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Chemometric Pattern Recognition:

Using machine learning to decipher complex patterns in chemical data

Leon Delwiche; Dr. Jonathan Nuwer

Introductions

Leon M Delwiche – Marine Scientist +20 years

Managing Technical Consultant – GIS Analyst

Newfields – (now ERM/Newfields) – 15 years

ldelwiche@ermnewfields.com

Dr. Johnathan Nuwer – Senior Chemist/Oceanographer

NewFields

jnuwer@ermnewfields.com

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Outline

1. **What is Machine Learning?**
2. **Machine Learning for Pattern Recognition**
3. **Thoughts and Questions**

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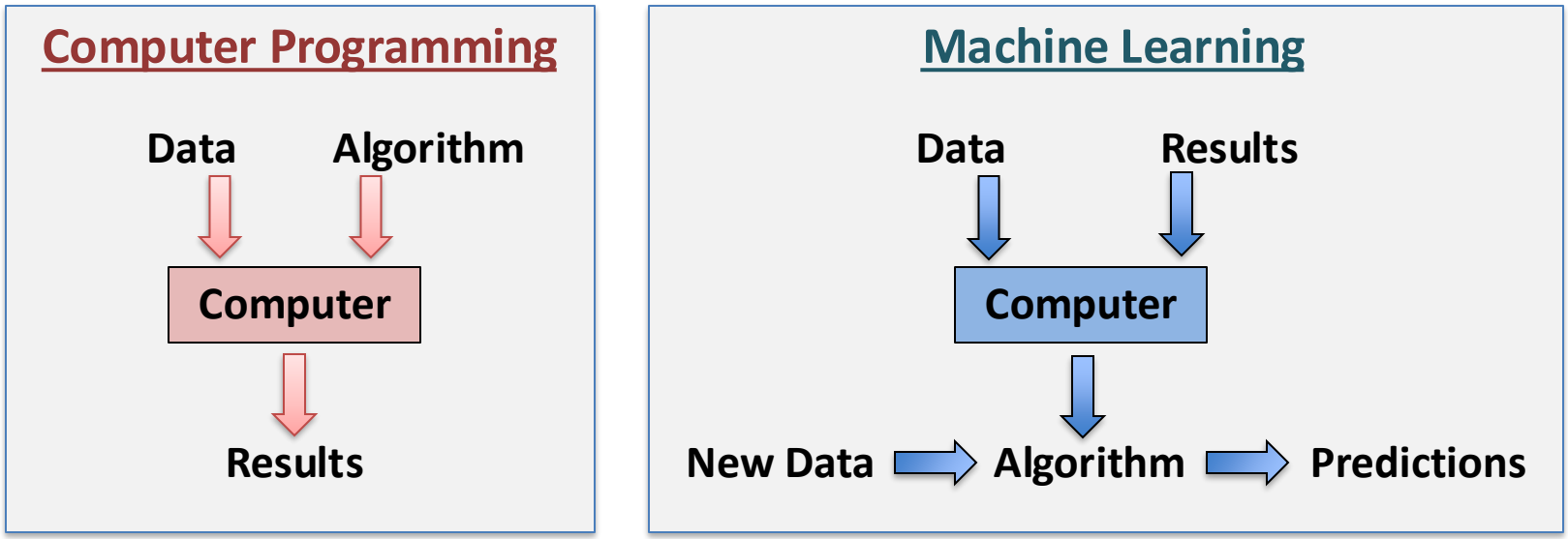
What is machine learning?



- Give the computer the ability to learn without being explicitly programmed
- Artificial Intelligence - computer makes educated decisions

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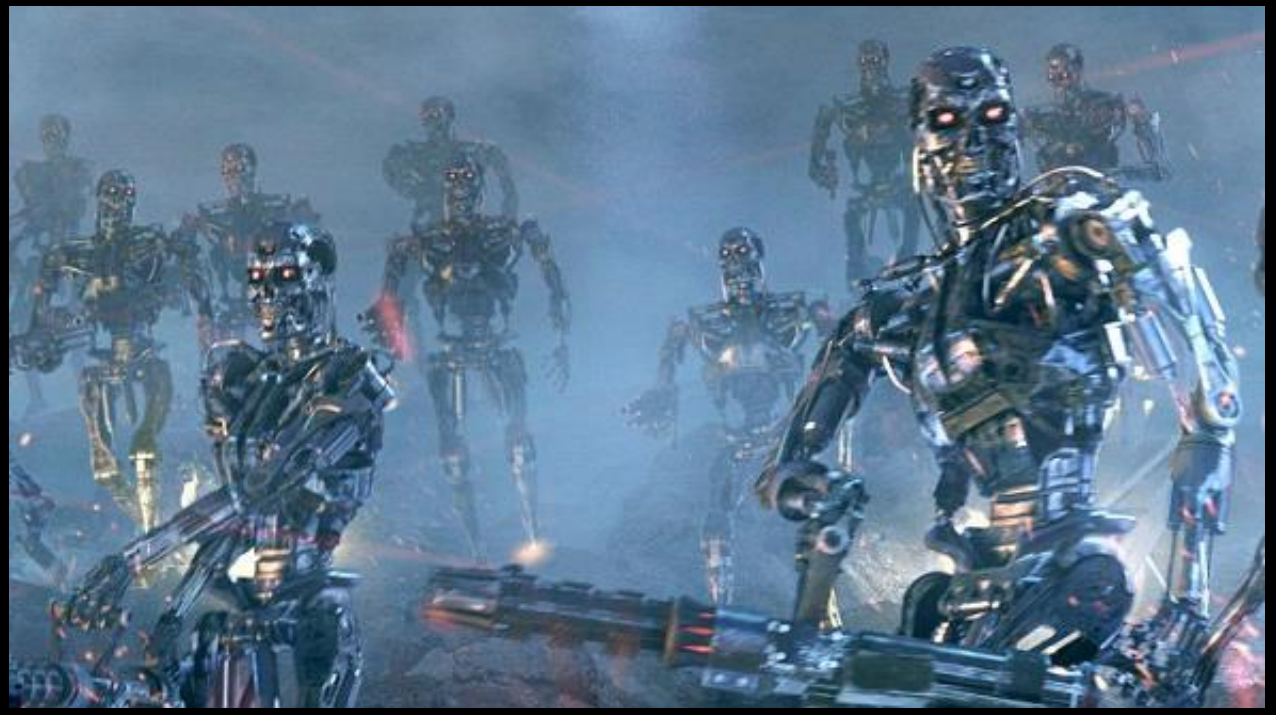
What is machine learning?

ROBOT APOCALYPSE



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Computer-assisted pattern recognition

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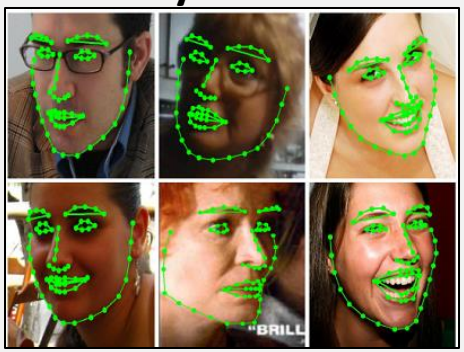
Computer-assisted pattern recognition

Unless processes are totally random, data has pattern

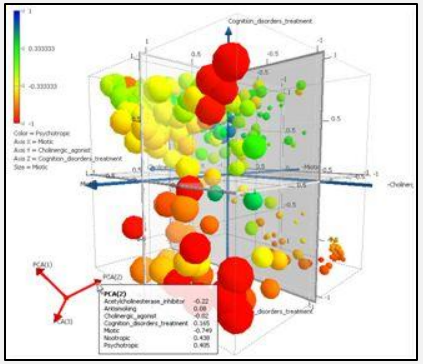
Identity Verification



Bioinformatics

Online Personalization

Chemometrics



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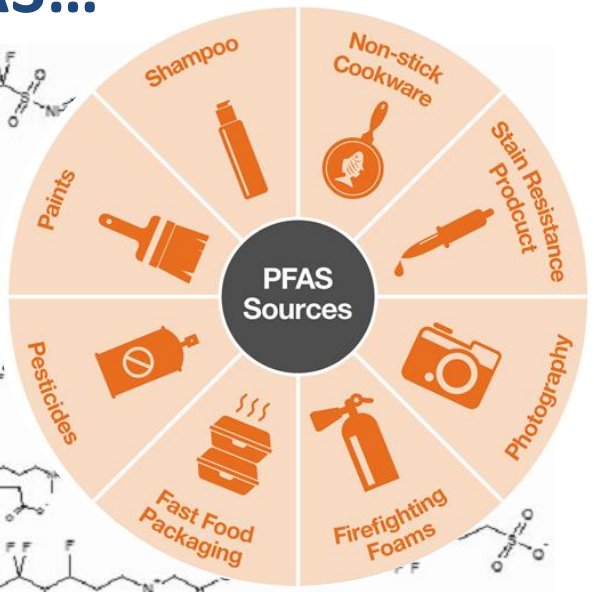
Perfluoroalkyl Substances (PFAS)

There are thousands of PFAS…



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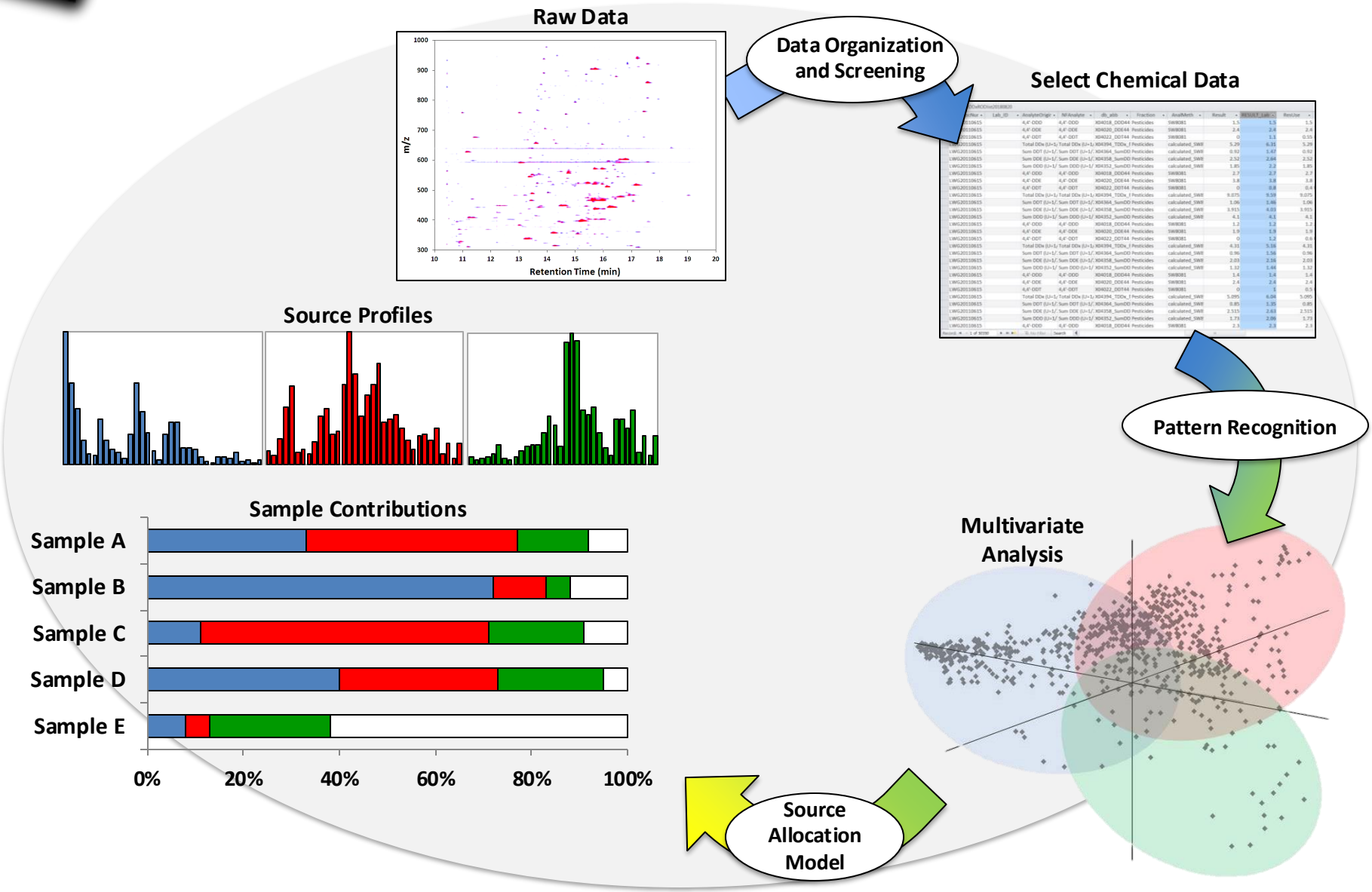
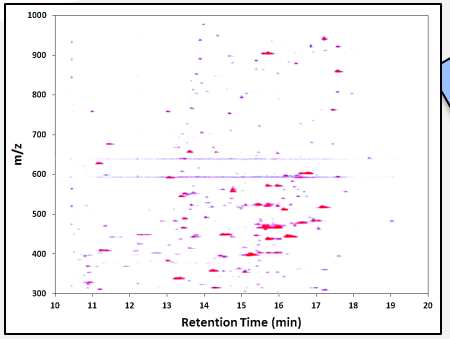
Chemometrics



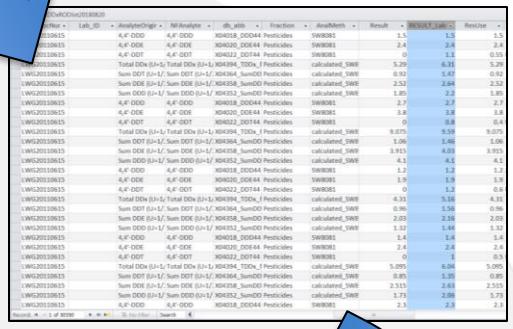
Chemometrics

Raw Data



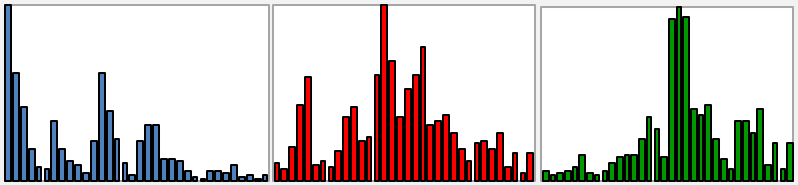
Data Organization and Screening

Select Chemical Data



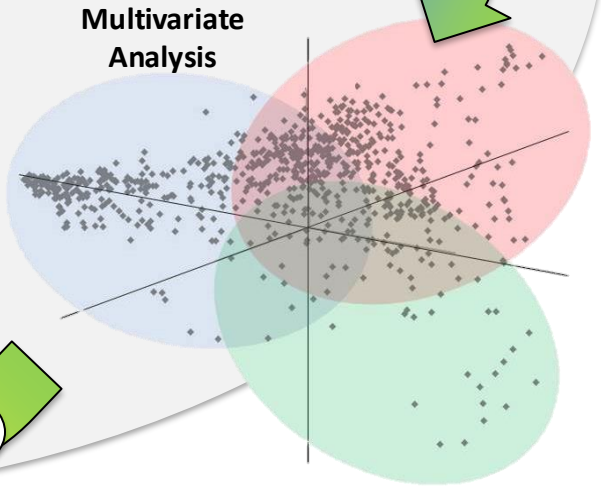
Machine Learning

Source Profiles

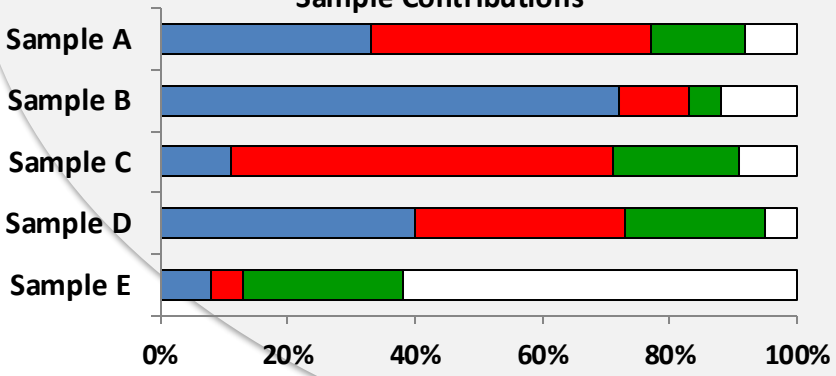


Pattern Recognition

Multivariate Analysis

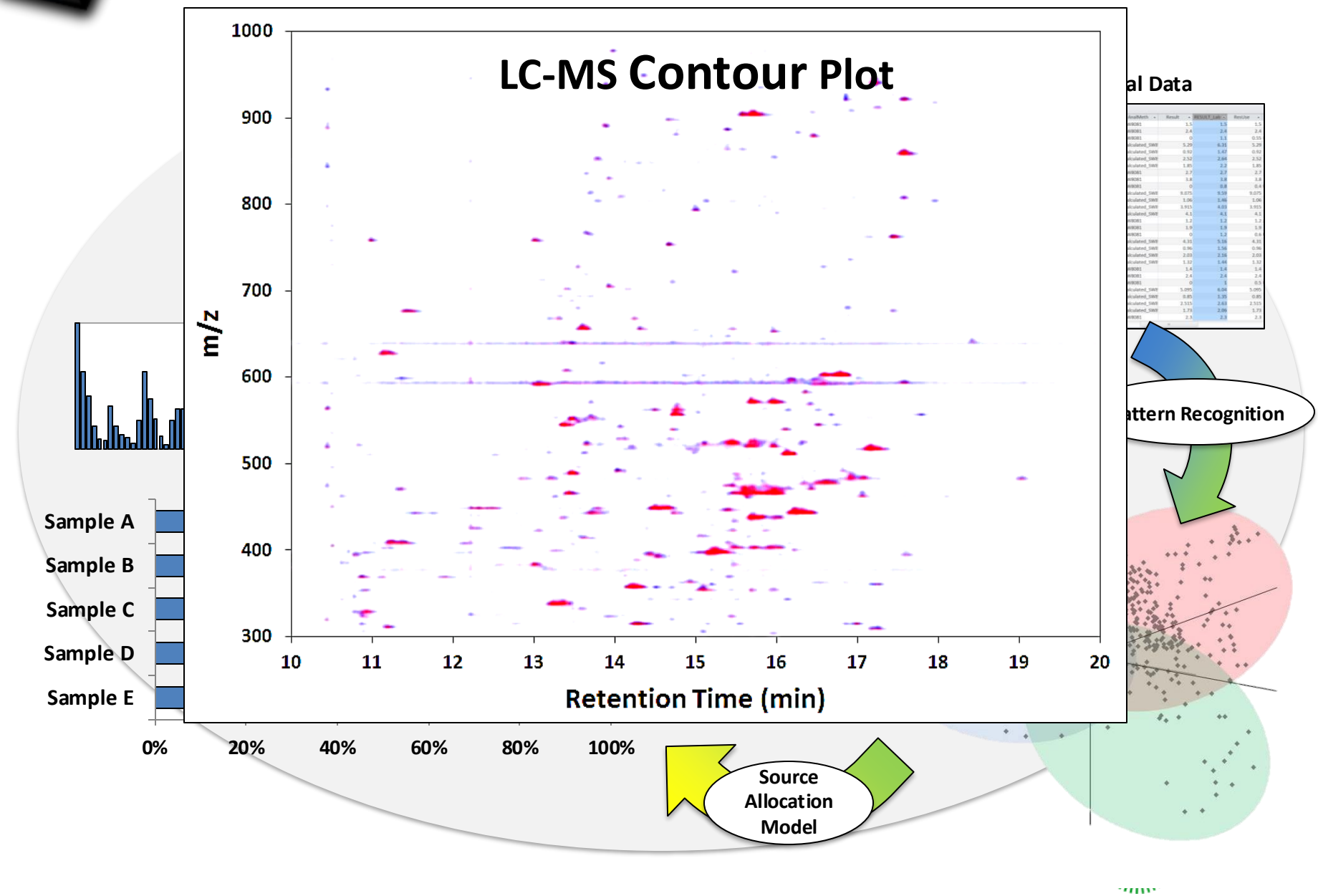


Sample Contributions

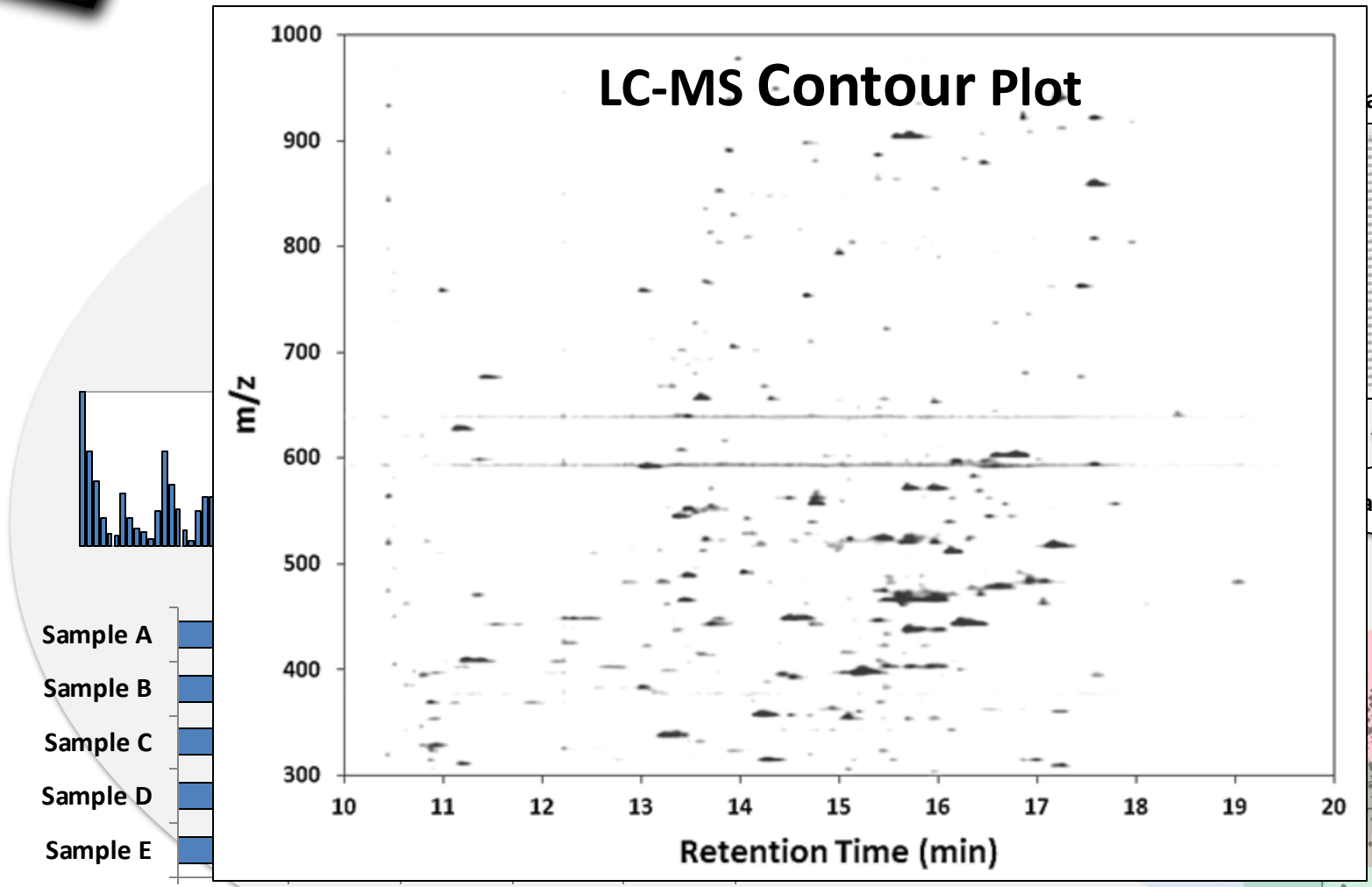


Source Allocation Model

Chemometrics



Chemometrics



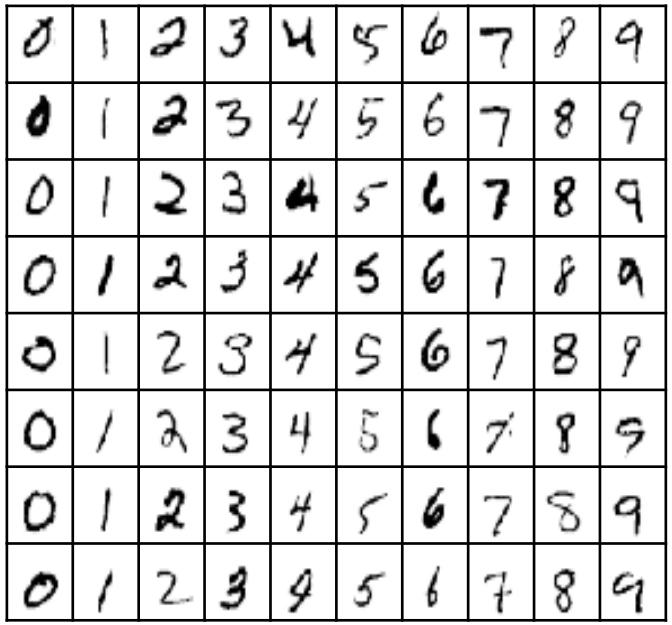
How does machine learning work?

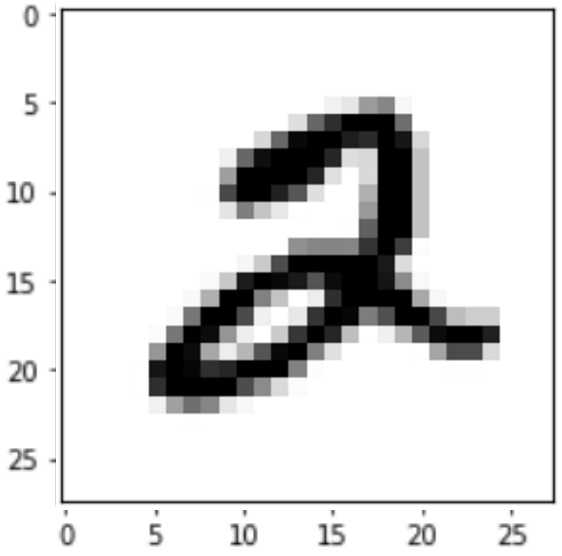
MNIST Dataset:

- **Handwritten digits (0-9)**
- **100 people**

Each image:

- **28 x 28 pixels**
- **Pixel values 0-100**





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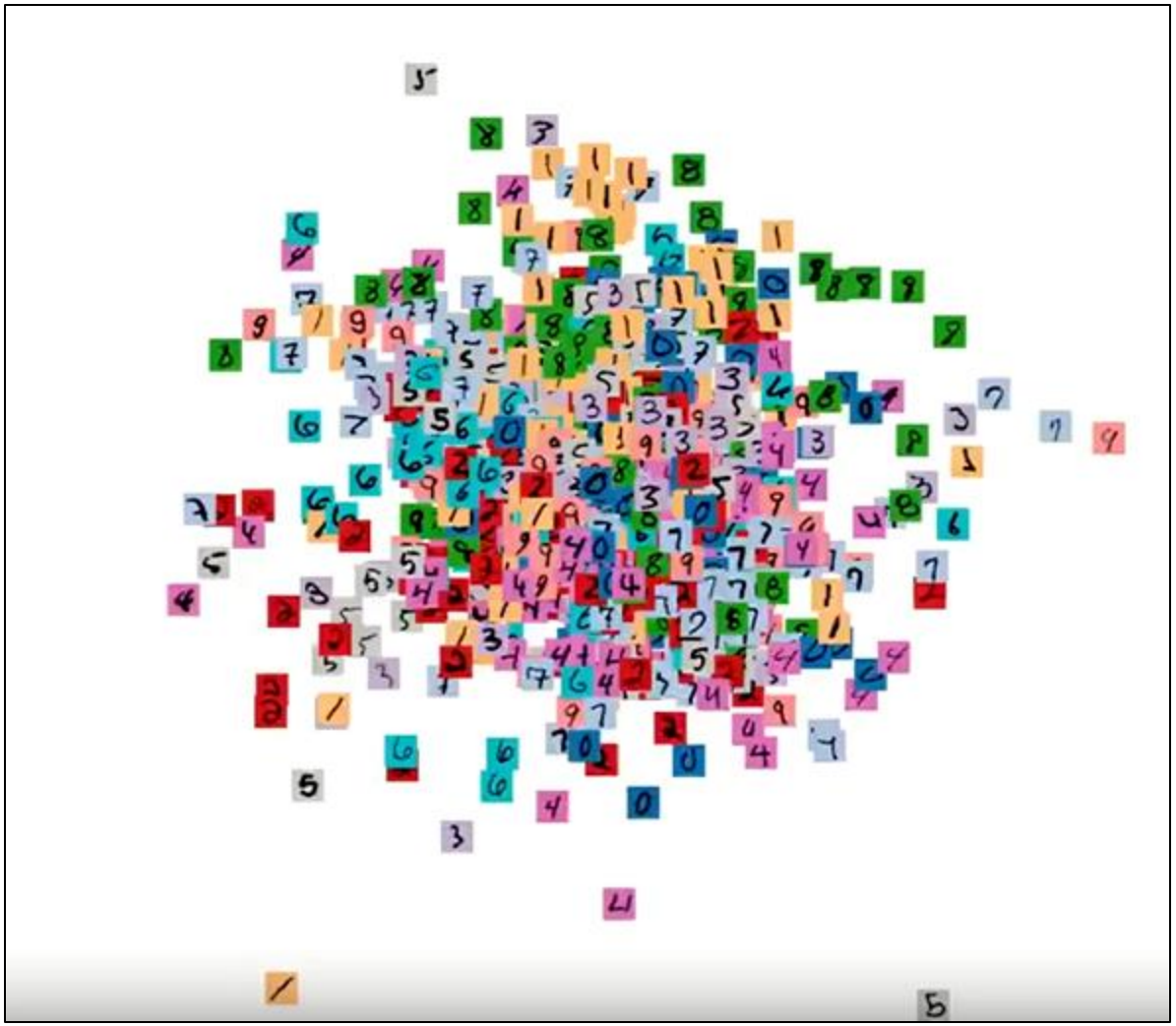
Machine Learning with R's MXNet



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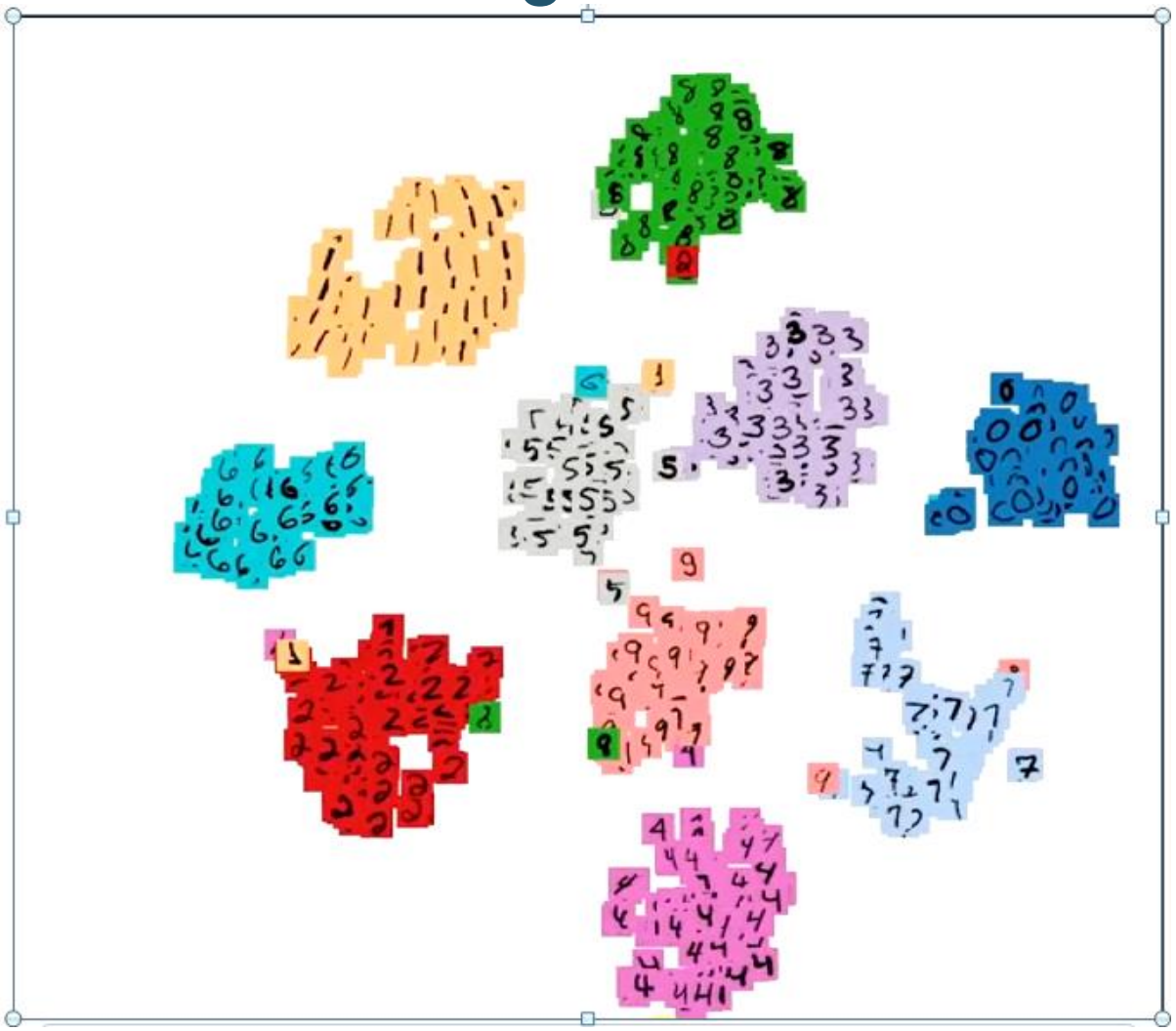

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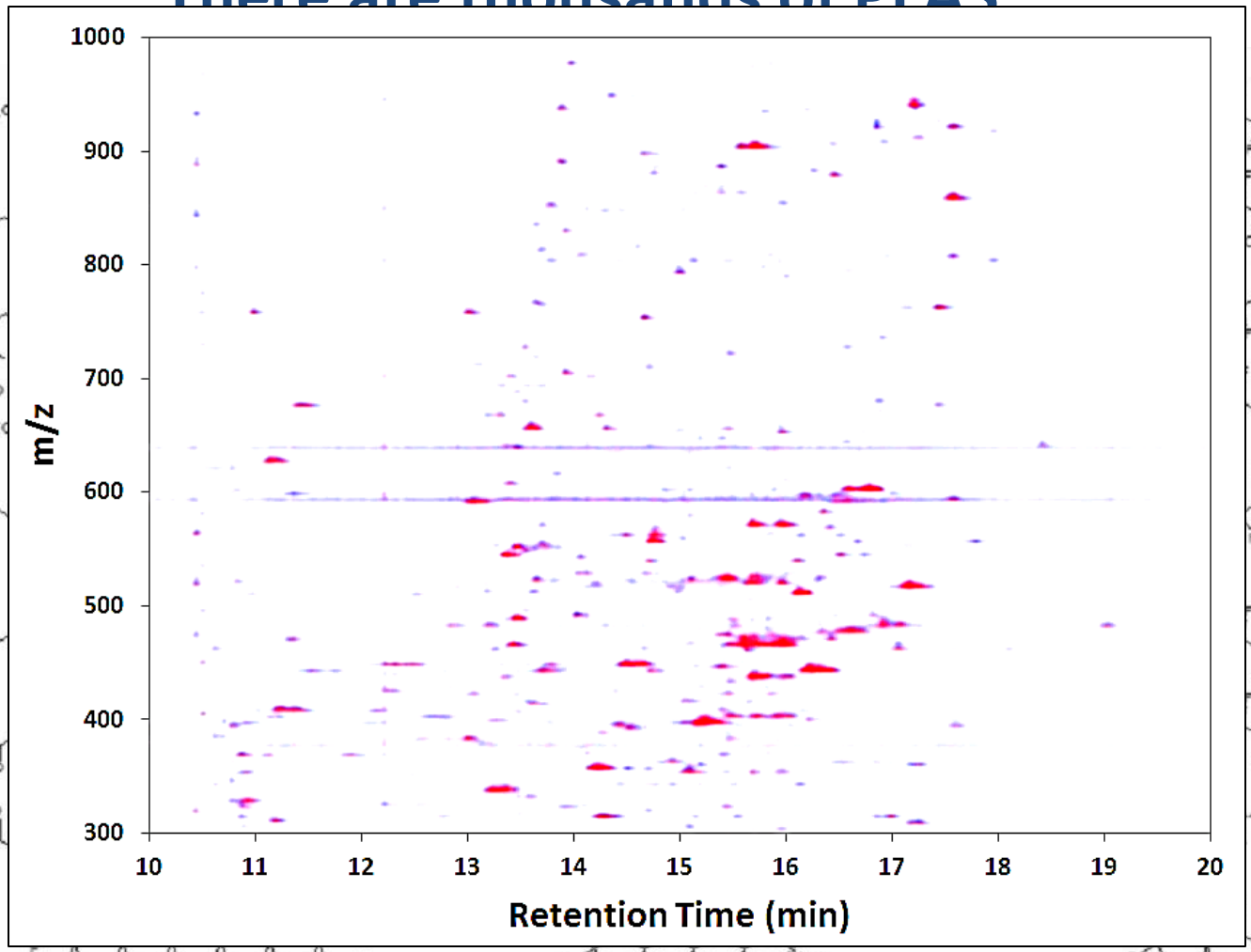
PFAS Patterns – From the LC-MS?

There are thousands of PFAS



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How I will use Machine Learning

1. Check on manual data interpretation
    - What are the diagnostic compounds?
    - Did you bias the results?

2. Instant Knowledge (relative to sample library)
    - Identify outliers
    - Assess similarity
    - Source mixture composition

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Questions?

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