AI and Machine Learning in the Discovery of New Materials

Lincoln To

https://www.technologyreview.com/s/612388/a-robot-scientist-will-dream-up-new-materials-to-advance-computing-and-fight-pollution/

Overview

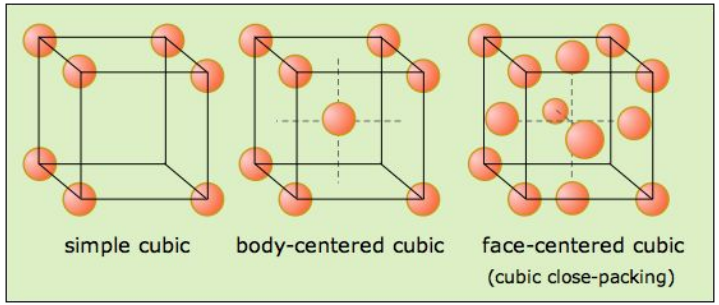
- Introduction
  - Materials Science
  - Applications in Computer Science & Engineering
- Current Approach to Materials Research
- Machine Learning in Materials Discovery and Design
  - Kebotix's Approach - AI & Automation
- Conclusion

Introduction

- Materials Science and Engineering
  - Interrelationships between the structures and properties of materials
    - Microstructures of materials
    - Mechanical, thermal, optical, electrical, etc
  - General paradigm
  - Inherently interdisciplinary
- Materials Genome Initiative (NIST)
- Applications in Computer Science & Engineering
  - Semiconductors
  - Integrated Circuits
  - Quantum computing

Figure 1.1 The four components of the discipline of materials science and engineering and their interrelationship.

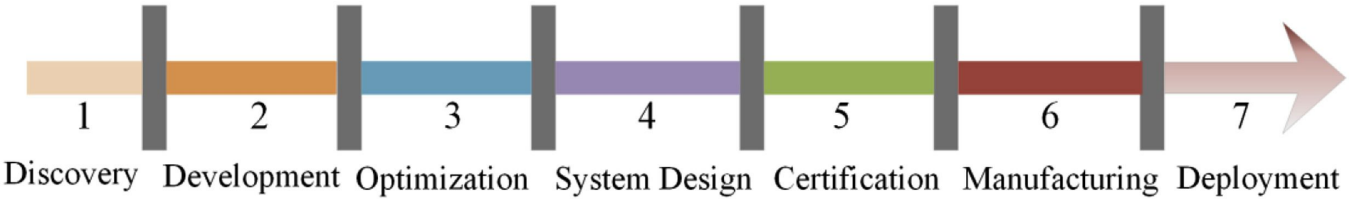
Callister, William D., and David G. Rethwisch. *Materials Science and Engineering: An Introduction*. Wiley, 2018.



https://chem.libretexts.org/Textbook_Maps/General_Chemistry/Book%3A_Chem1_(Lower)/07%3A_Solids_and_Liquids/7.08%3A_Cubic_Lattices_and_Close_Packing

Current Approach to Materials Research

- Traditional Process - 7 discrete stages
  - Discovery
  - Development
  - Property Optimization
  - System Design and Integration
  - Certification
  - Manufacturing
  - Deployment

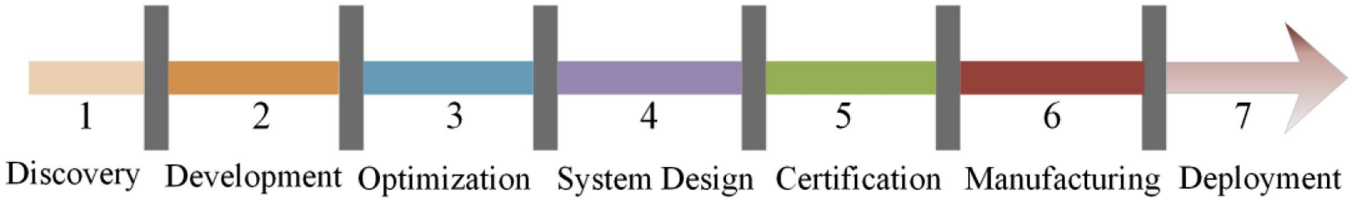


The process of finding new materials using traditional methods

https://www.sciencedirect.com/science/article/pii/S2352847817300515?via%3Dihub

Current Approach to Materials Research

- Current approach is essentially a blind search
  - Limited by:
    - Time
    - Resources
    - Experimental Conditions
    - Theoretical Foundations
- Time Frame from Initial Research to First Use
  - 10-20 years



The process of finding new materials using traditional methods

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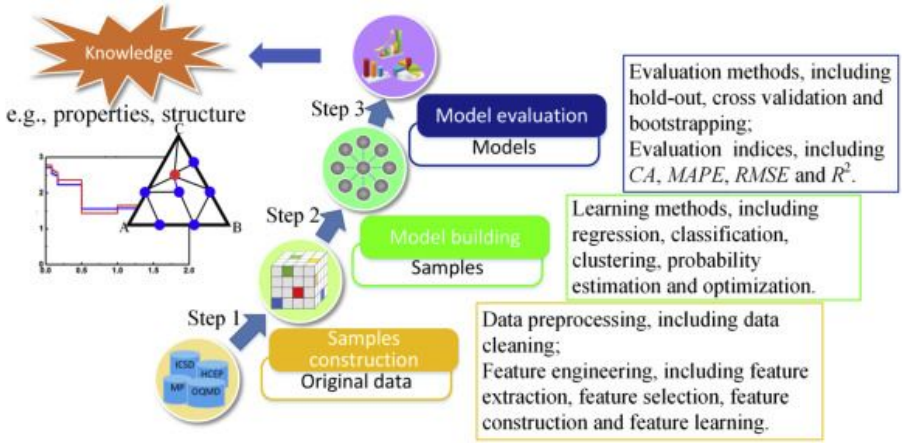
Machine Learning in Materials Discovery & Design - Paradigm

- Classical Definition of Machine Learning:
  - Performance, Task, Experience (<P,T,E>)
    - Program learns from E with respect to class T and performance measure P if…
      - Performance on T, as measured by P, improves with E
- Paradigm: [Goal + Sample + Algorithm = Model]
  - Goal
    - The given problem
  - Sample
    - Population selected for study
    - Data preprocessing
      - Data cleaning
      - Feature engineering
  - Algorithm
    - Machine learning algorithm
      - Support Vector Machine (SVM)
      - Artificial Neural Network (ANN)
      - Decision Tree (DT)
    - Model optimization algorithm
      - Genetic Algorithm (GA)
      - Simulated Annealing Algorithm (SAA)
      - Particle Swarm Optimization (PSO)

Machine Learning in Materials Discovery & Design - Methodology

- Step 1: Sample Construction
  - Original data collected from computational simulations & experimental measurements
  - Data Preprocessing, Feature Engineering
- Step 2: Model Building
  - Complex relationships between conditional factors and target attributes
  - Machine learning methods valuable here
  - “Core” algorithms in this step
- Step 3: Model Evaluation
  - Model must be effective on new datasets
  - Hold-out, cross validation, bootstrapping
    - Selection based on data volume



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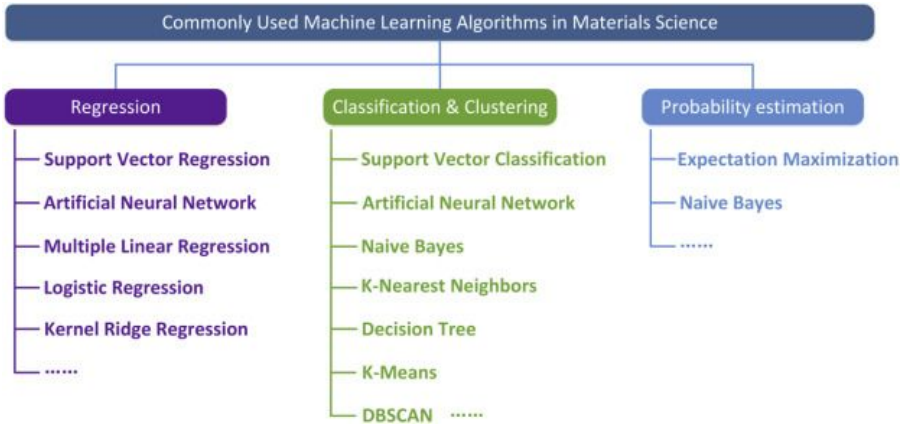
Machine Learning in Materials Discovery & Design - Algorithms

- Select appropriate machine-learning algorithm (4 categories)
  - New materials discovery:
    - Probability estimation
  - Material property prediction:
    - Regression
    - Clustering
    - Classification
- Optimization Algorithms
  - Optimize model parameters
  - GA, SAA, PSO



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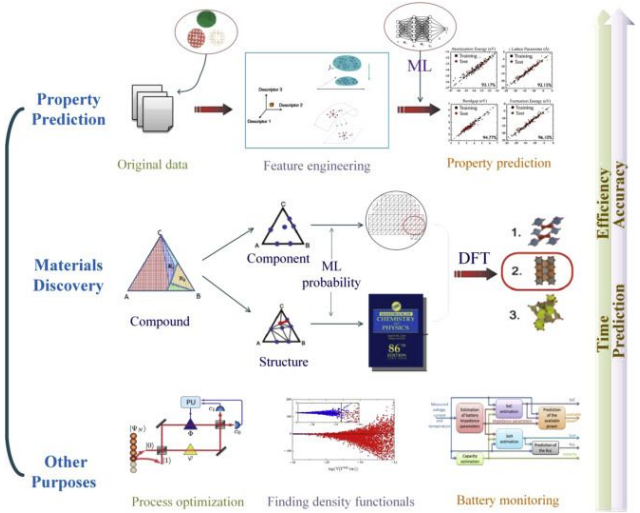
Machine Learning in Materials Discovery & Design - Application

- Property Prediction
  - Regression analysis
    - Predicts macro and microscopic properties
- New Materials Discovery
  - Probabilistic models
    - Screen combinations of structures and components
    - Select material with good performance from candidate set
      - Density Functional Theory based validation
- Other Applications
  - Process Optimization
    - Design process parameters in materials synthesis



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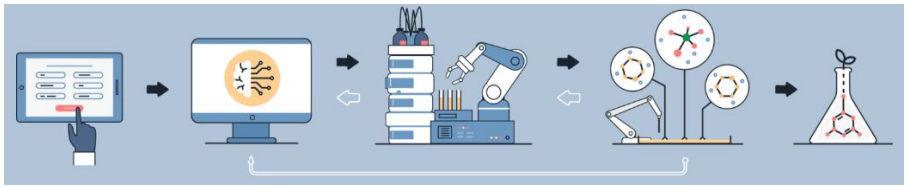
Kebotix's Approach - AI & Automation

- Kebotix Self-Driving Lab (AI and Robotics)
  - Robotics
    - Sample preparation
    - Materials property measurements
  - AI
    - Analyze experiment results
    - Formulate new hypothesis
- Methodology
  - Feed molecular models of compounds with desirable properties into neural network
  - Learns statistical representation of these properties
  - Comes up with new examples that fit this model



https://www.kebotix.com/

Conclusion

- Machine learning has extensive applications in Materials Science
  - New materials discovery
  - Material property prediction
- Machine Learning methodologies
  - Artificial Neural Networks
  - Support Vector Machine
  - Decision Tree
- Real world applications
  - Kebotix's Self-Driven Lab

Questions?