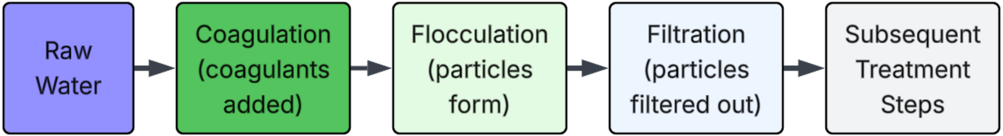
Predicting Water Treatment Plant Chemical Doses

Ethan Schilling, Joshua Tobey, Dawson Carney, Reece Carmody

11 December 2025

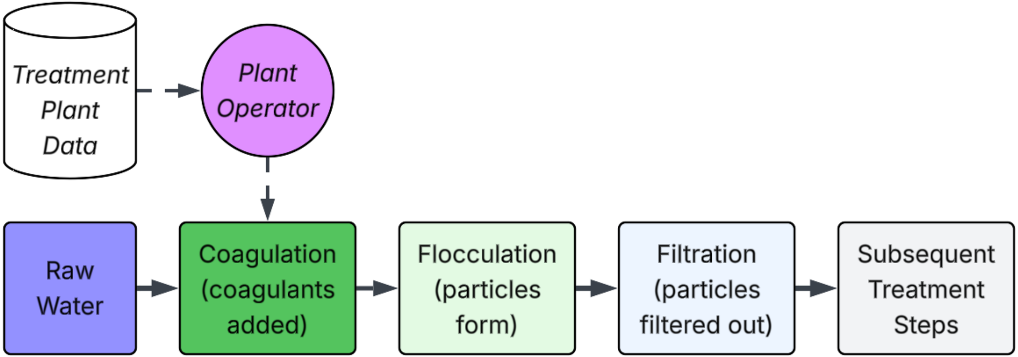
Background and Motivation

The drinking water treatment process takes water from a river, lake, reservoir, or other source, and purifies it to have it reach drinking water standards.


Raw Water
Coagulation (coagulants added)
Flocculation (particles form)
Filtration (particles filtered out)
Subsequent Treatment Steps

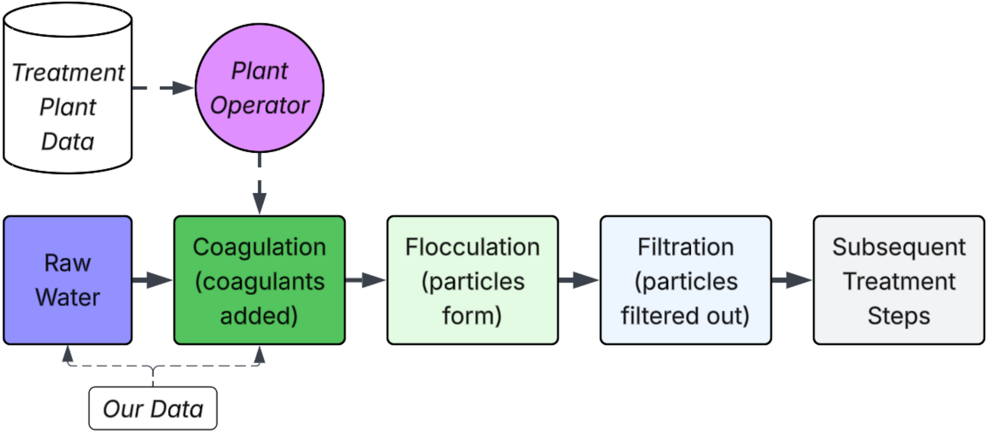
Background and Motivation

One role of an operator in the water treatment process is to look at a wide array of data and make decisions about how to adjust chemical doses.


Treatment Plant Data
Plant Operator
Raw Water
Coagulation (coagulants added)
Flocculation (particles form)
Filtration (particles filtered out)
Subsequent Treatment Steps

Background and Motivation

OUR GOAL: Create a model that serves the role of an "operator," taking raw water data and making predictions of chemical doses.


Treatment Plant Data
Plant Operator
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Our Data

Data Overview

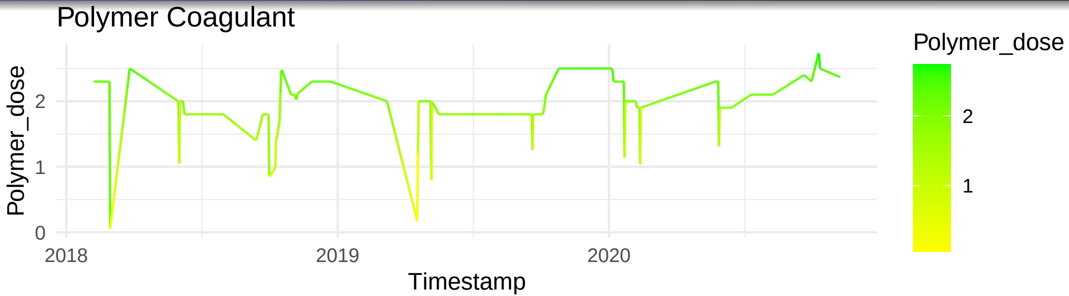
Three years of data from 2018-2020, provided by a Colorado water treatment plant.

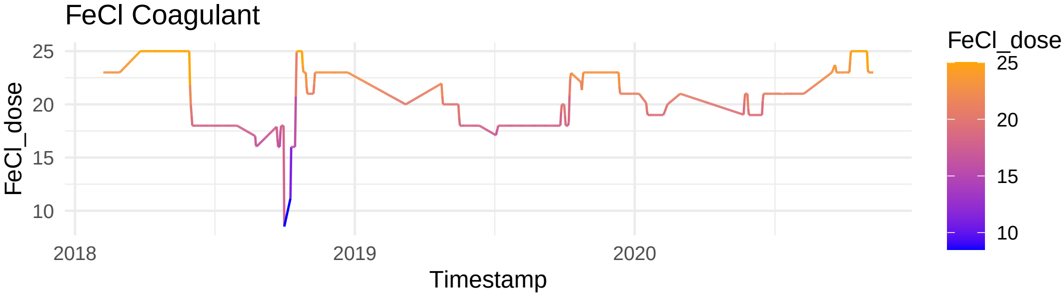
- Raw Water Data
  - pH
  - Temperature (of the water)
  - Turbidity
  - Conductivity
  - Suspended Grain Size
  - Alkalinity
  - Hardness
- Chemical Dosing Data
  - Ferric Chloride Dose: primary additive
  - Cationic Polymer Dose: secondary additive

Data Cleaning

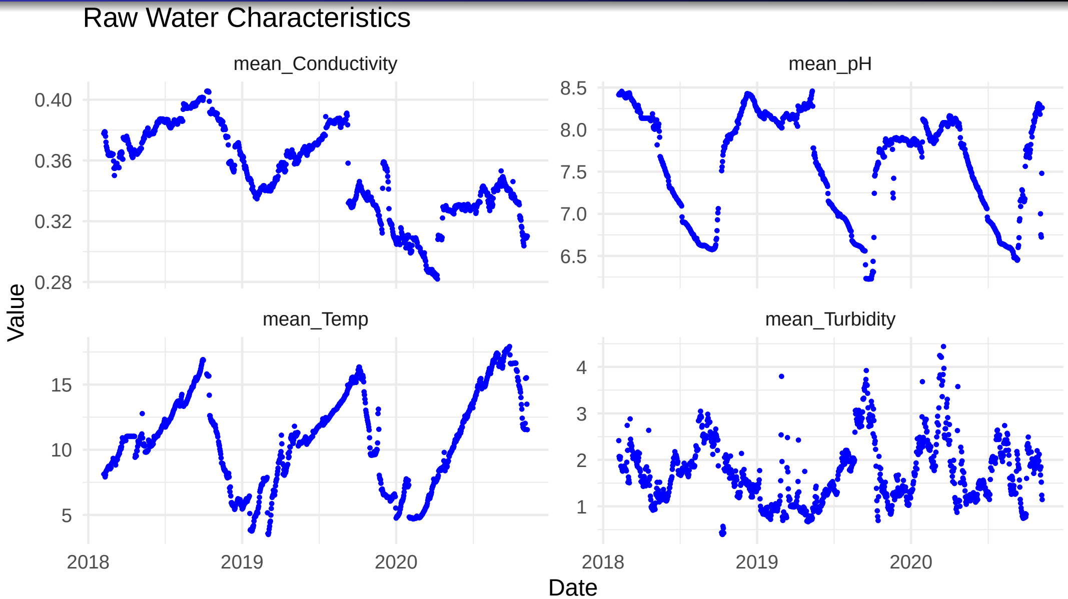
- Dropped Data
  - Suspended grain size was not used as it was highly variable
  - Alkalinity and hardness were not used because of missing data chunks and differing time ranges
- Processing
  - Daily averages were taken for raw water data to match the dosing data's timestep
  - Significant outliers (likely caused by equipment malfunction) were removed or interpolated
  - Dosing and raw water data merged

Exploratory Analysis


Polymer Coagulant


FeCl Coagulant

Exploratory Analysis



Predictor Selection

Temperature and pH seem to have the strongest relationship to dose, consistent with feedback from treatment plant operators. Other data were either highly variable or had minimum availability with large gaps. We will focus on the following to predict dose:

- pH
- Temperature
- Conductivity (lots of noise, weaker)
- Turbidity (lots of noise, weaker)

Focus: **FeCl Dose**. Polymer dose is not changed significantly in plants.

Added Variables

Similar to the stock dataset we've seen in labs and homeworks, our time series dataset needs **lagged variables**.

- For each of the main four parameters:
  - Introduce two lagged variables
  - First represents the day before
  - Second represents two days before

We also introduced a **categorical predictor** indicating whether the dose increased, decreased, or stayed the same compared to the day before.

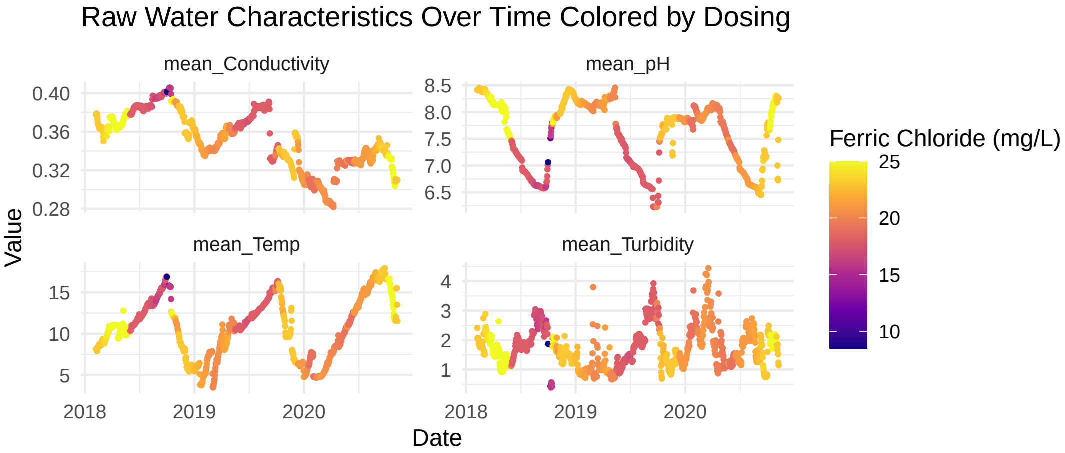
Summary of Modeling

Priorities: Interpretability, Capturing of Nonlinear Behavior

- Training and Testing
  - Training: 2018-2019
  - Testing: 2020
  - Approximately 70/30 split
- Coagulant Dose Prediction
  - Linear Regression
  - Tree-based Models
  - GAM
- Coagulant Dose Change Prediction
  - Linear methods: Multinomial, LDA
  - Nonlinear methods: QDA, Random Forest

Coagulant Dose Prediction

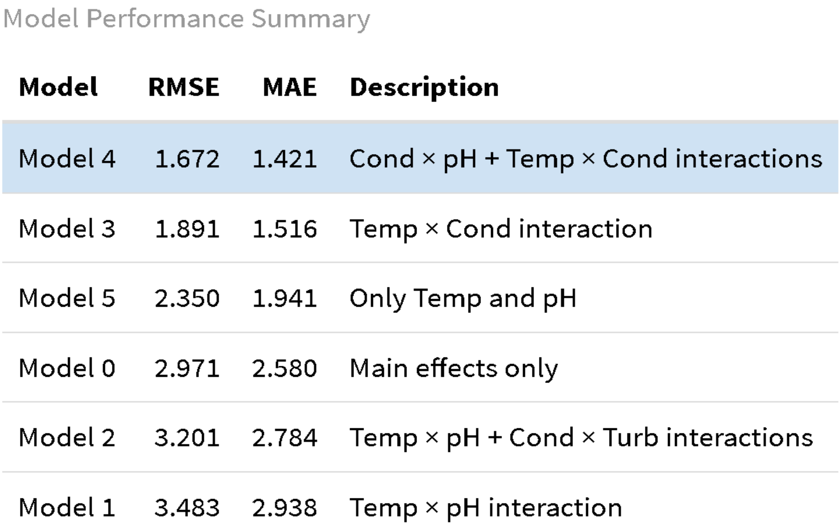
GOAL: Predict coagulant doses based on raw water characteristics.



Coagulant Dose Prediction: Linear Regression

- Created 6 models with different predictors and combinations of interaction terms
- Used lag variables for temp, pH, conductivity, turbidity
- Dropped Turbidity as it was not a good predictor for FeCL dosing
- Difficult to determine what factors of the dataset are driving the predictions
- RMSE and MAE vary widely depending which predictors are selected and the interactions

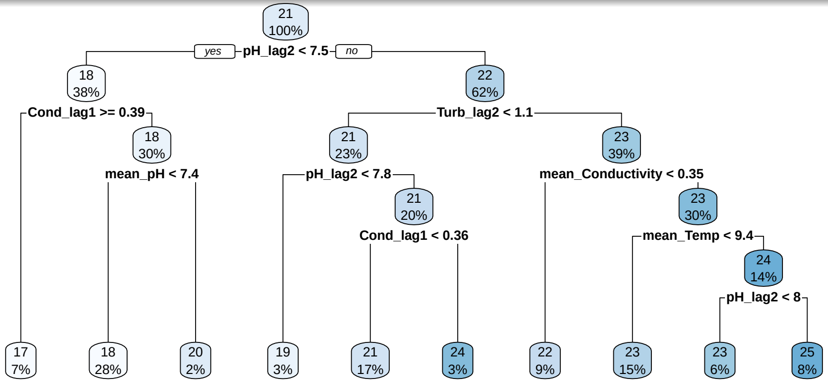
RMSE & MAE Table



Model Performance Summary

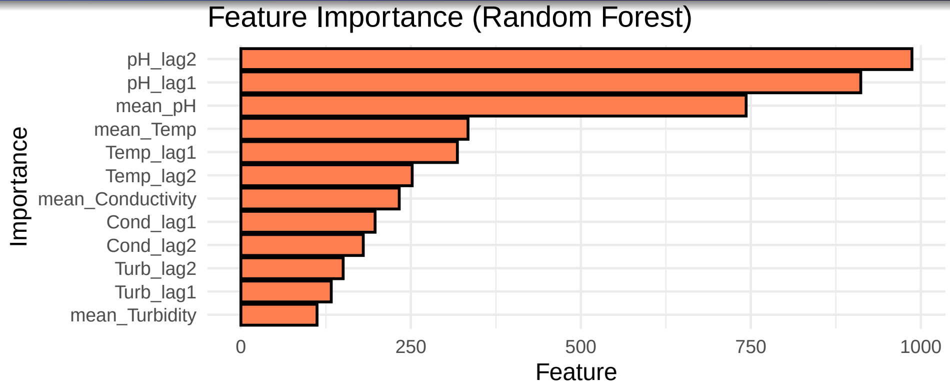
Model	RMSE	MAE	Description
Model 4	1.672	1.421	Cond × pH + Temp × Cond interactions
Model 3	1.891	1.516	Temp × Cond interaction
Model 5	2.350	1.941	Only Temp and pH
Model 0	2.971	2.580	Main effects only
Model 2	3.201	2.784	Temp × pH + Cond × Turb interactions
Model 1	3.483	2.938	Temp × pH interaction

Coagulant Dose Prediction: Decision Tree



Metric	Value
RMSE	2.756
R-Squared	0.012
MAE	2.484

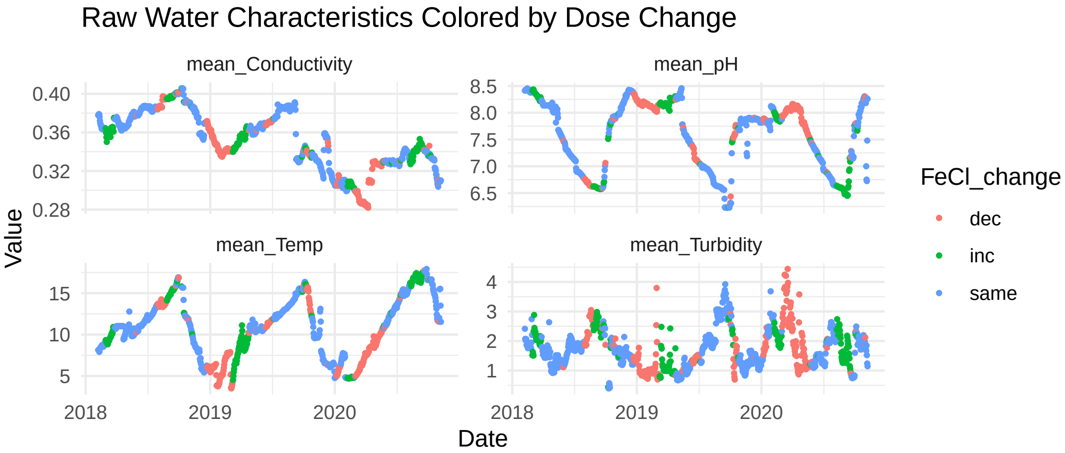
Coagulant Dose Prediction: Random Forest



Metric	Value
RMSE	2.811
R-Squared	0.021
MAE	2.283

Coagulant Dose Change Prediction

GOAL: Predict whether coagulant dose increased, decreased, or stayed the same based on raw water characteristics.



Coagulant Dose Change Prediction: LDA

- Experimented with predictor sets and found that pH and temperature (plus the associated lagged variables) were the main effective predictors.
- Turbidity and conductivity did not improve prediction.

LDA ACCURACY: 43.7%

Table 3: LDA Confusion Matrix

True	dec	inc	same
dec	26	2	74
inc	22	6	44
same	17	16	104

Coagulant Dose Change Prediction: QDA

- Experimented with predictor sets and found that pH and temperature (plus the associated lagged variables) were the main effective predictors.
- Turbidity and conductivity did not improve prediction.

QDA ACCURACY: 35.7%

Table 4: QDA Confusion Matrix

True	dec	inc	same
dec	71	2	29
inc	57	5	10
same	86	16	35

Coagulant Dose Change Prediction: Multinomial Classification

- Experimented with predictor sets and found that pH and temperature (plus the associated lagged variables) were the main effective predictors.
- Turbidity and conductivity did not improve prediction.

MULTINOMIAL ACCURACY: 46.3%

Table 5: Multinomial Regression Confusion Matrix

True	dec	inc	same
dec	31	2	69
inc	22	2	48
same	21	5	111

Coagulant Dose Change Prediction: Random Forest

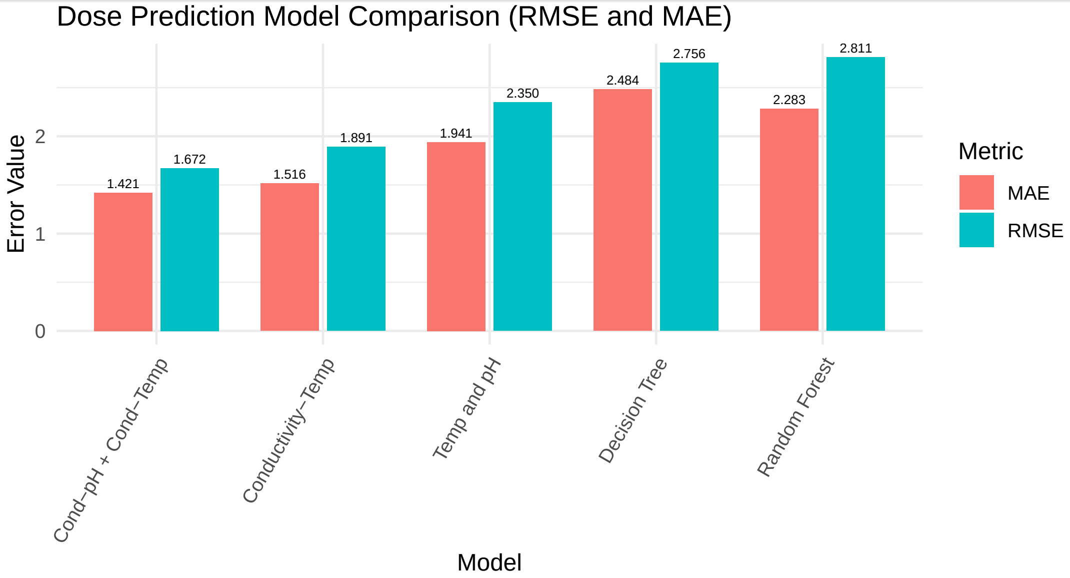
- Experimented with predictor sets and found that pH and temperature (plus the associated lagged variables) were the main effective predictors.
- Turbidity and conductivity did not improve prediction.

RANDOM FOREST ACCURACY: 39.2%

Table 6: Random Forest Confusion Matrix

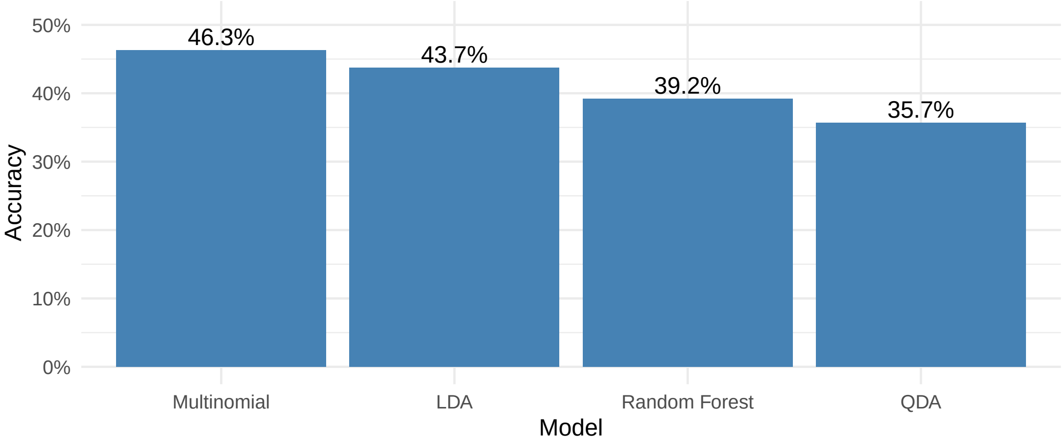
True	dec	inc	same
dec	37	6	59
inc	17	7	48
same	37	22	78

Summary of Dose Prediction Models



Summary of Dose Change Prediction Models

Overall ineffective, and prone to overfitting (especially random forest).
Model predicting no dose change would be more accurate.



Conclusion and Next Steps

- Predicting chemical doses based on these raw water characteristics proved to be ineffective
- Most likely reasons:
  - Limited size of dataset
  - Limited predictor set
  - Operator-dependent
  - Complexity of chemical relationships
  - Other factors (example: reservoir turnover)
- Operators make decisions based on variety of other factors: chemical waste production, filter performance, lab tests, etc.
- Incorporate more varieties and time ranges of data in future modeling efforts