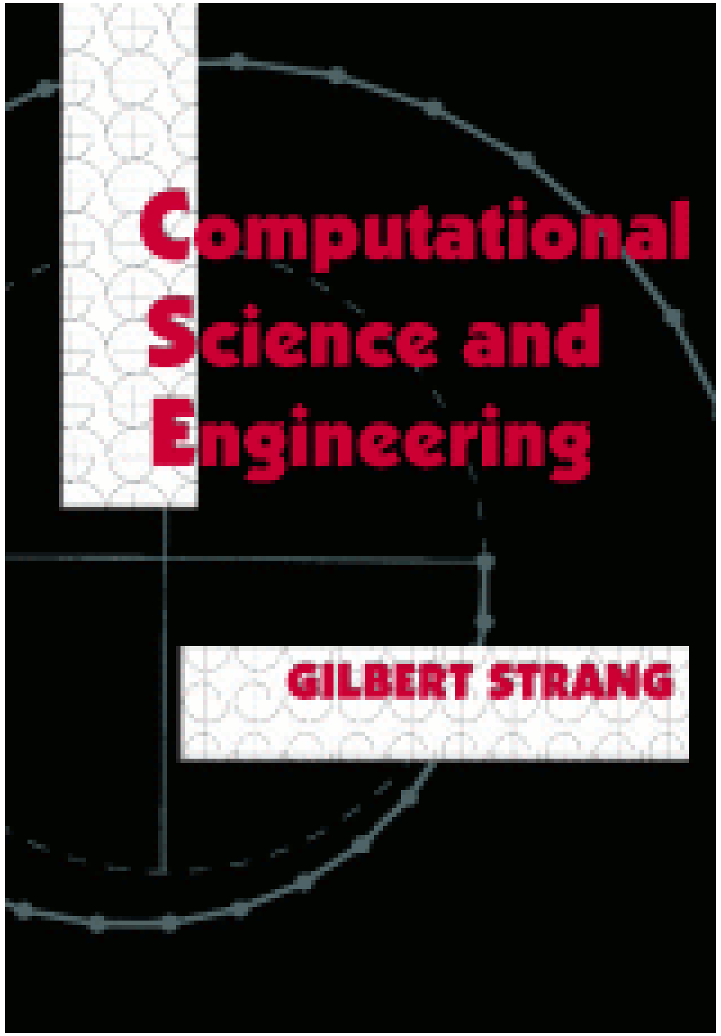
AY: 2008~2017



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	○

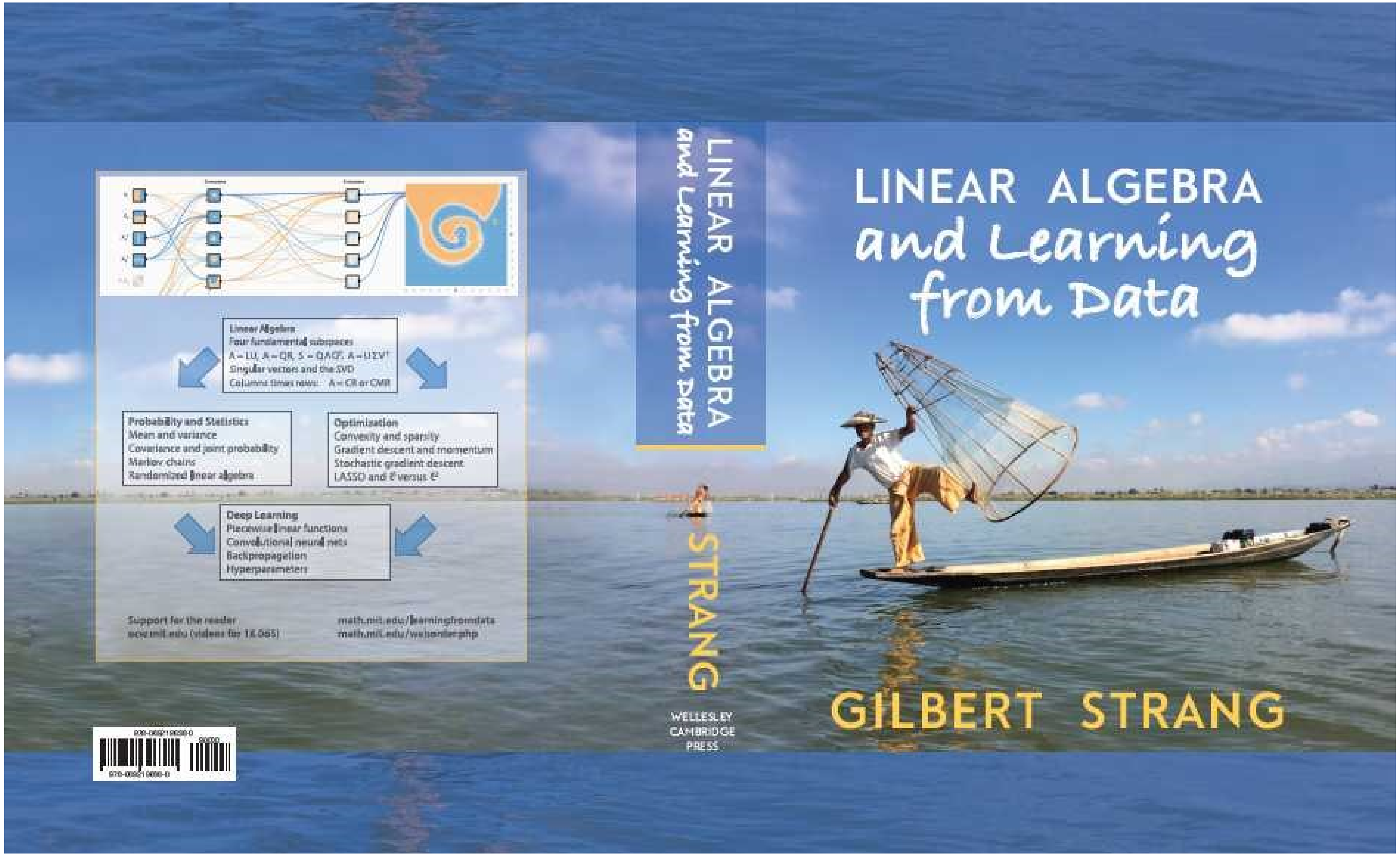
Advanced Numerical Methods in Engineering
수치해석특론

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/

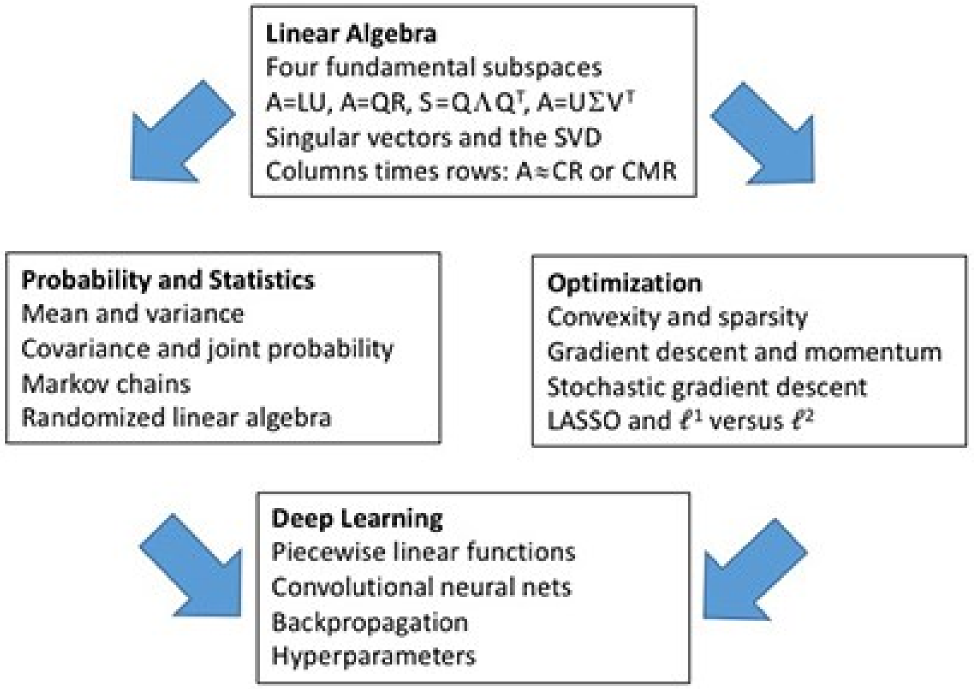
Applied Mathematics for Deep Learning
딥러닝수학

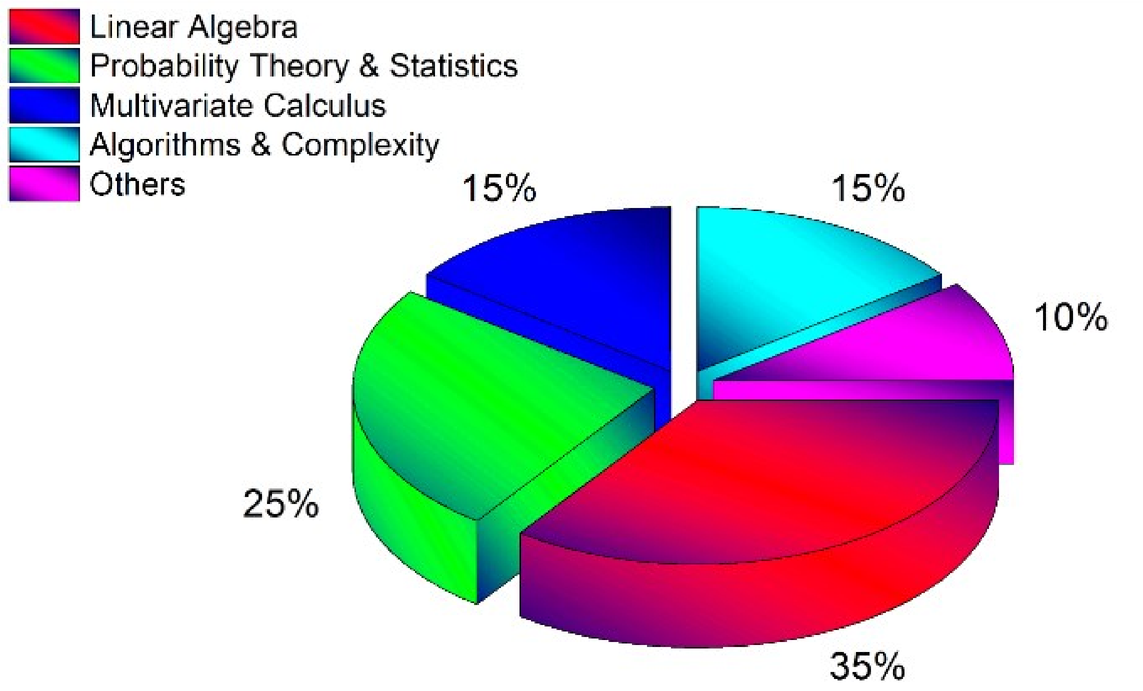
- MIT Math 18.065, Matrix Methods in Data Analysis, Signal Processing, and Machine Learning

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.





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

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

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)

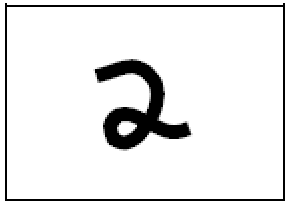
Linear and Nonlinear Learning Functions

- 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
  – II might be halfway between I and III (as linearity demands), what would be halfway between I and XIX?
  – Handwritten digits: two zeros→8, one and zero→9 or 6, images don't add
- Nonlinearity: squaring? (separate a circle from a point inside)
  – 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: $v_1=\mathrm{ReLU}(A_1 v+b_1)$
  - 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 $v =$



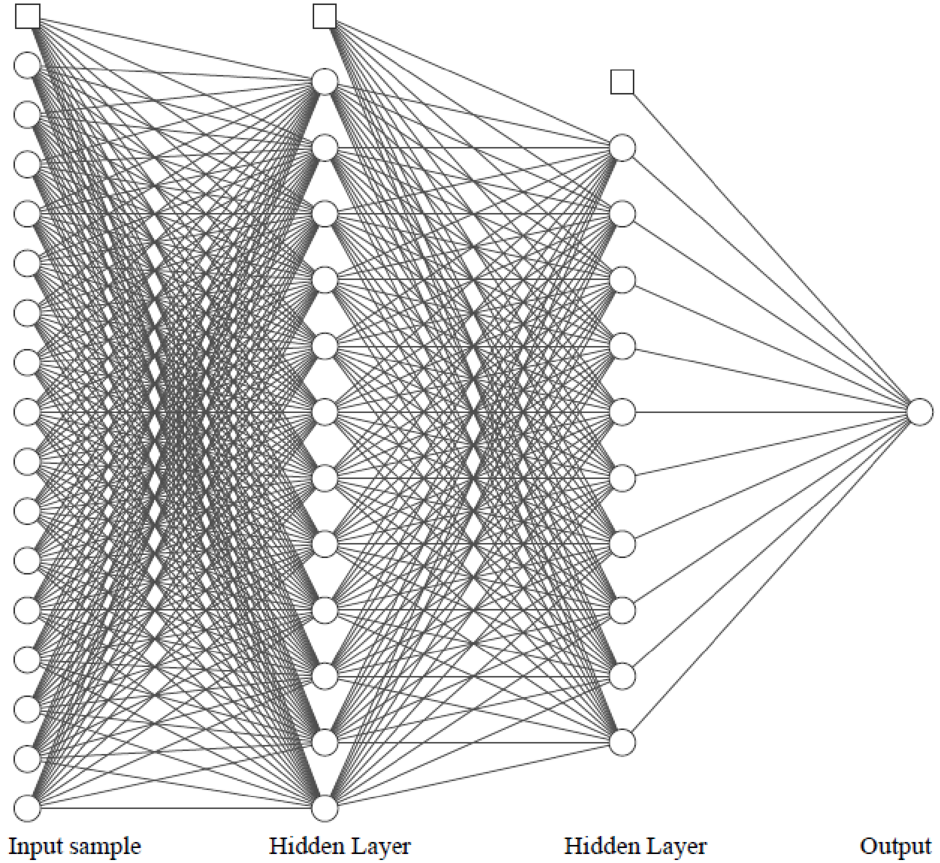
One output $w = 2$

Neural Nets (1)

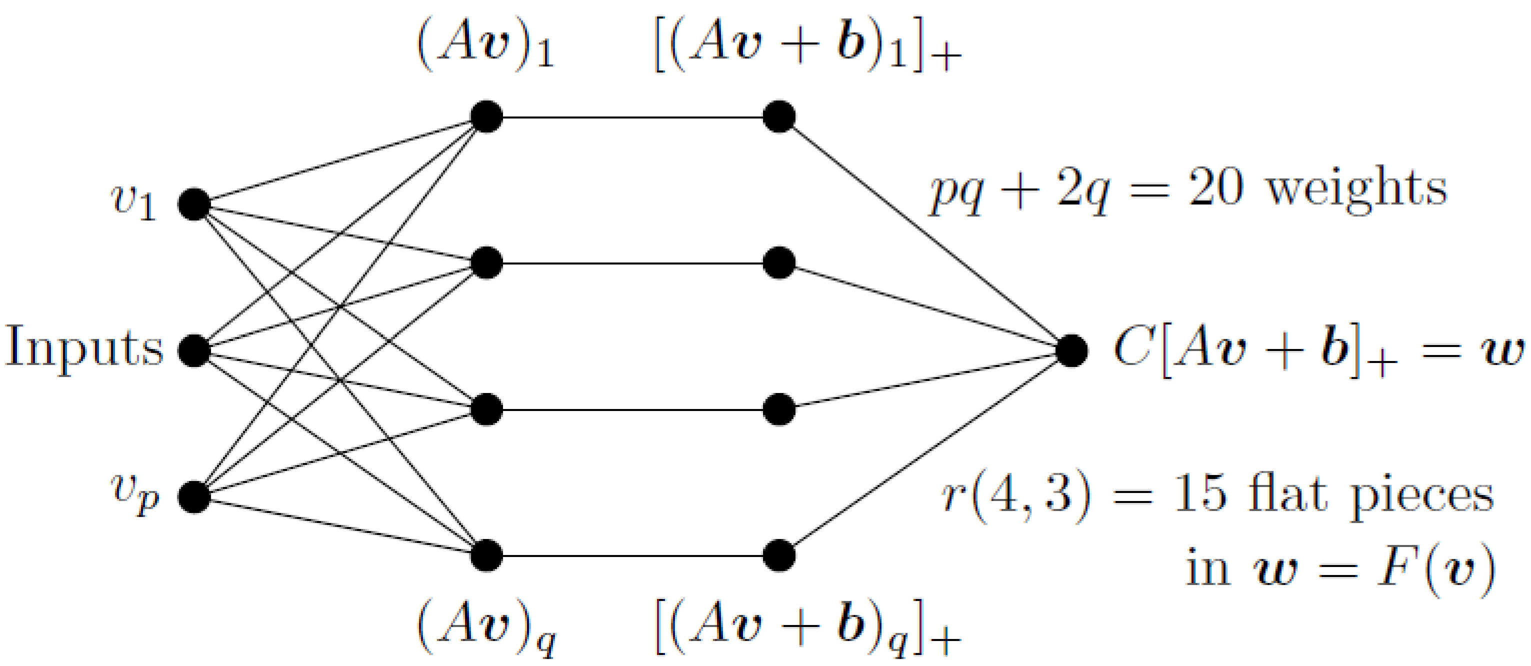
- Input layer: training samples $v=v_0$
- Output: their classification $w=F(v)$
- Hidden layers add depth to the network
  - Allow composite function F
- Feed-forwarded fully connected network
  - For images, convolutional neural net(CNN) is often appropriate and weights are shared, constant diag(A)
- 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 $\mathbf{x}_{k+1} = \mathbf{x}_k - s_k \nabla L$

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

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

Objectives

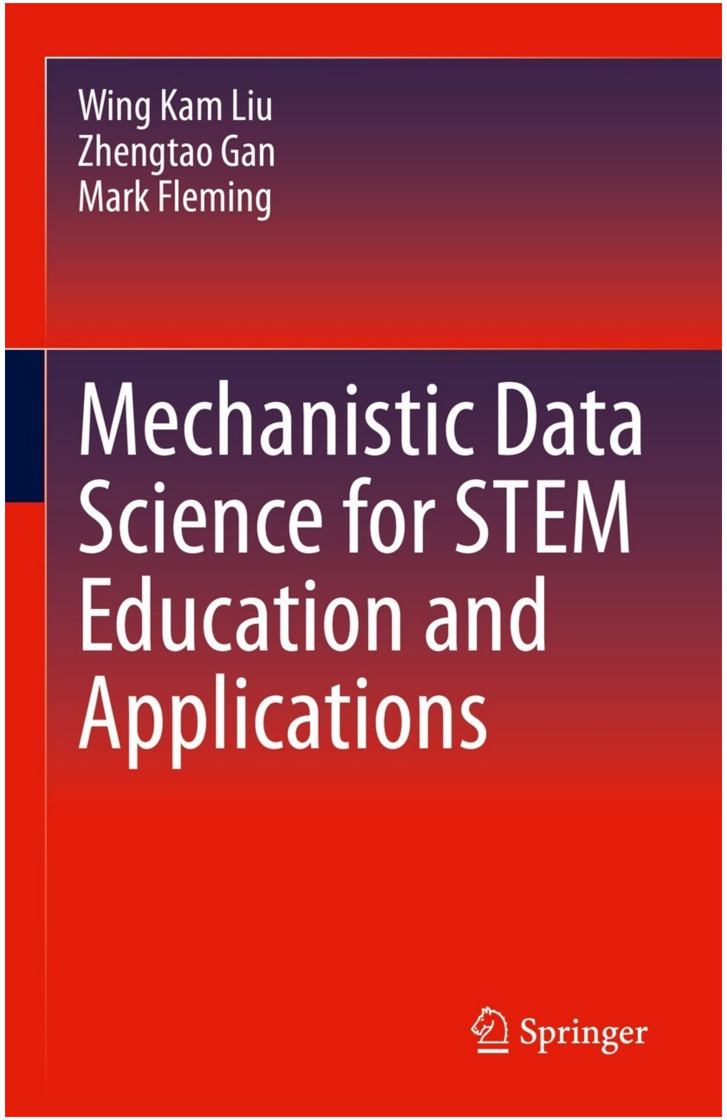
Machine Learning (ML) and Digital Twins (DT) are at the heart of today's different industries, ranging from advanced manufacturing to biomedical systems to resilient ecosystems, civil infrastructures, smart cities, and healthcare. They have become indispensable for solving complex problems in science, 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.**

MMLDT
CSET
2021

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

Examples

	Ch.1	Ch.2	Ch.3	Ch.4	Ch.5	Ch.6	Ch.7
Diamond		○			○	○	
Indentation testing		○					○
X-ray image				○		○	○
Signal							
Sound				○		○	○
Additive Manufacturing					○		○
Spring-mass motion					○		
Polymer matrix composite materials							○
Early warning of rainfall induced landslides							○