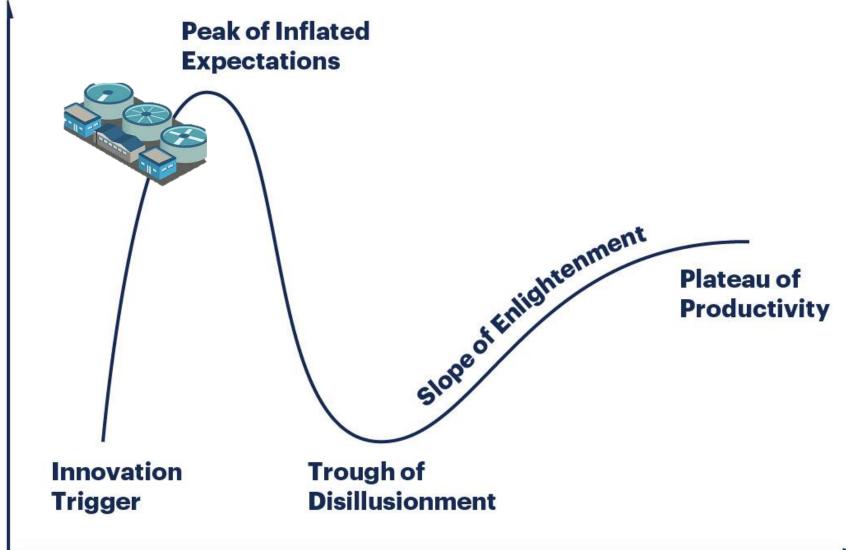




FINAL THOUGHTS



Hype Cycle: ML and Utilities

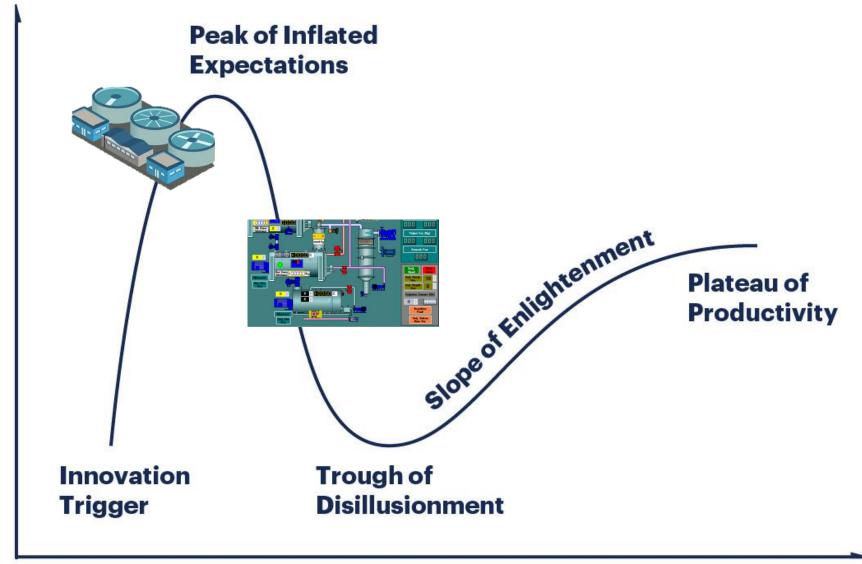


Expectations



Expectations

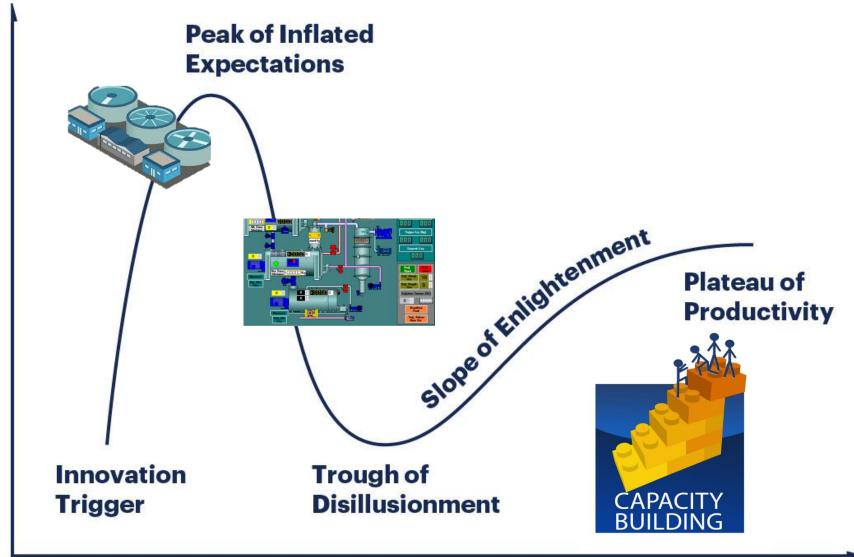
Hype Cycle: ML and Utilities



Time



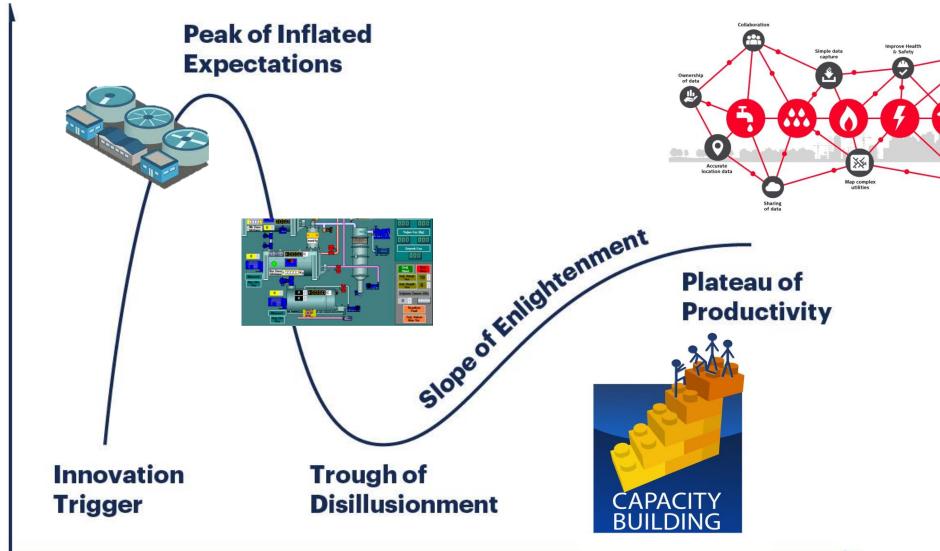
Hype Cycle: ML and Utilities



Expectations

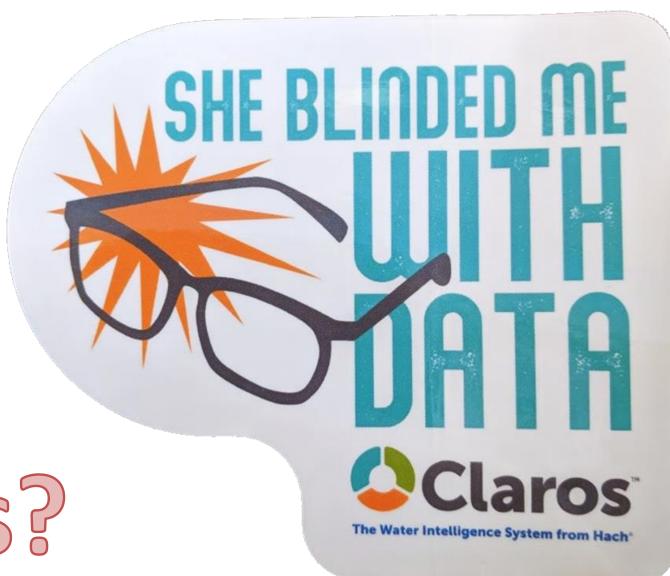


Hype Cycle: ML and Utilities



Expectations





Questions?