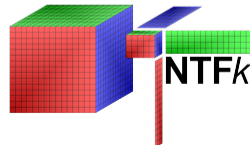


Unsupervised and Physics-Informed Machine Learning Analyses for Characterization of Energy Production from Unconventional Reservoirs

Velimir V. Vesselinov (monty) (vvv@lanl.gov)

Earth and Environmental Sciences Division
Los Alamos National Laboratory, NM, USA

<http://tensors.lanl.gov>



- ▶ **Supervised** ML: learns everything from data
 - ⇒ requires big training datasets
 - ⇒ highly impacted by noise
- ▶ **Physics-informed** ML: learns from data but includes preconceived knowledge about the governing processes
 - ⇒ requires smaller training datasets
 - ⇒ produces better predictability with lower uncertainty
 - ⇒ robust to data noise
- ▶ **Unsupervised** ML: extracts features from data that can be applied for categorization and prediction
 - ⇒ unbiased analyses not impacted by data labeling, subject-matter-expert opinions, and physics assumptions
 - ⇒ however, physics constraints can be added

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- ▶ **Supervised** ML: requires “labeling” (prior categorization (knowledge) about the processed data)

Example: Recognizes images of cats and dogs after extensive training; but cannot recognize horses if not trained

Cannot discover something that we do not know already

- ▶ **Unsupervised** ML: extracts hidden features (signals) in the processed data without any prior information (**exploratory analysis; data-driven science**)

Example: Identifies features that distinguish images of animals (e.g., cats, dogs, horses, etc.)

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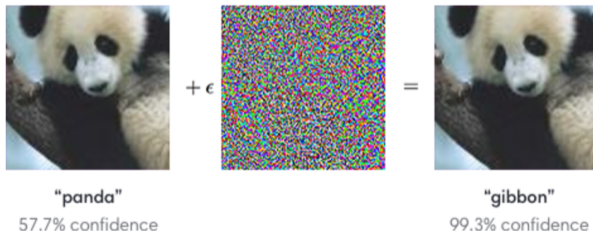
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▶ Supervised ML

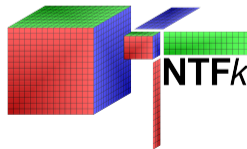
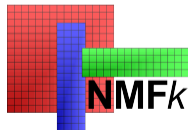
- ▶ introduces subjectivity (through the labeling process)
- ▶ does not provide insights why horses are different from dogs / cats
- ▶ cannot make predictions (that we do not know already)
- ▶ requires huge training (labeled) datasets
- ▶ we do not know why it works
- ▶ is impacted by “adversarial examples”



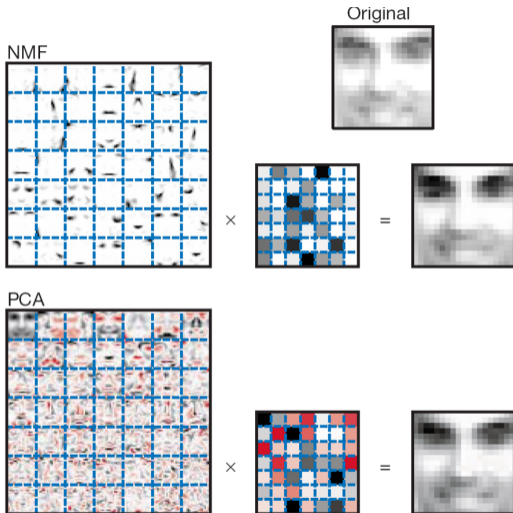
⇒ major limitations of the **supervised** ML methods for **science** applications

- ▶ Feature extraction (**FE**)
- ▶ Blind source separation (**BSS**)
- ▶ Detection of disruptions / anomalies
- ▶ Image recognition
- ▶ Separate physics processes
- ▶ Discover unknown dependencies and phenomena
- ▶ Develop reduced-order/surrogate models
- ▶ Identify dependencies between model inputs and outputs
- ▶ Guide development of physics models representing the data
- ▶ Make predictions
- ▶ Optimize data acquisition
- ▶ “Label” datasets for supervised ML analyses

- ▶ Novel LANL-patented, open-source, unsupervised Machine Learning (ML) methods and computational techniques
- ▶ Based in matrix/tensor factorization coupled with custom k -means clustering and nonnegativity/sparsity constraints:
 - NMF k : Nonnegative **Matrix** Factorization
 - NTF k : Nonnegative **Tensor** Factorization
 - <https://github.com/TensorDecompositions>
- ▶ Capable to efficiently process large datasets (TB's) utilizing GPU's, TPU's & FPGA's
⇒ **Julia**, Flux.jl, AutoOffLoad.jl, TensorFlow, PyTorch, MXNet

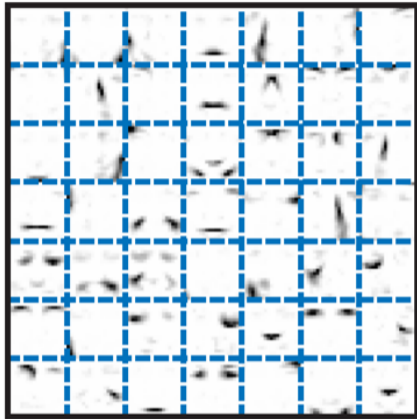


- ▶ NMF vs PCA (Lee & Seung, 1999)
- ▶ NMF: Nonnegative Matrix Factorization
- ▶ PCA: Principal Component Analysis

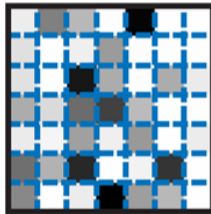


Nonnegativity constraints provide meaningful and interpretable results (+sparsity)

- ▶ **Tensors** (multi-dimensional/multi-modal/multi-way datasets) are everywhere:
 - ▶ observational data are typically a 5-D tensor (x, y, z, t, attributes)
 - ▶ model outputs are typically a 5-D tensor (x, y, z, t, attributes)
 - ▶ data dependency to N parameters will form a $(N + 5)$ -D tensor

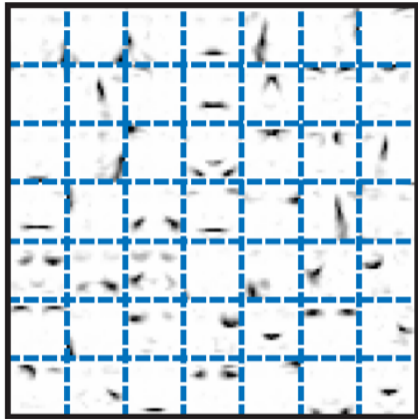


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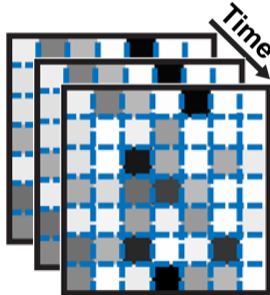


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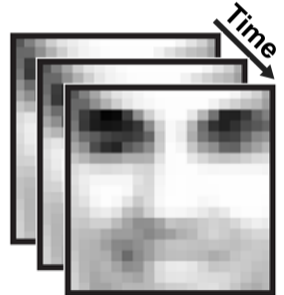


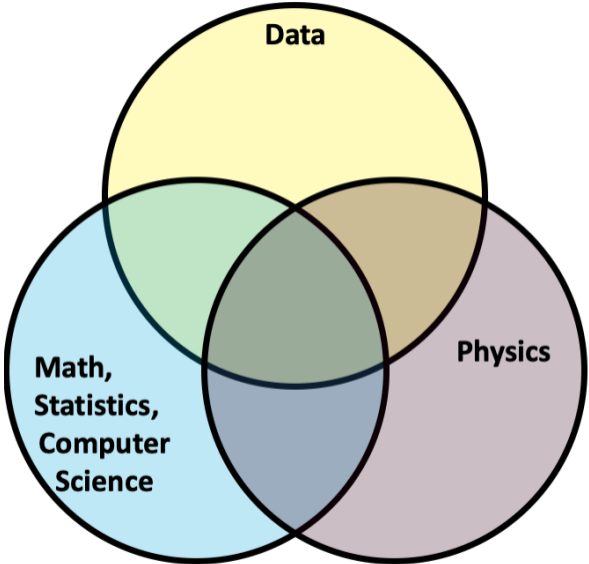


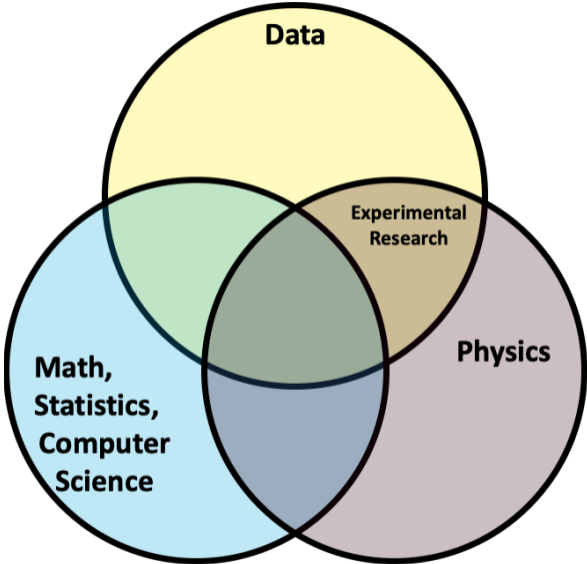
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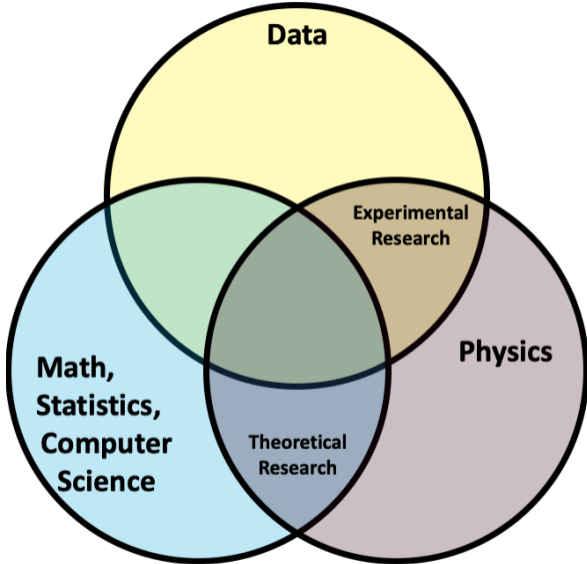


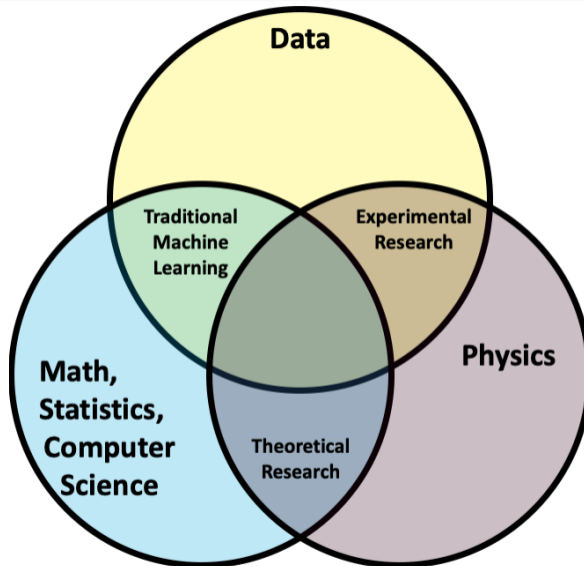
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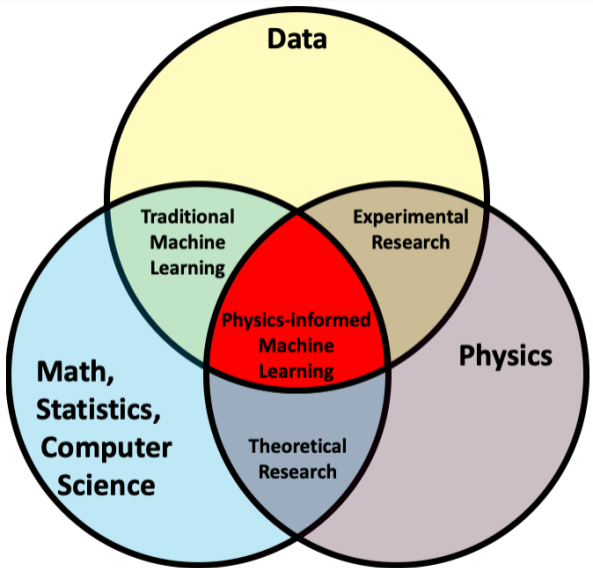




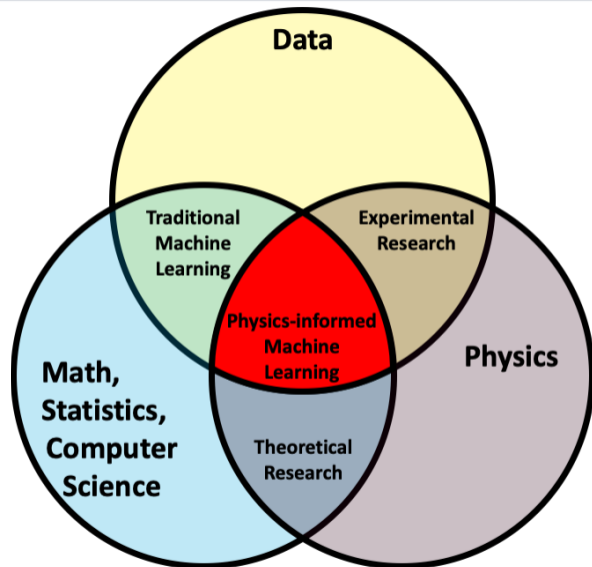


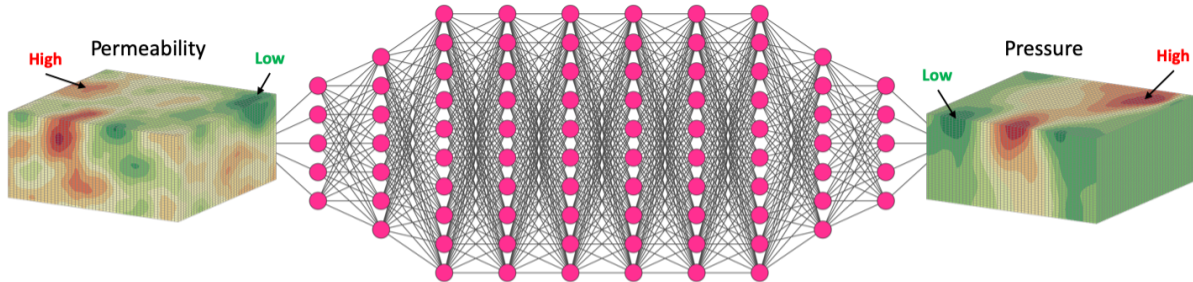




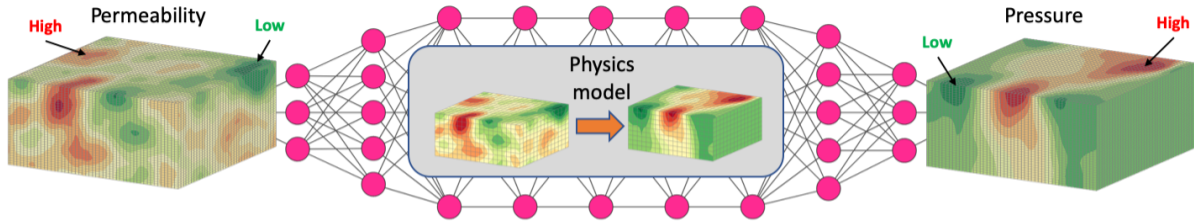


- ▶ **Empirical**: observations and experiments (since the cradle of our civilization)
- ▶ **Theoretical**: generalizations and models (since 1600's)
- ▶ **Computational**: analytical and numerical simulations (since 1950's)
- ▶ **Data-exploration**: unify data, simulations, and theory (since 2000's)

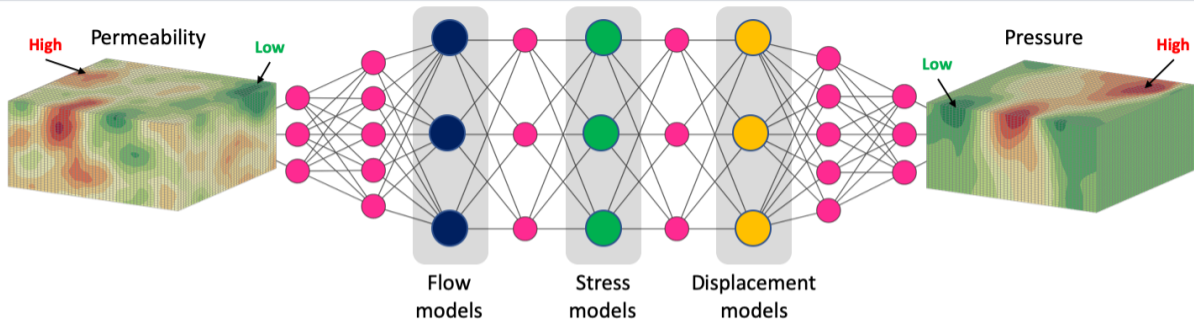




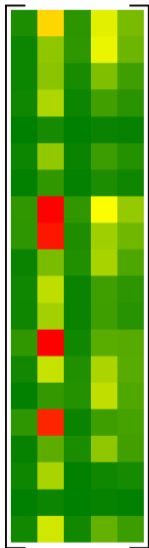
- ▶ it is a **black box**, **ad hoc** approach
- ▶ no preconceived knowledge about analyzed problem (general)
- ▶ all the neurons are $relu(Ax + b)$; A and b have no physical meaning; $relu()$ does not impose physics constraints
- ▶ neural networks needs to be very **deep** and **wide** to represent complex physics



- ▶ include preconceived knowledge about analyzed problem (problem specific)
- ▶ neurons can represent $PhysicsModel(Ax + b)$; A and b have physical interpretation; $PhysicsModel()$ imposes physics constraints (e.g. conservation of mass/species)
- ▶ **PIML** models can be **trained (optimized) faster** and with **less training data**

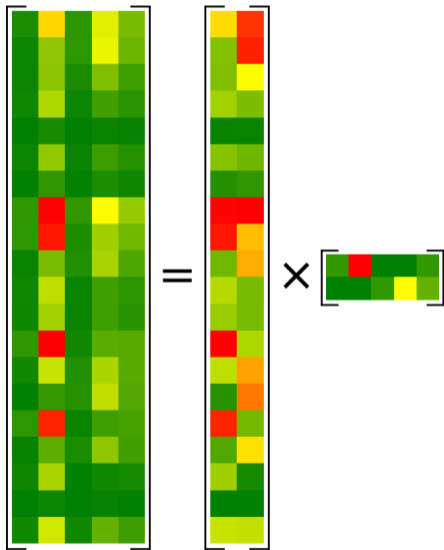


- ▶ physics-informed layers (“**fat**” **neurons**) capture important governing processes (e.g., flow, stress, deformation, and displacement)
- ▶ can be done efficiently only through differentiable programming in **julia**
- ▶ ongoing projects with **JuliaComputing** to further develop novel **PIML** theory, methods, and tools



$$\mathbf{X}$$
$$[20 \times 5]$$

\mathbf{X} – data matrix
[attributes × observations]



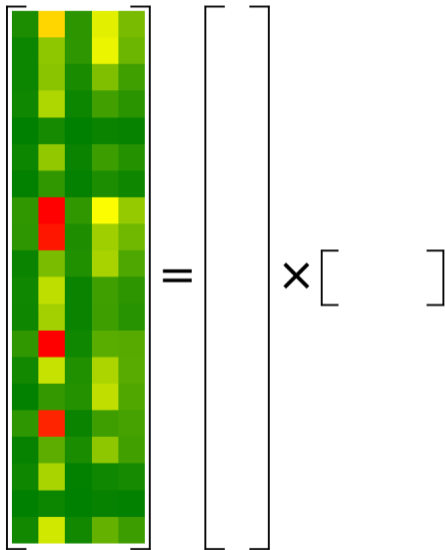
$$X = W \times H$$

$$[20 \times 5] = [20 \times 2] \times [2 \times 5]$$

X – **data** matrix
 [attributes × observations]

W – **feature (signal)** matrix
 [attributes × features]

H – **mixing** matrix
 [features × observations]



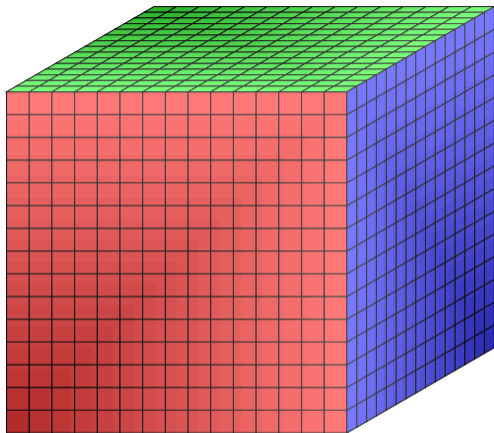
$$X = W \times H$$

$$[20 \times 5] = [20 \times ?] \times [? \times 5]$$

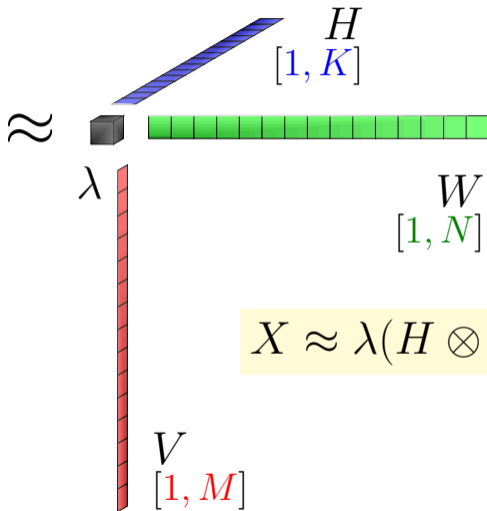
⇒ 100 **knowns**

⇒ **unknown** number of features
(2 or more)

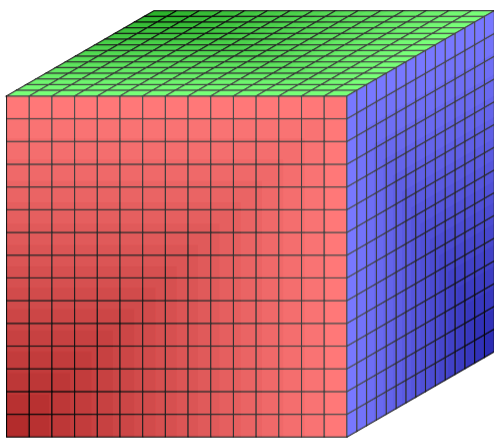
⇒ **unknown** matrix elements of W and H
(50 or more)



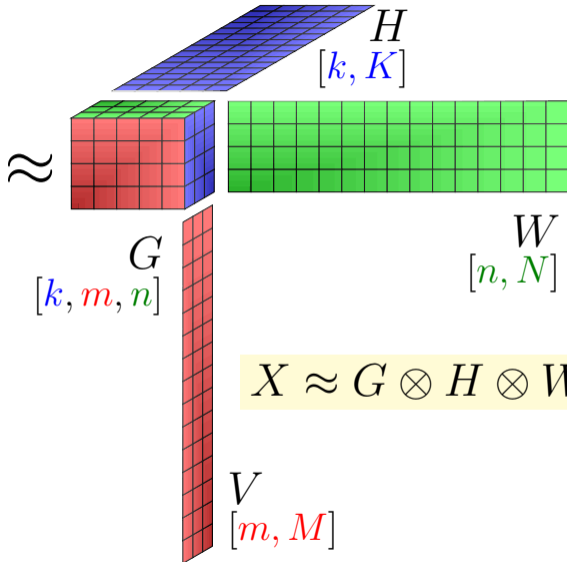
X
[K , M , N]



$$X \approx \lambda(H \otimes W \otimes V)$$

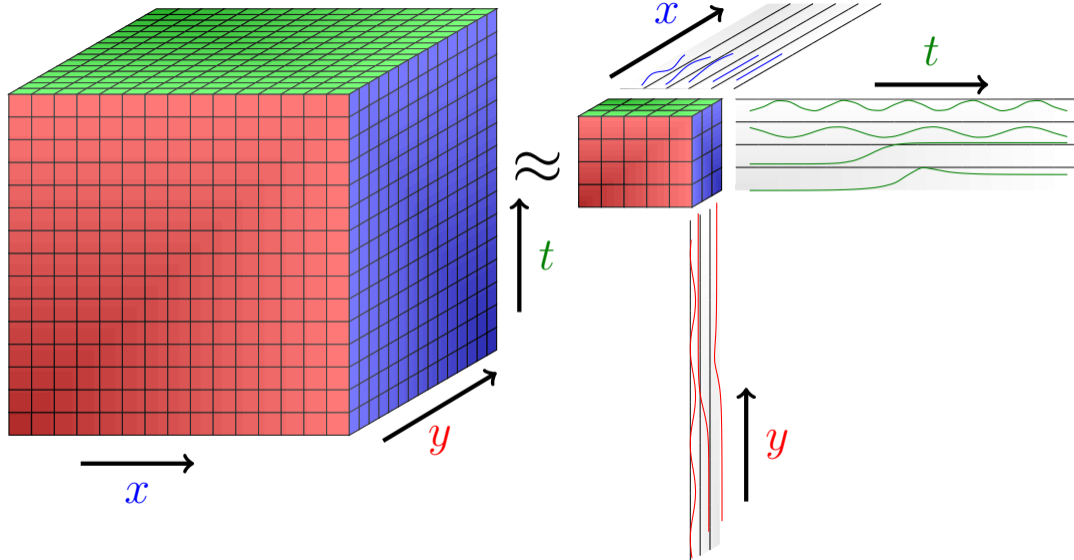


X
[K, M, N]



$$X \approx G \otimes H \otimes W \otimes V$$

Tucker Tensor Decomposition (3D): Rank-60 / Multirank-(3,4,5) tensor



▶ Field Data:

- ▶ Contamination
- ▶ Climate
- ▶ Geothermal
- ▶ Seismic
- ▶ Oil/gas production

▶ Lab Data:

- ▶ X-ray Spectroscopy
- ▶ UV Fluorescence Spectroscopy
- ▶ Microbial population analyses
- ▶ Isotope fractionation

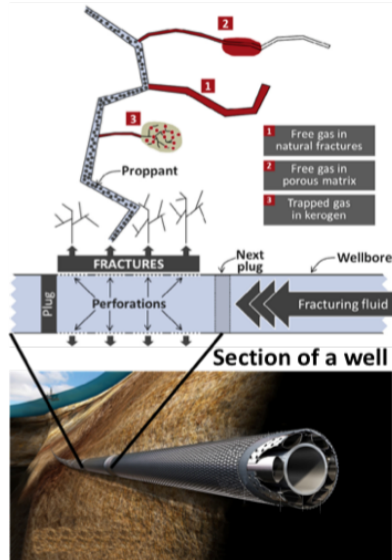
▶ Operational Data:

- ▶ LANSCE: Los Alamos Neutron Accelerator
- ▶ Oil/gas production

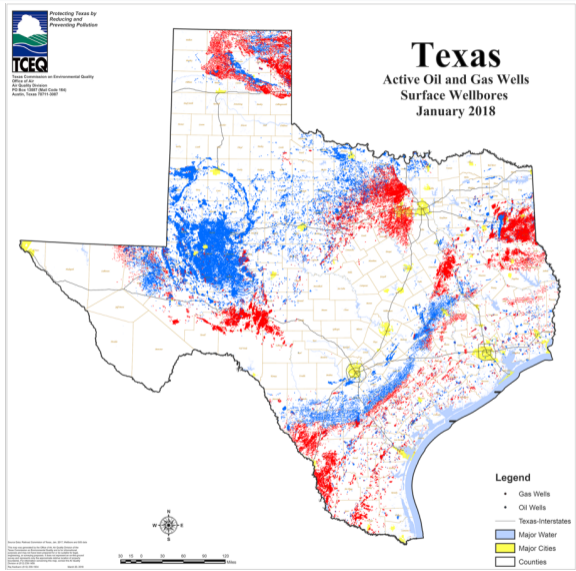
▶ Model Outputs:

- ▶ Reactive mixing $A + B \rightarrow C$
- ▶ Phase separation of co-polymers
- ▶ Molecular Dynamics of proteins
- ▶ Climate modeling

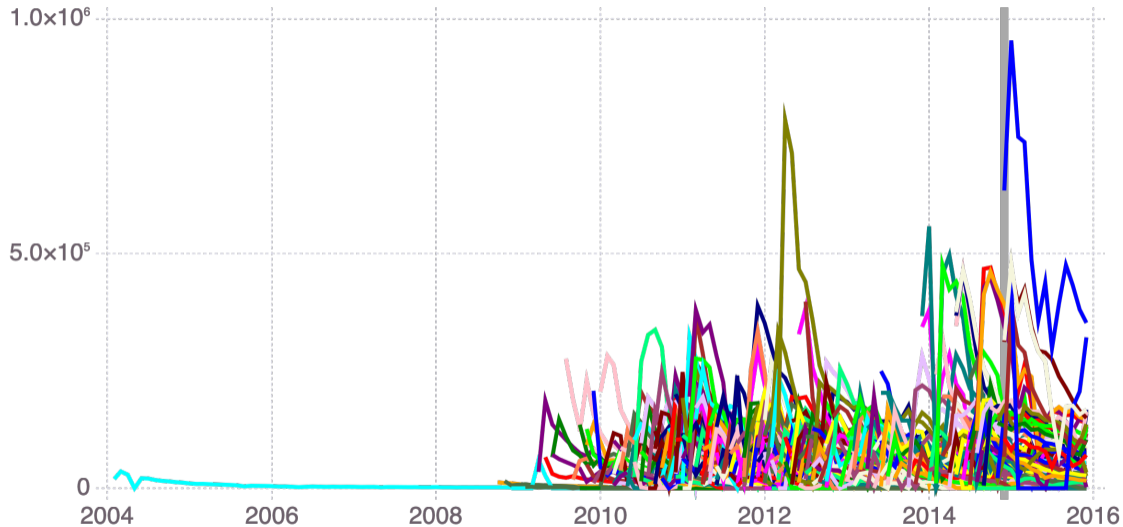
- ▶ Oil/Gas production from unconventional reservoirs extracts a small portion of the available resources (<10%)
- ▶ Oil/Gas production is challenging to predict and optimize
- ▶ Physics processes during well development (including hydrofracking) and extraction are poorly understood and challenging to simulate
- ▶ Alternative is to learn to predict system behavior based on the observed oil/gas production at existing wells



- ▶ Large public datasets are available representing unconventional oil and gas production (U.S. and world wide)
- ▶ Data represent monthly production rates (oil, gas, water) + many other well attributes
- ▶ ~ 2,000,000 wells in U.S.
- ▶ > 300,000 wells in Texas
- ▶ > 20,000 wells in Eagle Ford Shale Play
- ▶ 327 gas wells in Eagle Ford Shale Play selected for preliminary analyses

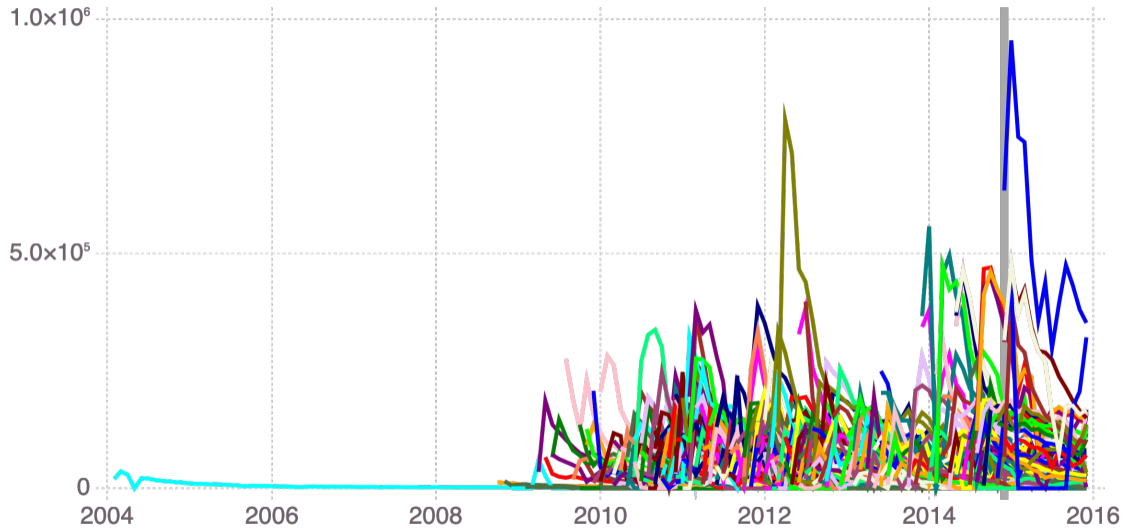


Eagle Ford Shale Play: Monthly production volumes [MCF] of 327 gas wells

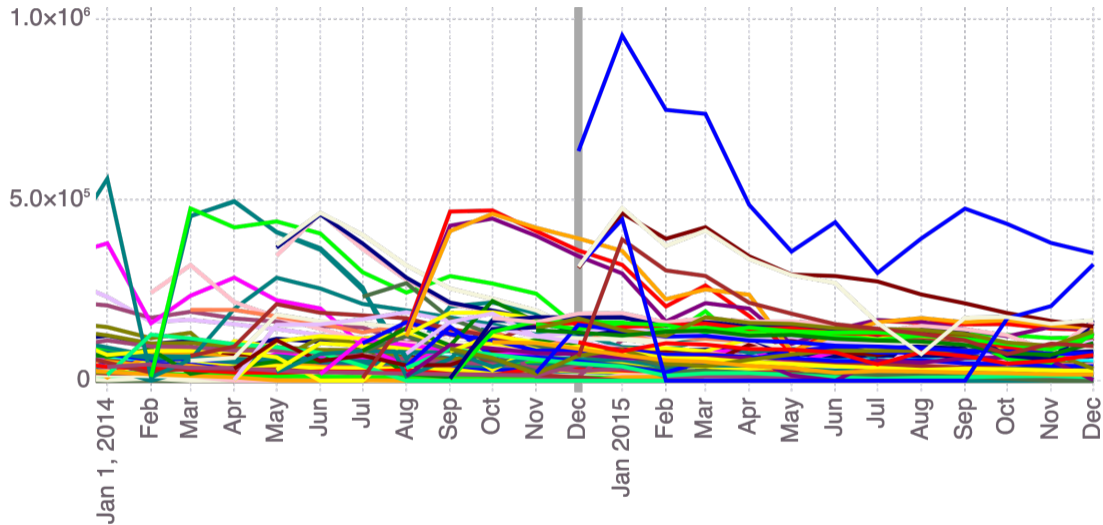


- ▶ Use all the data up to a given cutoff date (e.g. 2015)
- ▶ Apply ML to learn behavior of the “known“ well transients
 - Identify and group wells which behave similarly (having similar production transients)
 - Discover the optimal number of **master decline curves** required to reproduce the observed transients
 - **master decline curves** represent production **features/signatures**
- ▶ Apply ML to predict **blindly** the unknown production transients beyond the cutoff
- ▶ Prediction is obtained by discovering to which type (group) the wells producing beyond the cutoff belong
- ▶ i.e., discovering what combinations of the **master decline curves** can represent the wells producing beyond the cutoff
- ▶ Unsupervised ML analyses performed using **SmartTensors (NMFk/NTFk)**

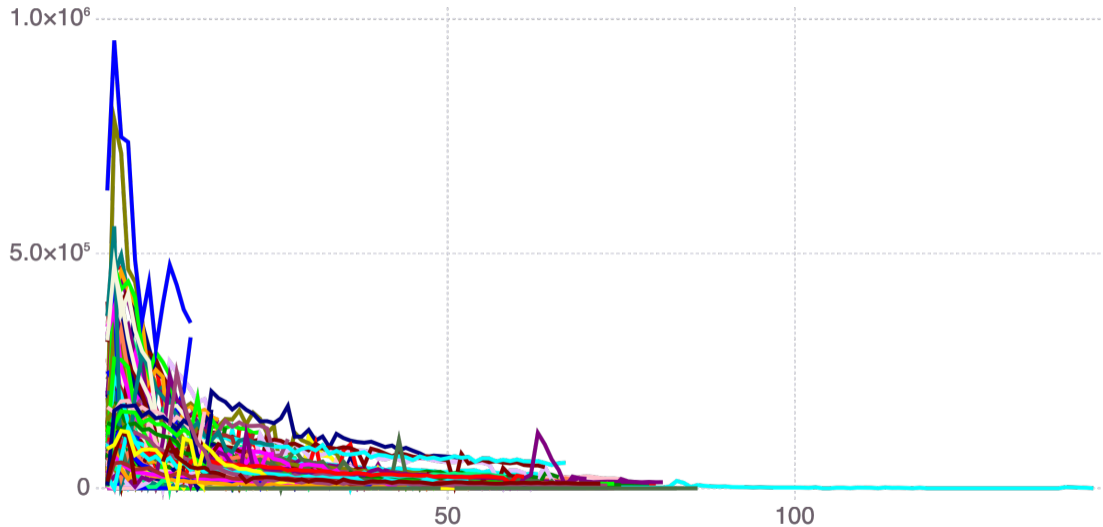
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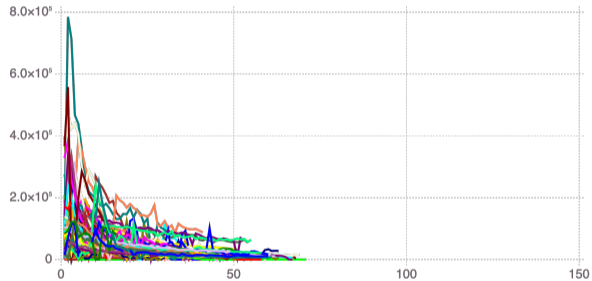
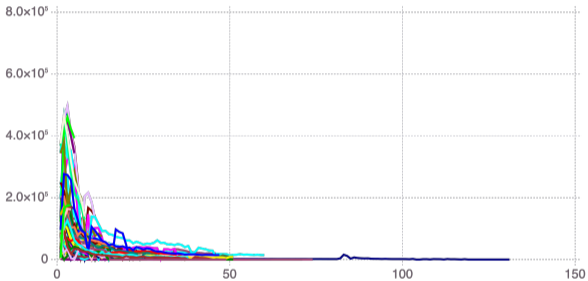


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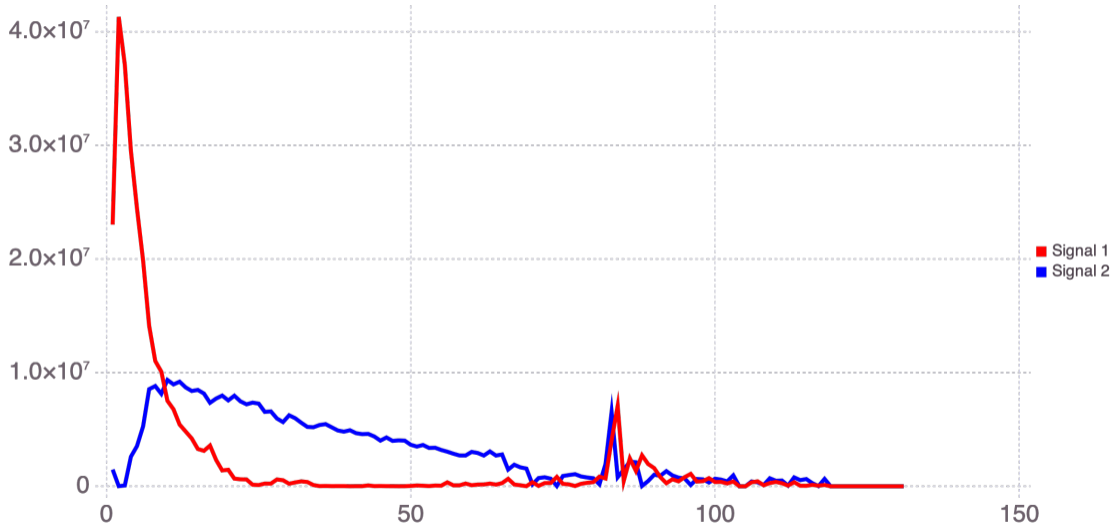


'Fast' declining (135)

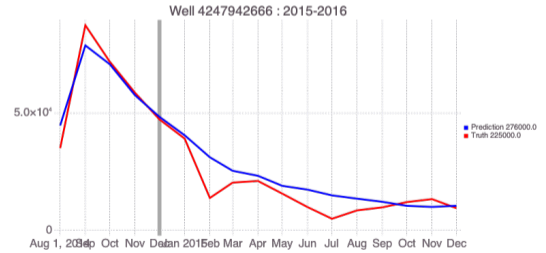
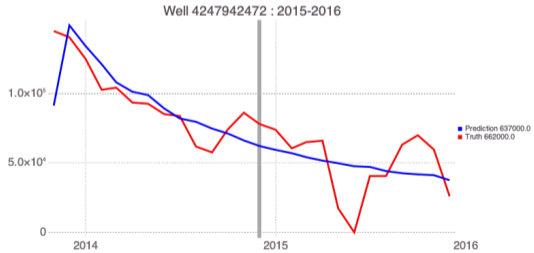
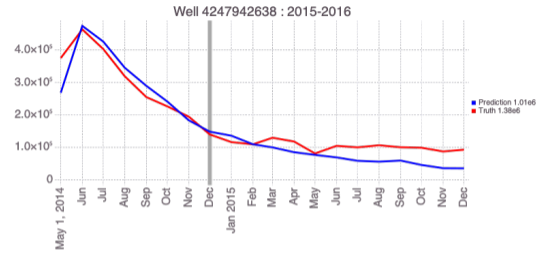
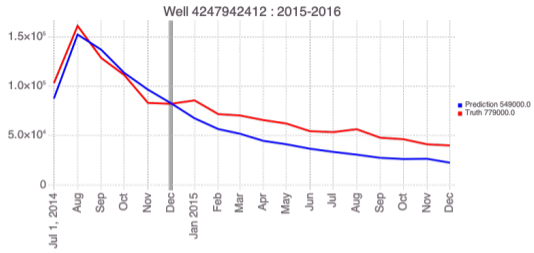
'Slow' declining (192)



Eagle Ford Shale Play: Master Decline Curves [MCF over months]

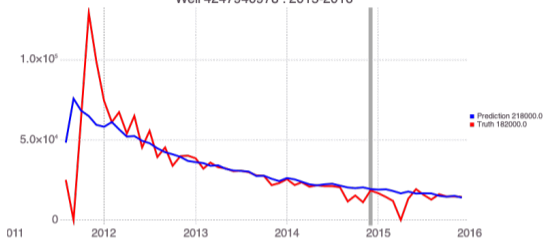


Eagle Ford Shale Play: Blind predictions beyond 2015

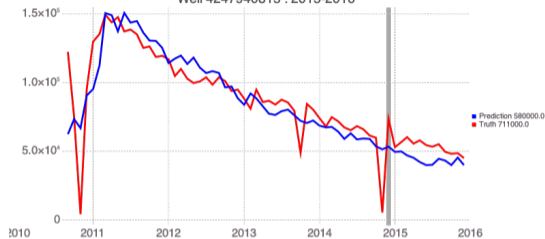


Eagle Ford Shale Play: Blind predictions beyond 2015

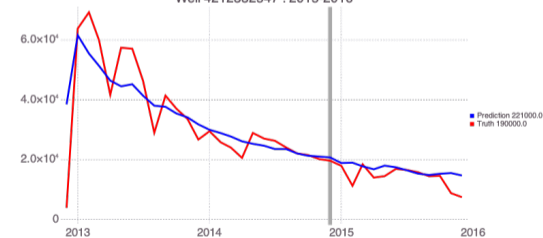
Well 4247940978 : 2015-2016



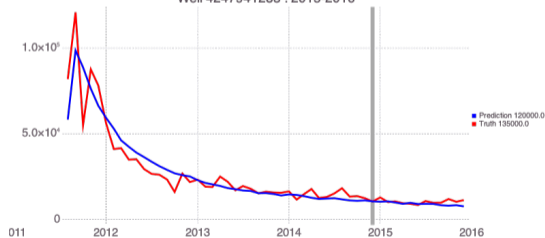
Well 4247940815 : 2015-2016



Well 4212332547 : 2015-2016



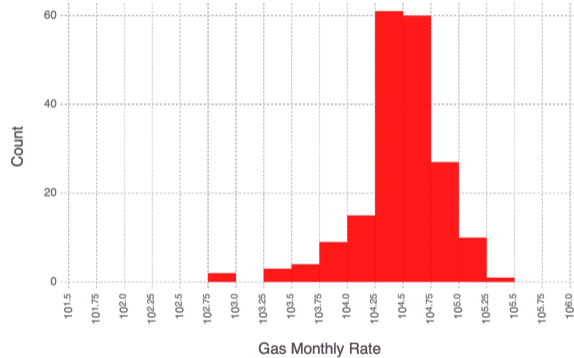
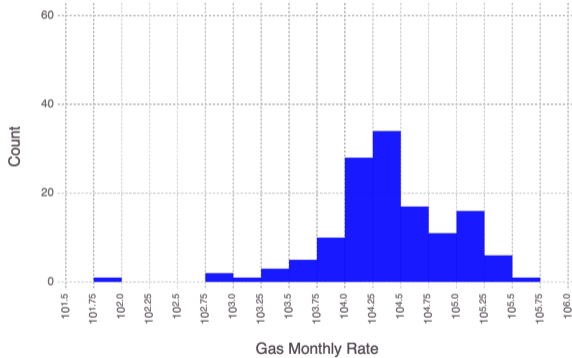
Well 4247941283 : 2015-2016



Monthly rate histograms

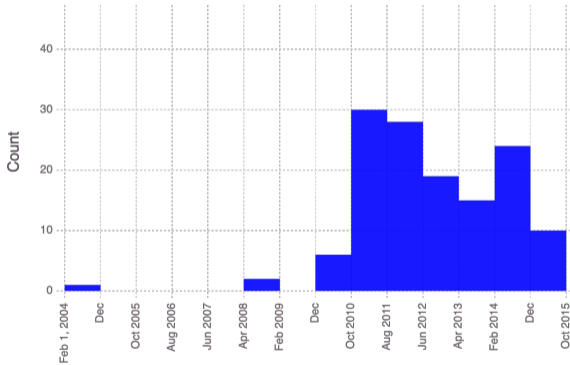
'Fast' declining (135)

'Slow' declining (192)

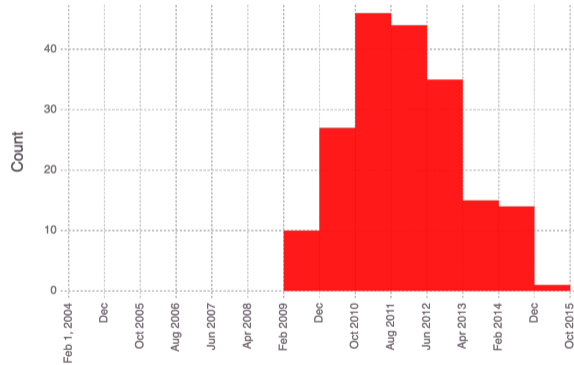


Drilling date histograms

'Fast' declining (135)

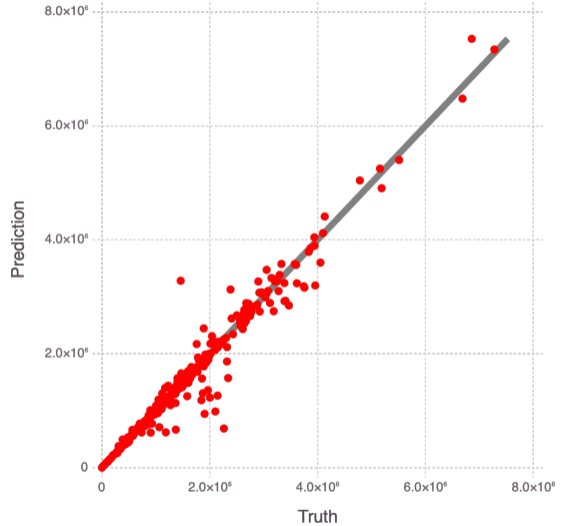


'Slow' declining (192)

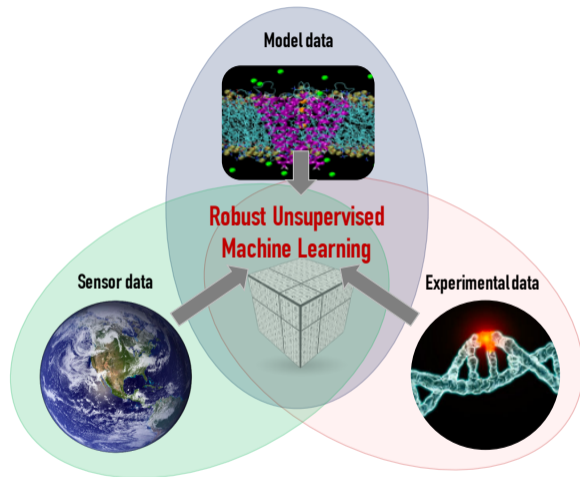


- ▶ Other well attributes also differ between the 2 groups
- ▶ For example:
 - Operators
 - Proppant mass
 - Injected fluid volumes
 - ...

- ▶ 300 wells continue producing beyond 2015
- ▶ $r^2 = 0.96$

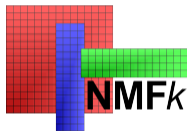


- ▶ Developed **novel** unsupervised and physics-informed ML methods and computational tools
- ▶ Some of our tools have been recently patented
- ▶ Our ML methods have been used to solve various real-world problems (brought breakthrough discoveries related to human cancer research)
- ▶ Several ongoing projects (DOE, ARPA-E, ...)



► Codes:

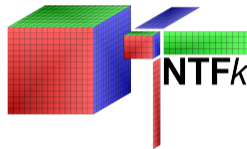
NMF_k



MADS



NTF_k



► Examples:

http://madsjulia.github.io/Mads.jl/Examples/blind_source_separation

<http://tensors.lanl.gov>

<http://tensordecompositions.github.io>

<https://github.com/TensorDecompositions>

<https://hub.docker.com/u/montyvesselinov>



- ▶ Vesselinov, Munuduru, Karra, O'Malley, Alexandrov, Unsupervised Machine Learning Based on Non-Negative Tensor Factorization for Analyzing Reactive-Mixing, **Journal of Computational Physics**, Special issue: Machine Learning, 2019.
- ▶ Stanev, Vesselinov, Kusne, Antoszewski, Takeuchi, Alexandrov, Unsupervised Phase Mapping of X-ray Diffraction Data by Nonnegative Matrix Factorization Integrated with Custom Clustering, **Nature Computational Materials**, 2018.
- ▶ Vesselinov, O'Malley, Alexandrov, Nonnegative Tensor Factorization for Contaminant Source Identification, **Journal of Contaminant Hydrology**, 2018.
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