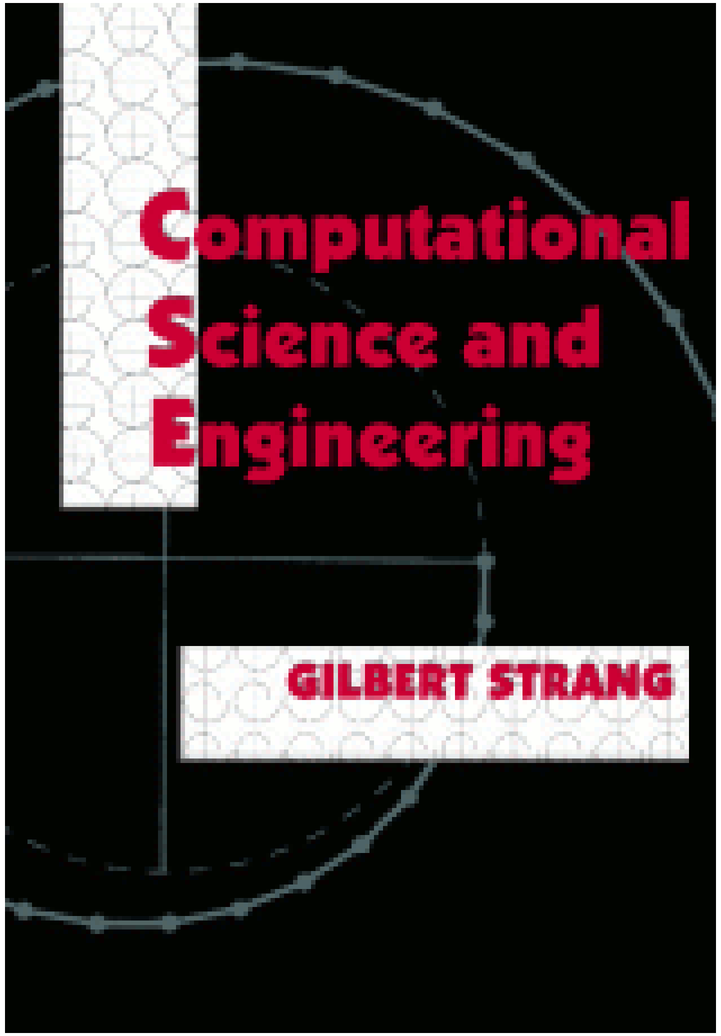
AY: 2008~2017



http://math.mit.edu/~gs/cse/

Applied Mathematics for Computational Design and Analysis
전산설계 및 해석을 위한 응용수학

- MIT Math 18.065 Computational Science and Engineering I

Ch	Contents	
1	Applied Linear Algebra	○
2	A Framework for Applied Mathematics	○
3	Boundary Value Problems	○
4	Fourier Series and Integrals	
5	Analytic Functions	
6	Initial Value Problems	
7	Solving Large Systems	
8	Optimization and Minimum Principles	○

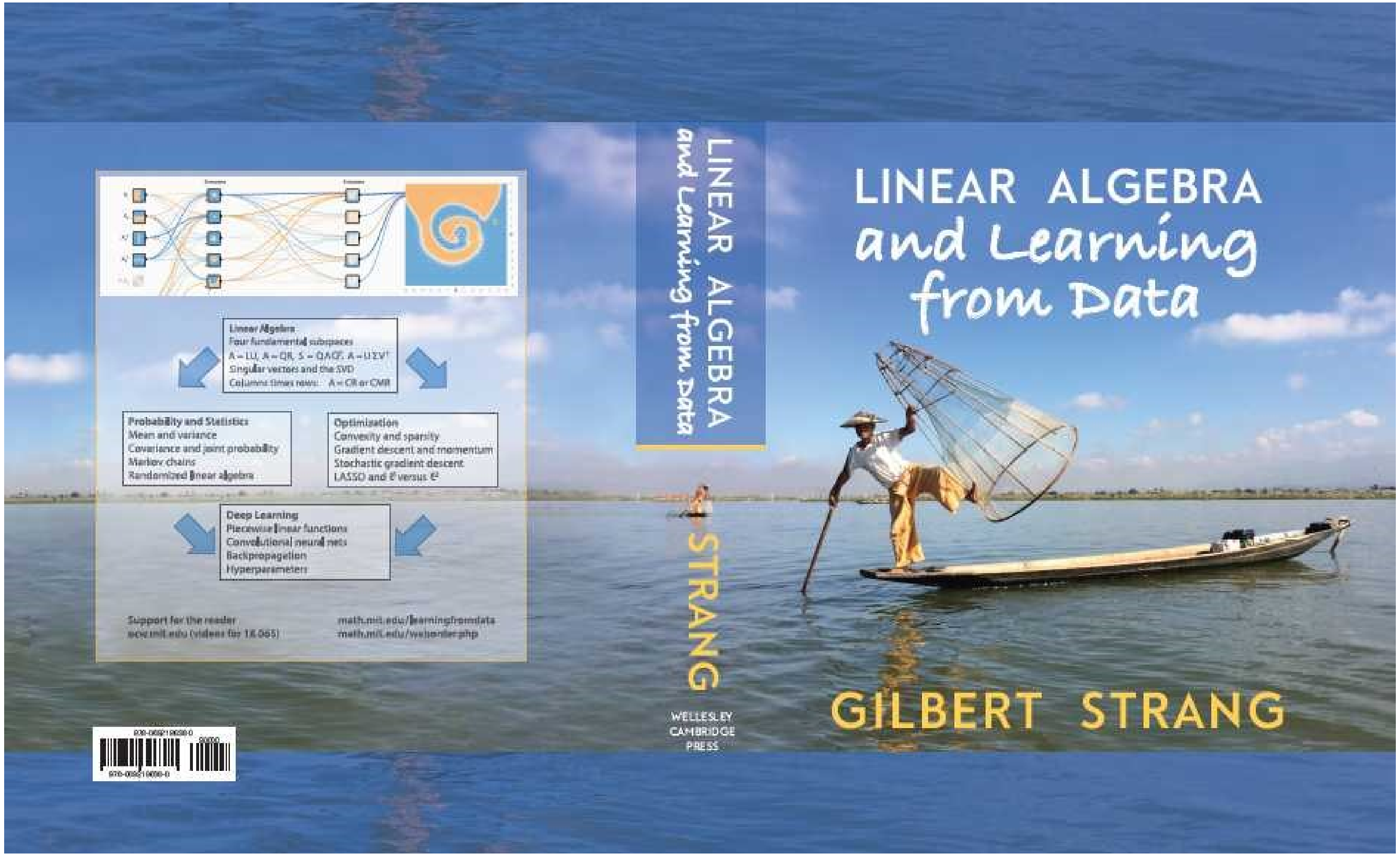
Advanced Numerical Methods in Engineering
수치해석특론

Ch	Contents	
1	Applied Linear Algebra	
2	A Framework for Applied Mathematics	
3	Boundary Value Problems	
4	Fourier Series and Integrals	◯
5	Analytic Functions	
6	Initial Value Problems	◯
7	Solving Large Systems	◯
8	Optimization and Minimum Principles	
	Variational Method	◯

Motivation

- New master's program in data science?
- Introductory course in mathematical fundamentals for a quantitatively oriented but heterogeneously group of students
  - What data science exactly is
  - What kind of mathematics plays a role
  - What is most important when there is not enough time

AY: 2020



https://math.mit.edu/~gs/learningfromdata/

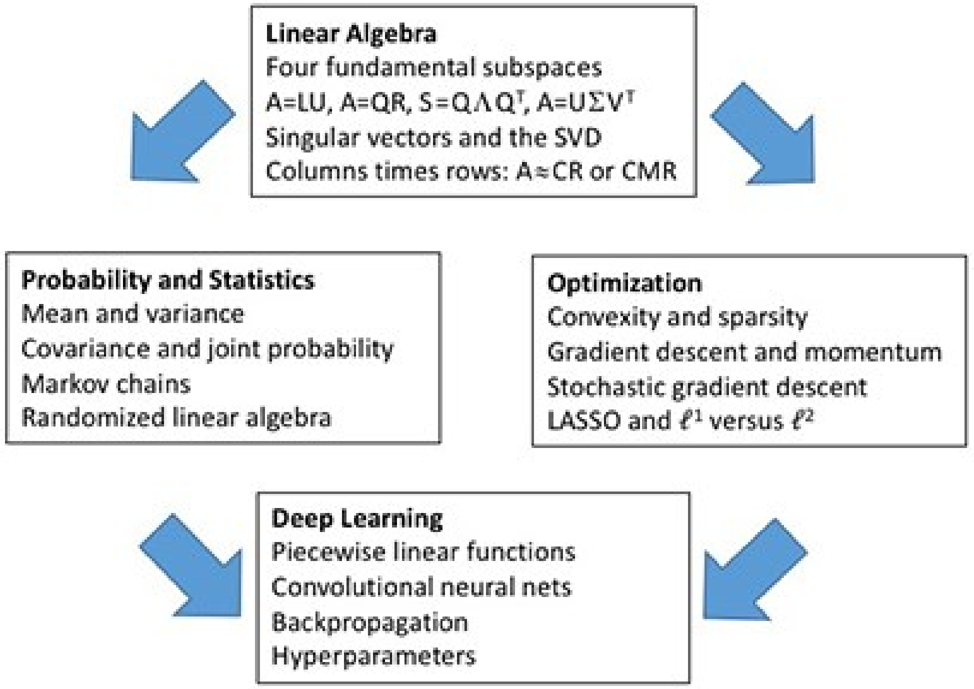
Applied Mathematics for Deep Learning
딥러닝수학

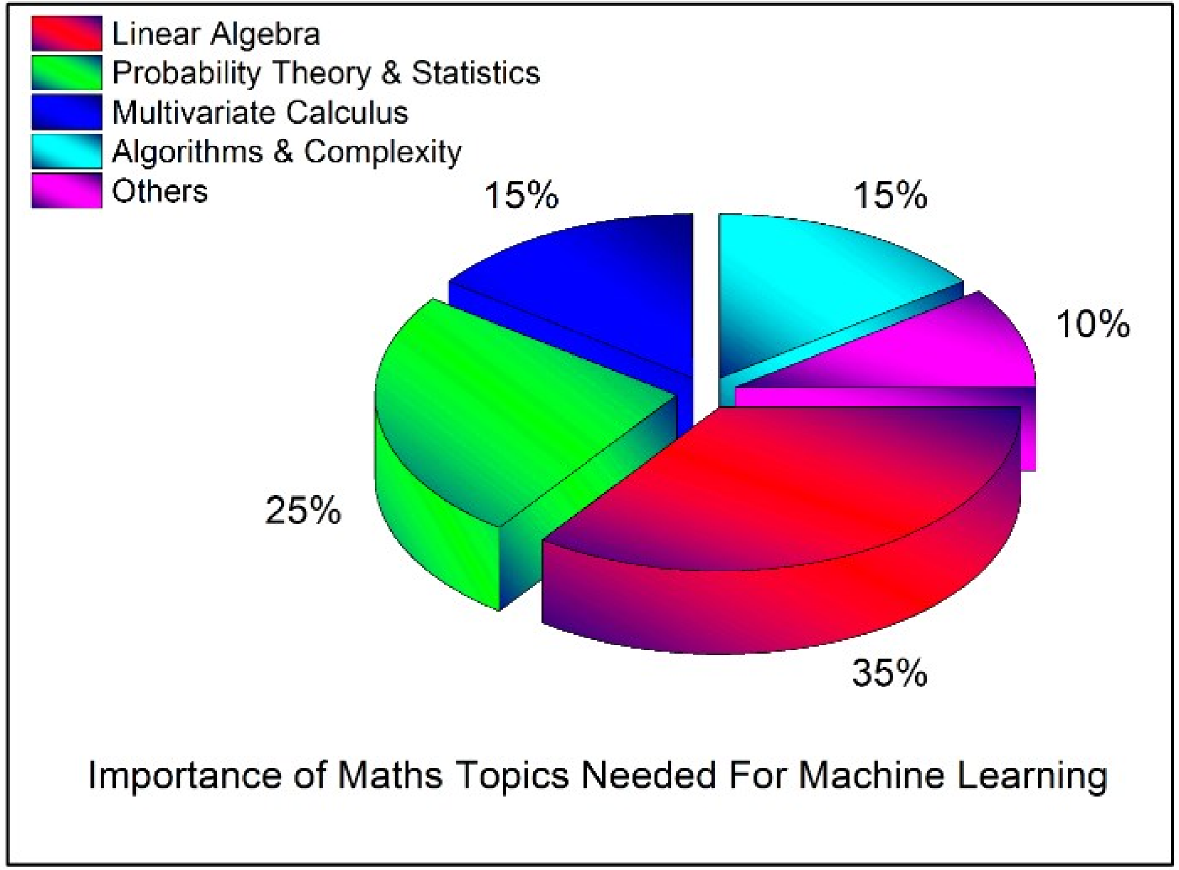
- MIT Math 18.065, Matrix Methods in Data Analysis, Signal Processing, and Machine Learning

Ch	Contents	
1	Highlights of Linear Algebra	○
2	Computations with Large Matrices	○
3	Low Rank and Compressed Sensing	
4	Special Matrices	
5	Probability and Statistics	○
6	Optimization	○
7	Learning from Data	○

Course Description

- Linear algebra concepts are key for understanding and creating machine learning algorithms, especially as applied to deep learning and neural networks.
- This course reviews linear algebra with applications to probability and statistics and optimization–and above all a full explanation of deep learning.




Linear Algebra
Probability Theory & Statistics
Multivariate Calculus
Algorithms & Complexity
Others
15%
15%
10%
25%
35%
Importance of Maths Topics Needed For Machine Learning

Two Essential Topics

- Linear Algebra
  - Symmetric, orthogonal
  - Factorization
- Deep Learning
  - Create a(learning) function
  - Input: image (driverless car: pedestrian, pole, handwriting: zip-code)
  - Speech: Siri

$$\begin{bmatrix} \text{input} \\ (\text{data}) \end{bmatrix} \rightarrow \underbrace{[\text{function}]}_{\substack{\text{matrix multiplication} \\ \text{all linear? fail} \Rightarrow \text{nonlinear}}} \rightarrow [\text{output}]$$

Two Supporting Subjects

- Optimization
  - Find entities in those matrices → learning function
  - Minimizing error → multivariable calculus, giant calculation
- Statistics
  - Keep the mean and variance at the right spot
  - Numbers: good range
    - Bad news for learning function
    - Grow out of sight exponentially
    - Drop to zero

Linear Algebra

- Basic Course
  - Elimination to solve Ax=b
  - Matrix operations, inverses, determinants
  - Vector spaces and subspaces
  - Independence, dimension, rank of a matrix
  - Eigenvalues and eigenvectors
- Stronger Course
  - Ax=b in all cases: square system, too many equations and unknowns
  - Factor A in LU, QR, $U\Sigma V^T$, CMR: columns times rows
  - Four fundamental subspaces: dimensions, orthogonality, good bases
  - Diagonalizing A by eigenvectors and left and right singular vectors
  - Applications: graph, convolution, iteration, covariance, projection, filter, network, image, matrices of data

Deep Learning and Neural Nets

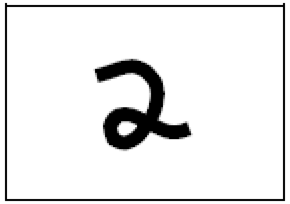
- Mathematical pillars of machine Learning
  - Linear algebra, Probability/Statistics, Optimization
- Goal: to construct a (learning) function that classifies the training data correctly, so it can generalize to unseen test data
- For the problem of identifying handwritten digits
  - Input: image (a matrix of pixels)
  - Output: ten numbers from 0 to 9
  - Function: create by assigning weights to different pixels in the image (architecture of an underlying neural nets)
  - Big problem of optimization to choose weights
  - MNIST set: 70,000 handwritten digits (60,000 for training data, 10,000 for test data)

Linear and Nonlinear Learning Functions

- Inputs: samples v
- Outputs: computed classifications w=F(v)
- Simplest learning function: w=Av
- Affine functions: F(v)=Av+b (b: bias vector), too simple
- Linearity: very limiting requirement
  - halfway between I and III, I and XIX
  - Handwritten digits: two zeros→8, one and zero→9 or 6, images don't add
- Nonlinearity: squaring?
  - sigmoidal functions with S-shaped graphs: A(S(Bv))
  - Simple ramp function: ReLU(x)=max(0,x)

Structure of F(v)

- Functions that yield deep learning
  - Composition of affine functions Lv=Av+b with nonlinear functions R
  - F(v)=L(R(L(R(…(Lv)))))
  - A, b: weights in the learning function
  - Output from first hidden layer: $v_1=\text{ReLU}(A_1v+b_1)$
  - More layers in F → typically more accuracy in F(v)
- Choose weights A_k and b_k to minimize the total loss over all training samples
  - Least squares: $||F(v)-(\text{true output})||^2$

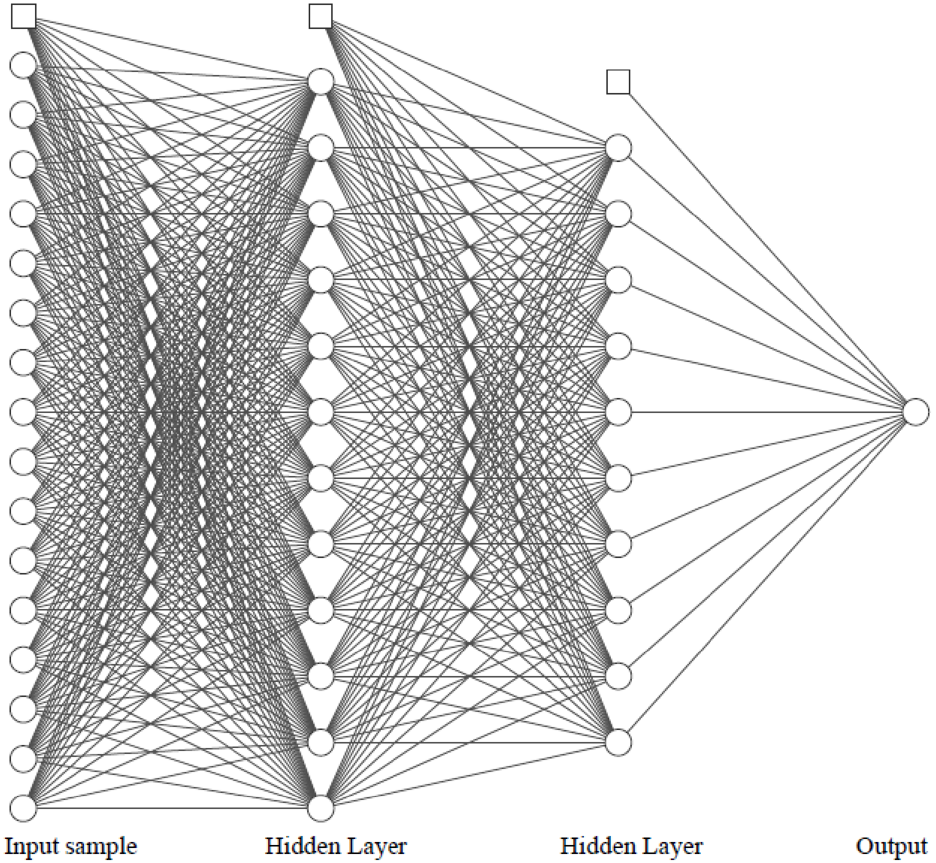
One input $v =$  **One output** $w = 2$

Neural Nets (1)

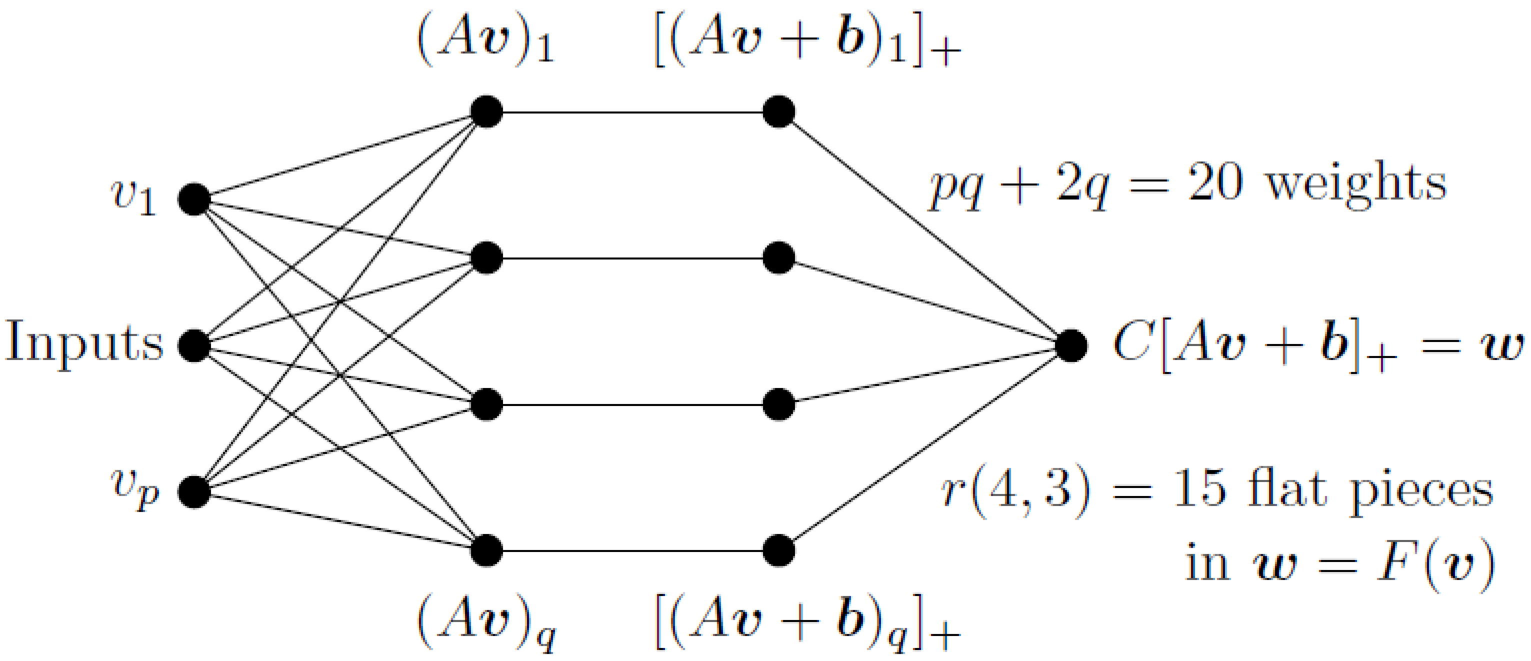
- Input layer: training samples $v=v_0$
- Output: their classification $w=F(v)$
- Hidden layers add depth to the network
  - Allow composite function F
- Feed-forwarded fully connected network
  - For images, convolutional neural net(CNN) is often appropriate and weights are shared, constant diag(A)
- Deep learning works amazing well, when the architecture is right

Neural Nets (2)

- Each diagonal: weight to be learned by optimization
  - Edges from the squares contain bias vector b
  - The other weights are in A



Functions of Deep Learning



– If A is q by p, the input space R^p is sliced by q hyperplanes into r pieces → measure the "expressivity" of the overall function F(v)

$$r(q,p) = \binom{q}{0} + \binom{q}{1} + \cdots + \binom{q}{p}$$

DL: Linear Algebra and Calculus

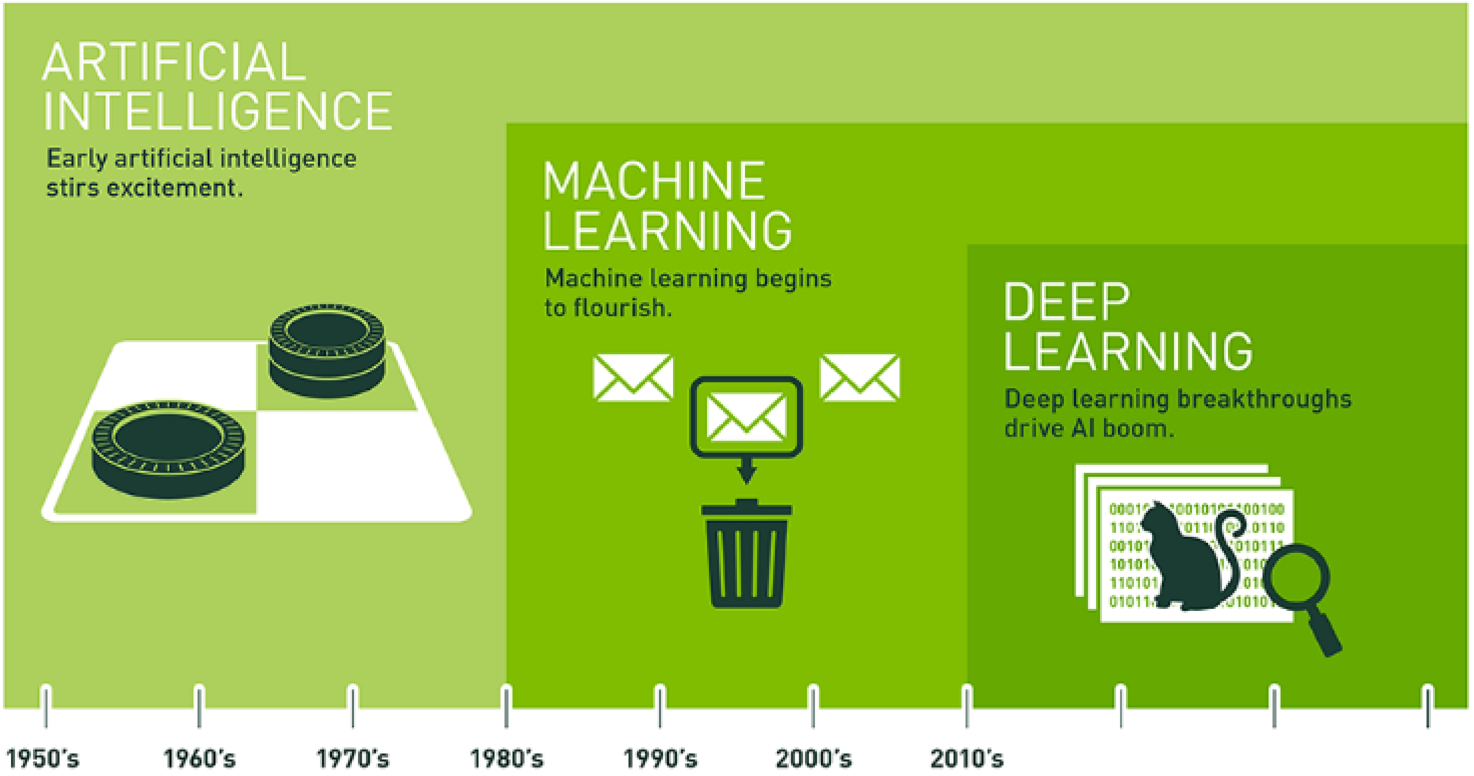
- Linear algebra
  - Compute “weights” that pick out the important features of the training data, and those weights go into matrices
  - Form of learning function
- Calculus
  - Show the direction to move in order to improve the current weights
  - Reduce the loss function L(x) by moving in the direction of fastest decrease
  - Reduce the error L(x) by $\mathbf{x}_{k+1} = \mathbf{x}_k - s_k \nabla L$

$$\text{minus sign}: \text{downhill}$$

$$s_k : \text{step size}\left(\text{learning rate}\right)$$

What's the Difference Between AI, ML and DL?

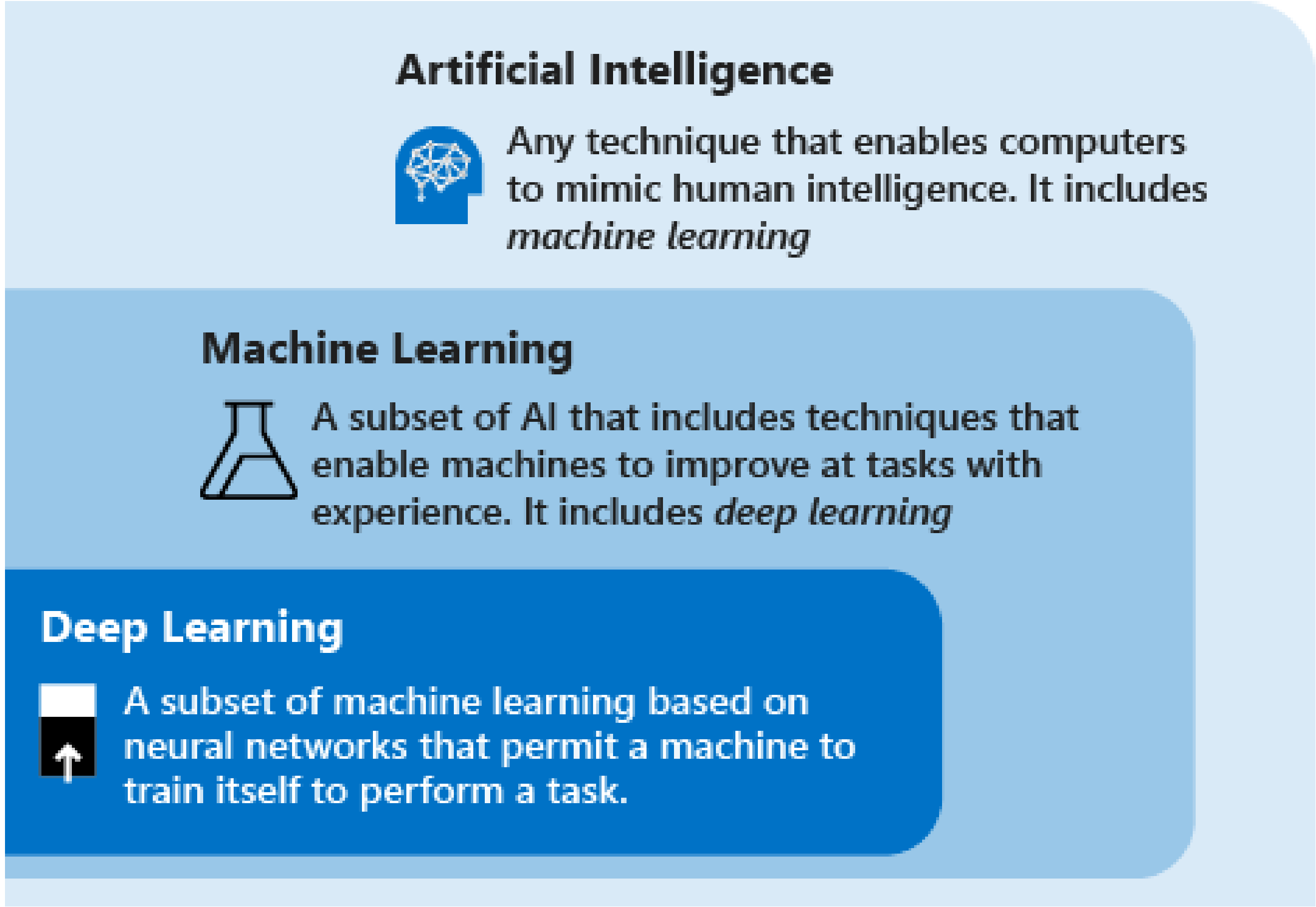
– (blogs.nvidia.com) July 29, 2016 by [MICHAEL COPELAND]()



Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence – first machine learning, then deep learning, a subset of machine learning – have created ever larger disruptions.

Deep Learning vs. Machine Learning

- (docs.microsft.com) 03/05/2020



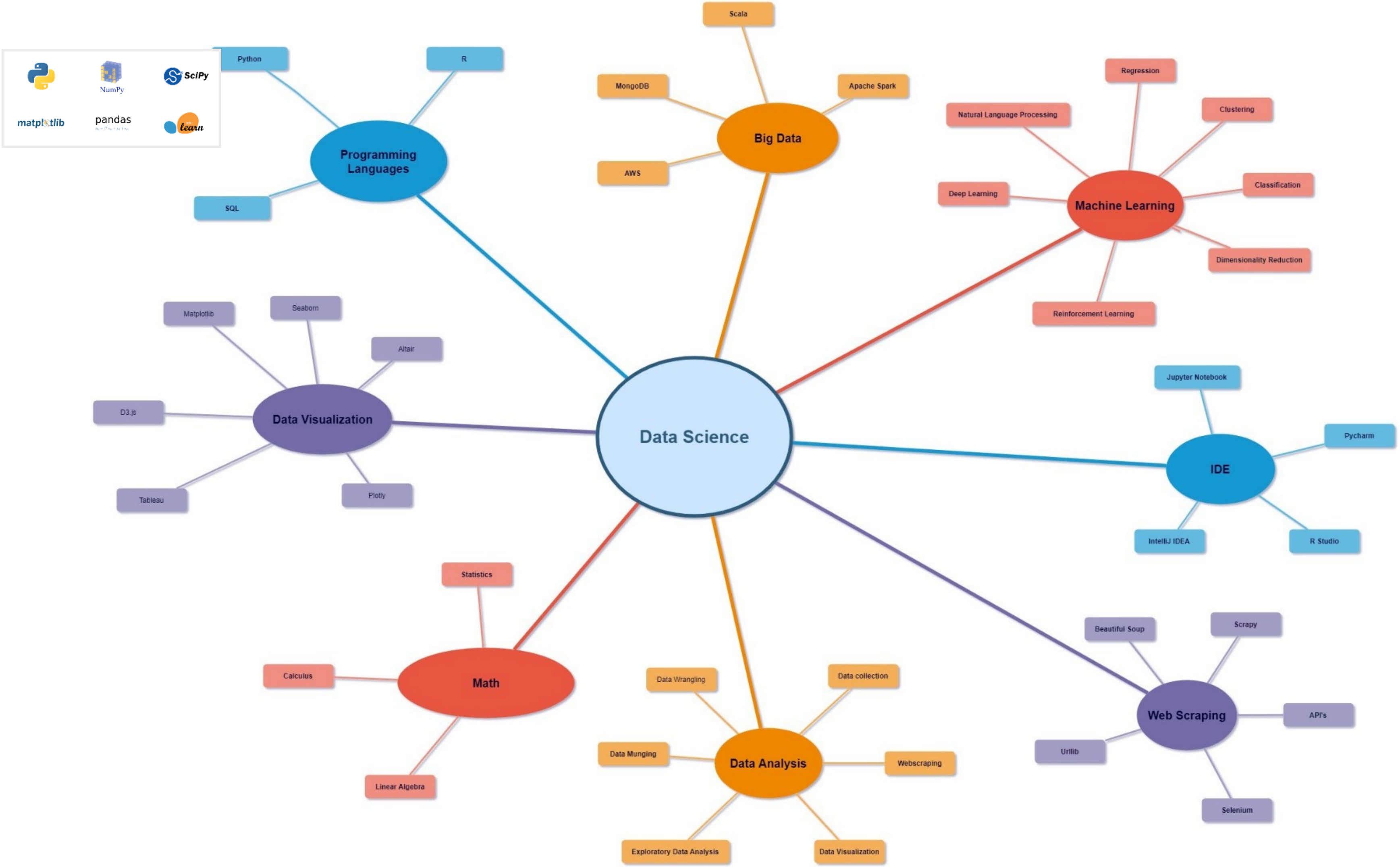
Current Status of CAE

- CAD for designing a product, CAE for testing and simulating it
- Computer-Aided Engineering (CAE)
  - Tool that supports finding the outcome by applying a discrete solution of partial differential equations for the phenomena to be analyzed
  - ☺ reduce the potential for errors in design, avoid over-engineering, and study the effect of altering a few parameters on the product
  - ☹ sufficiently accurate results come rather late in the design cycle to really drive the design
  - ☹ cost of computational resources (hardware, software, engineer time and computing time): major obstacle to improve design process
  - Mature technology(over half a century)? Limited synergies?
- Challenge → Enabler?
  - Smart systems lead to an increased need for multi-physics analysis including controls and contain new materials, to which engineers are often less familiar

https://medium.com/swlh/bridging-the-gap-between-machine-learning-and-cae-cf5cf4fd4017

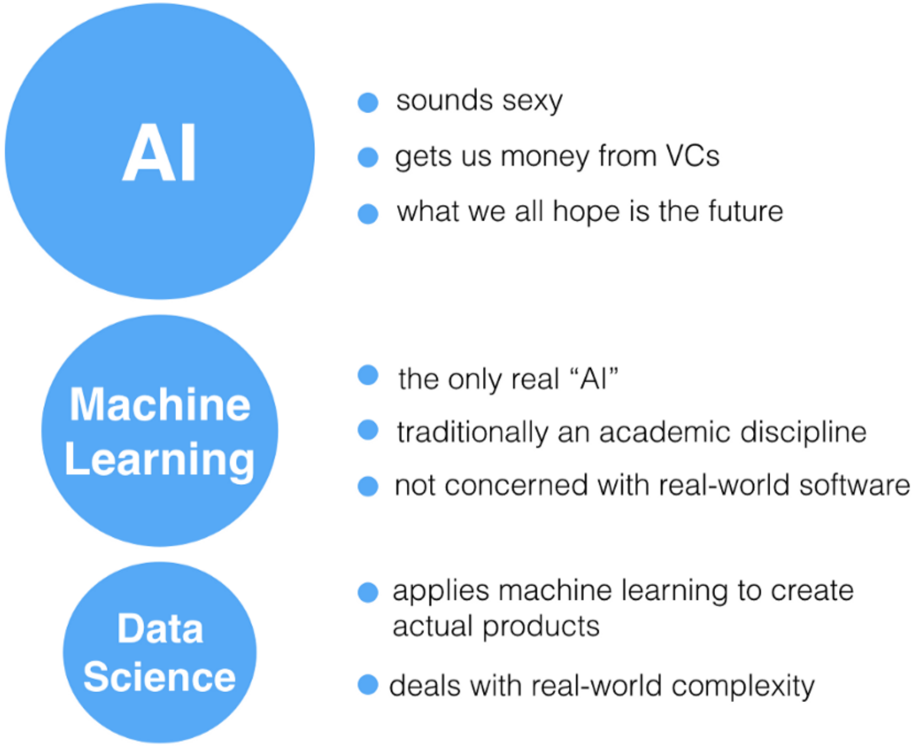
- Upcoming Analysis Agenda Topics
    - Engineering Data Science: The Fourth Paradigm
    - Designer-Oriented Simulation: Putting Simulation Upfront
    - Simulation Supporting Certification: Relying Less on Test
    - Communicating Complexity: Ensuring Simulation is Understood
    - Generative Design: Making the Impossible a Reality
    - Autonomous Things: Artificial Intelligence becomes Real
    - System-Level Simulation: Modelling the Sum of the Parts
    - Simulation Governance: Building a Simulation Capability
    - Multiscale Simulation: Analysis Great and Small
    - Simulating Tomorrow: Ensuring a Sustainable Future
    - The Digital Twin: Connecting Virtual with Physical
    - Code Verification: Keeping you Accurate
    - The Failure Test: Modelling Structural Failure
    - Rapid Manufacturing: Towards Distributed Digital Production
    - Process Simulation: Predicting and Optimizing Systems

How to Learn Data Science

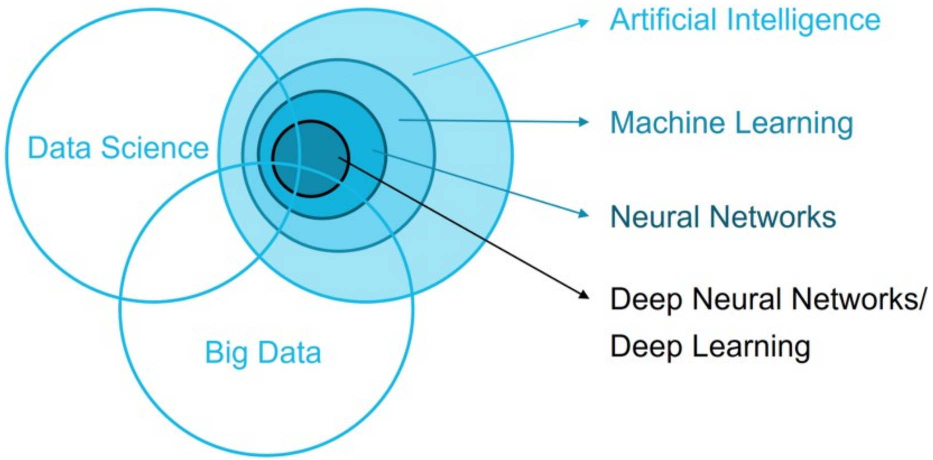


https://towardsdatascience.com/how-to-learn-data-science-my-path-ba7b9aa94f63

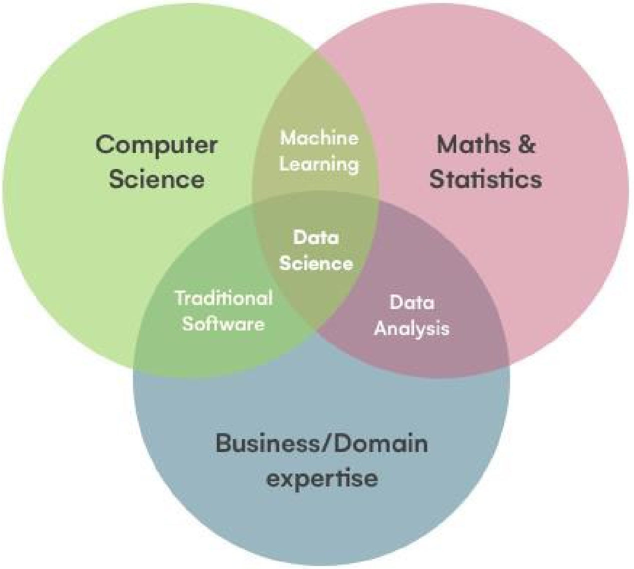
Data Science vs. Machine Learning vs. AI



A simplified explanation of AI, Machine Learning, and Data Science.
Source: Suraj Jena, June 10, 2018

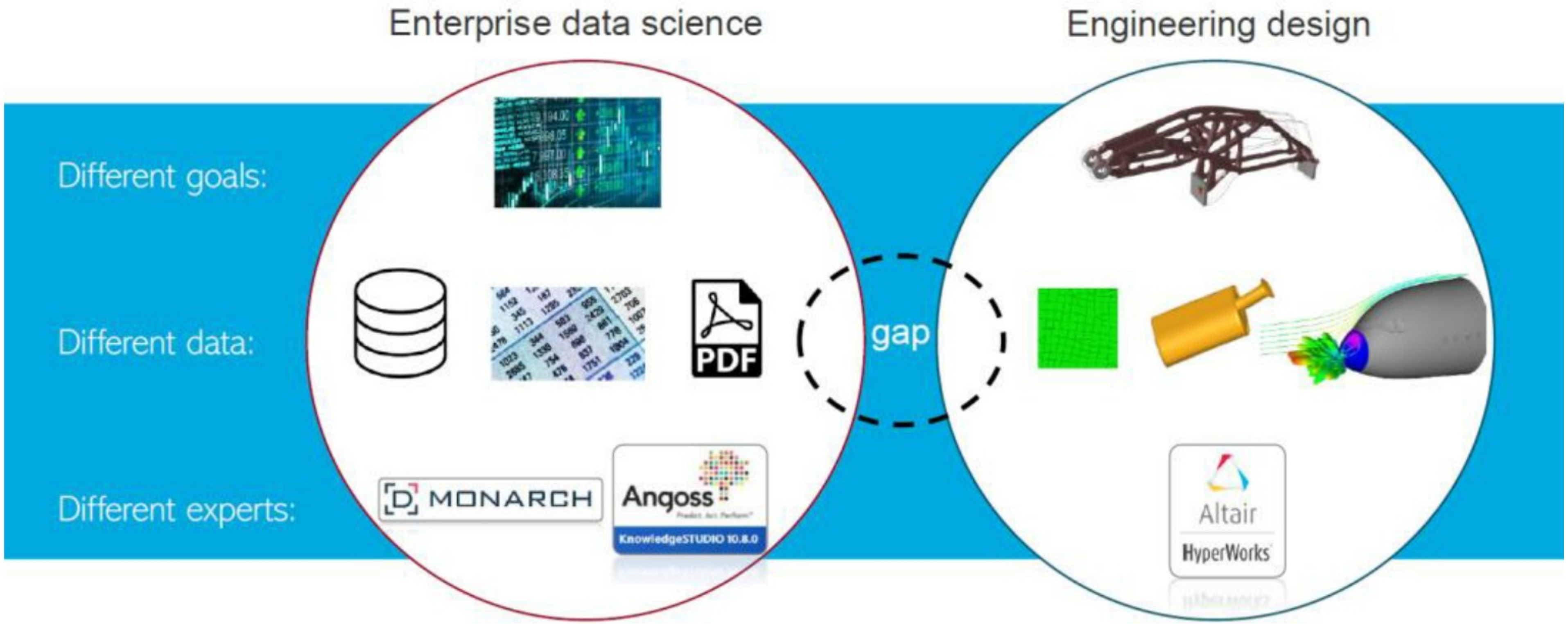


VENN diagram of AI, Big Data and Data Science Fraunhofer FOKUS



https://towardsdatascience.com/role-of-data-science-in-artificial-intelligence-950efedd2579

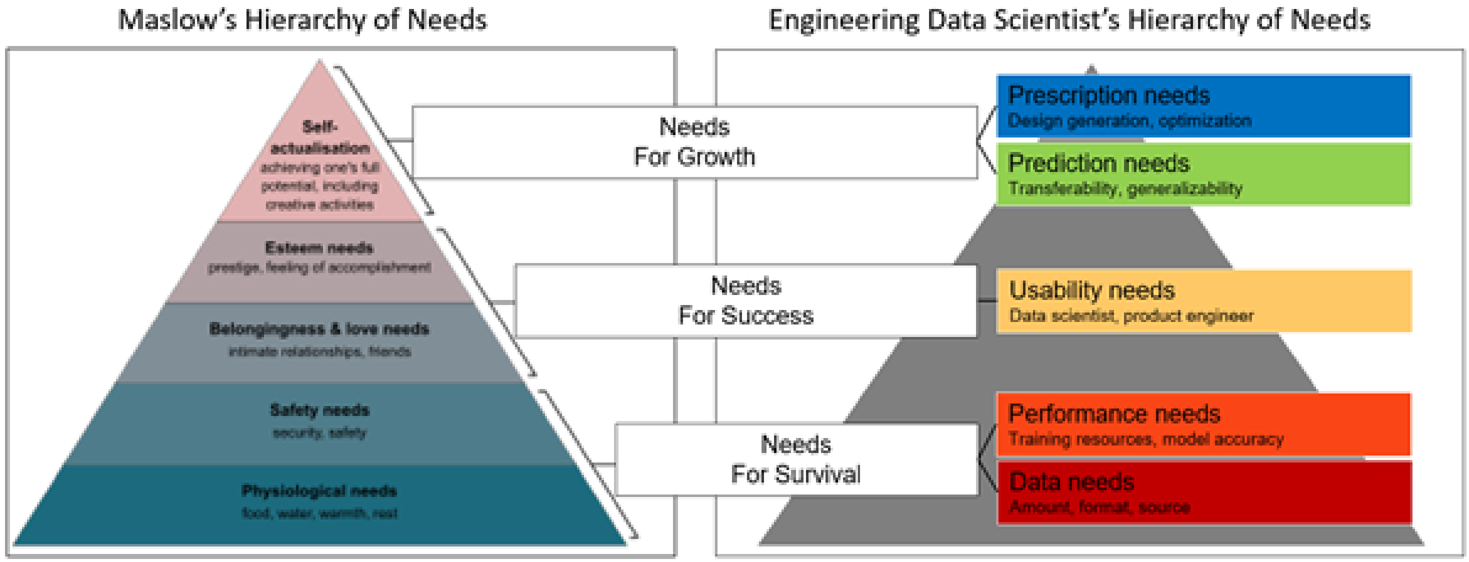
Data Science vs. Engineering Design



- What are customers interested in purchasing?
- How is the business doing with a particular product or in a geographic region?
- Is the COVID-19 pandemic straining or growing resources?

Engineering Data Scientist

- an engineer (with CAE expertise and data science knowledge)
- leverages design exploration, optimization and machine learning
- to improve CAE processes and results
- including model build, design optimization, manufacturing assessment and product operation (can identify the use cases for data science and plan data extraction, preparation, modelling and visualization)



https://community.altair.com/community?id=community_blog&sys_id=0429d5781bfc7c50c4dfdbd9dc4bcb2f

Application of Machine Learning to Solve Engineering Problems

- Idea of Artificial Intelligence
  - Replace human made evaluations and decisions by a software based automatic process
  - Rule-based software system: expert knowledge is implemented in a very explicit way, disadvantage?
  - Complex engineering systems: physical laws, input-output behavior is not obviously well known
  - Real world systems: stochastic inputs (noise)
  - Simulations and testing activities: complex unpredictable correlations between input and output
- Idea to learn these correlations from existing data: Machine Learning
  - Improve the performance of an existing system based on their learning from past experience
  - What if the CAE software asked the user for feedback on the generated simulation?

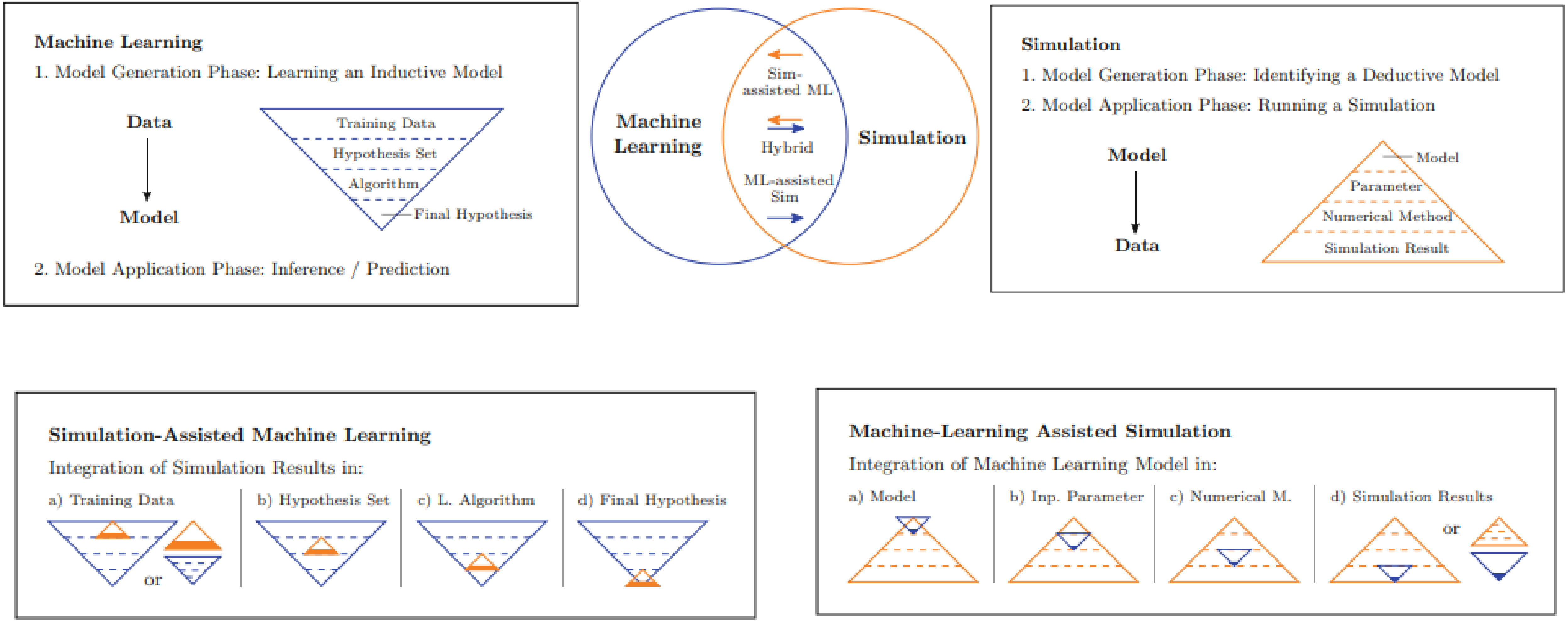
Machine Learning in CAE

- Machine Learning for future of CAE in the product development process
- Predictive Engineering Analytics (PEA)
  - Refinement of simulation and testing processes to improve collaboration between analysis teams that handle different applications
  - Predict the behavior of the complete system for all functional requirements and including physical aspects from the very beginning of the design cycle
  - Design driven by simulation, where product behavior is predicted from start (rather than reacting late)
- Fundamental steps of Machine Learning
  - Data preparation: quality of data, process of collecting and providing the complete set of data
  - Feature engineering: skillful choice of extracted data features
  - Appropriate choice of the machine learning model: model selection and model parameter optimization

Why Machine Learning in Simulation?

- Machine learning and simulation have a similar goal
  - To predict the behavior of a system with data analysis and mathematical modeling
- Hybrid modeling approach to bridge the knowledge gap between
  - Machine Learning: bottom-up approach that generates an inductive, data-based model
  - Simulation: top-down approach that applies a deductive, knowledge-based model
- Learning simulation engine
  - Hybrid system that combines machine learning and simulation in an optimal way
  - Can automatically decide when and where to apply learned surrogate models or high-fidelity simulations

Hybrid Modeling Approach

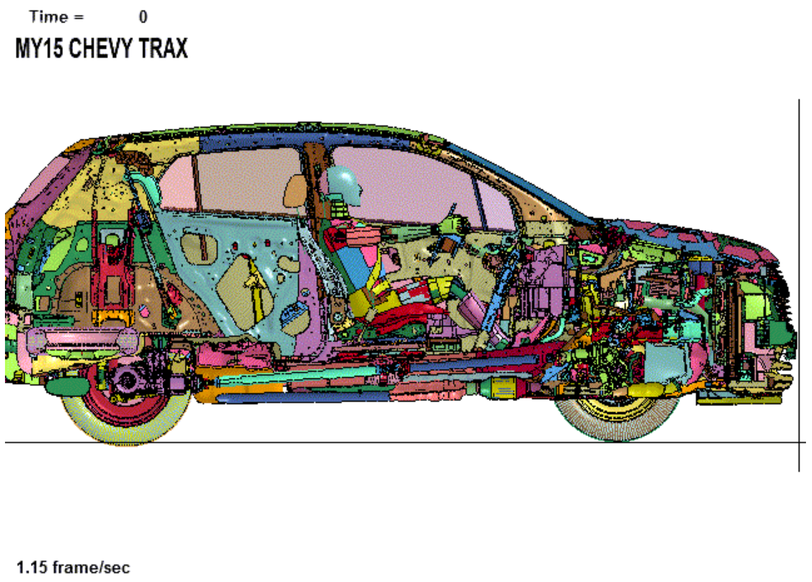


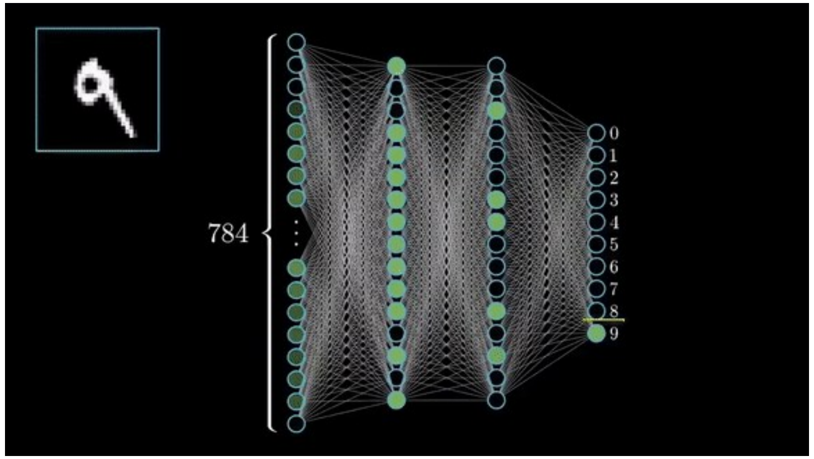
Combining Machine Learning and Simulation to a Hybrid Modelling Approach: Current and Future Directions (2020)

Bridging the gap between Machine Learning and CAE

- innovative Design Support System (DSS): Decision Support System
  - prediction and estimation of machine specification data such as machine geometry and machine design on the basis of heterogeneous input parameters
- Machine learning algorithm
  - Propose the characteristics of the new possible versions of the product or service
  - By learning, correlating, and interpreting the parameters of a database, which represents the characteristics of a product
- Machine Learning-based Simulation systems
  - Analyze every type of data: continuous variables, discrete variables and non-numerical classes: superior to other tools (e.g. operating on the mathematical basis)
  - Be more robust and allow a broader and complete set of solutions
  - Possibility to re-train the model every time new data are inserted, optimizing and refining predictive capacity over time

Types of Predictive Modeling Technologies





- Physics-based modeling
- Computational Engineering
- CAE
- Modeling & Simulation

- Data-driven modeling
- Machine Learning
- AI
- Statistical Modeling

Modeling: Physics-Based vs. Data-Driven

Physics-Based Modeling	Data-Driven Modeling
• Solid foundation based on physics and reasoning • Generalize well to new problems with similar physics • interpretability, robust foundation and understanding	• Take into account long term historical data and experiences • Once the model is trained, it is very stable and fast for making predictions • accuracy, efficiency, and automatic pattern-identification capabilities
• Difficult consistent engineering judgment with increasing complexity • Difficult to assimilate very long-term historical data into the computational models without a Simulation Data Management System • Sensitive to numerical instability when dealing with nonlinearities and ill-conditioned problems	• So far most of the advanced algorithms work like black boxes • Bias in data is reflected in the model prediction • Poor generalization on unseen problems
• Problem: PDE → u_{new} • Given: $M\ddot{u}+Ku=F$, M, K, F • Integration	• Problem: u_{old} → u_{new} • Given: u_{old} (← DOE?), M, K, F • Learning

Digital Twin: Values. Challenges and Enablers From a Modeling Perspective, IEEE Access (2020)

Objectives

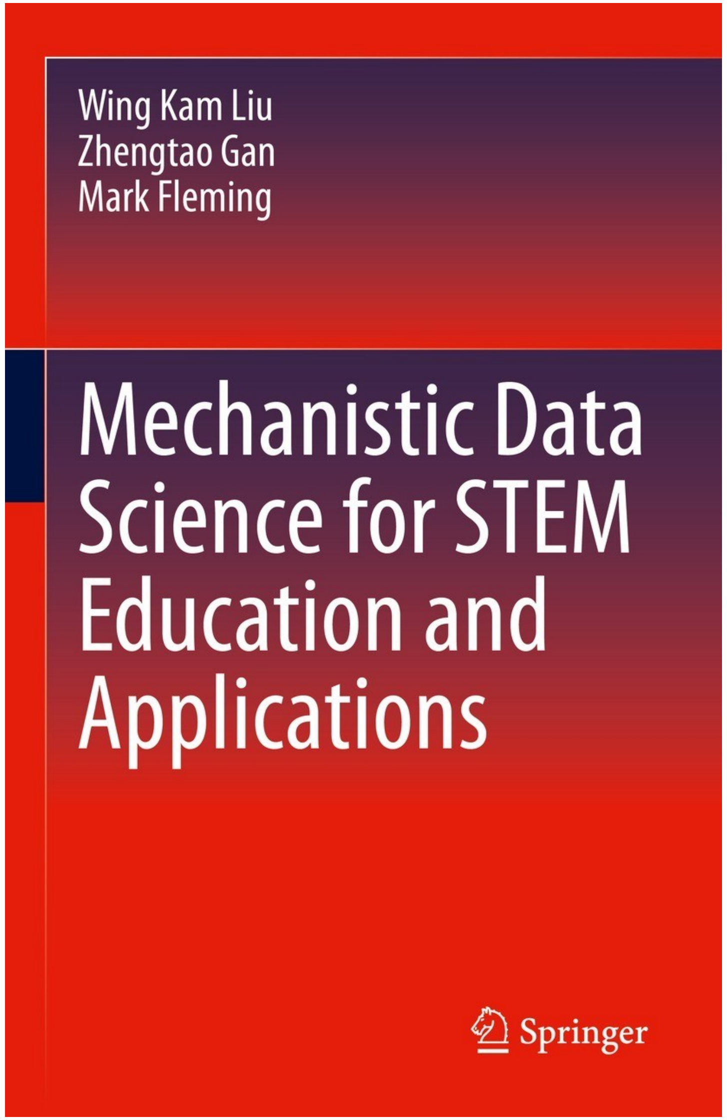
MMLDT CSET 2021

Machine Learning (ML) and Digital Twins (DT) are at the heart of today's different industries, ranging from advanced manufacturing to biomedical systems to resilient ecosystems, civil infrastructures, smart cities, and healthcare. They have become indispensable for solving complex problems in science, engineering, and technology development. The purpose of the MMLDT-CSET 2021 conference is to facilitate the transition of ML and DT from fundamental research to mainstream fields and technologies through advanced data science, mechanistic methods, and computational technologies. This 3-day conference features technical tracks of emerging ML-DT fields and applications, special public lectures, short courses, and demonstrations. **The conference will be held in a hybrid format, featuring both on-site and virtual sessions.**

Vision

The goal of this MMLDT-CSET Conference is to bring together the diverse communities that are interested in learning, developing, and applying mechanistic machine learning and digital twins via computational science and engineering tools to a broad range of engineering and scientific problems, and to promote collaborations between engineers, data and computer scientists, and mathematicians from federal agencies, academia, and industry in this field.

AY: 2023


Wing Kam Liu
Zhengtao Gan
Mark Fleming
Mechanistic Data Science for STEM Education and Applications
Springer

- Northwestern MECH_ENG 329: Mechanistic Data Science for Engineering

Ch	Contents	Pages
1	Introduction to Mechanistic Data Science	30
2	Multimodal Data Generation and Collection	14
3	Optimization and Regression	38
4	Extraction of Mechanistic Features	39
5	Knowledge-Driven Dimension Reduction and Reduced Order Surrogate Models	38
6	Deep Learning for Regression and Classification	42
7	Systems and Design	50