Machine Learning for Materials Science

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Course Syllabus

- Machine Learning Basics

- Applications to Materials Research:

Course Syllabus
Machine Learning Basics

- Machine Learning Introduction, Types of Machine Learning

- Linear Regression and Logistic Regression Decision Trees, Support Vector Machines (Linear SVM), Support Vector Machines (Soft SVM), Support Vector Machines (Non-Linear SVM), kNN,

- Loss functions, Gradient Descent Feature Engineering, Dataset split, Underfitting and Overfitting, Bias and Variance Regularization,

- k-Means, DBSCAN, PCA, tSNE,

- Neural Networks, Multilayer Perceptron Feedforward Neural Networks, Back-propagation, Deep Learning, Convolutional Neural Network.

Course Website:
https://www.niser.ac.in/~smishra/teach/ml-materialsc/2025/

Grading Scheme

- Exam (Written) - 30 marks

- Project - 70 marks

Grading - Projects Part A

- Own Project Group Size: Maximum 2 students per group

  - Introduction to their problem statement [5 marks]
    Deliverable: YouTube video (5 mins)
    Due: Sep 05, 2025

  - Midterm [10 marks]
    Deliverable: YouTube video (5 mins)
    Due: Oct 05, 2025

  - Endterm [25 marks]
    Deliverable: YouTube video (10 mins)
    Due: Dec 01, 2025

Grading - Projects Part B

- Each group will critically review 5 other projects. Each review must be a maximum 1-page report.

  - Introduction Review: 5 marks -
    Due - Sep 15, 2025

  - Midterm Review: 10 marks -
    Due - Oct 15, 2025

  - Endterm Review: 15 marks -
    Due - Dec 12, 2025

Artificial Intelligence (AI)

- What is AI ?

- Where are we with AI?

- Types of AI ?

Artificial Intelligence (AI)

- What is AI ?

  - Oxford Dictionary: "the capacity of computers, or other machines, to exhibit intelligent behaviour"

  - Artificial entity which is as good as human being (intelligence)

  - Critical thinking?

Artificial Intelligence (AI)

- Where are we with AI?

AI Painting (2018)
Edmond de Belamy

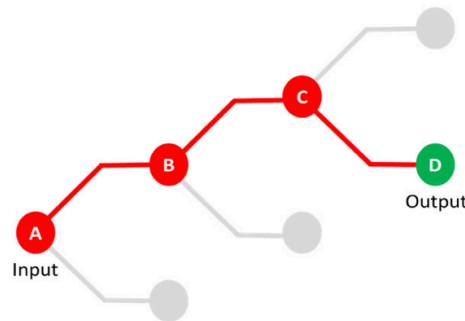**AI Painting (2023)**
Girl with Glowing Earrings

AI Photo (2023)
Pseudomnesia : The Electrician

Reference : INTRODUCTION TO ARTIFICIAL INTELLIGENCE (AI) TECHNOLOGY https://cdn-dynmedia-1.microsoft.com/is/content/microsoftcorp/microsoft/final/en-us/microsoft-brand/documents/2024-wttc-introduction-to-ai.pdf

Artificial Intelligence (AI)

- Where are we with AI?

  - Algorithms
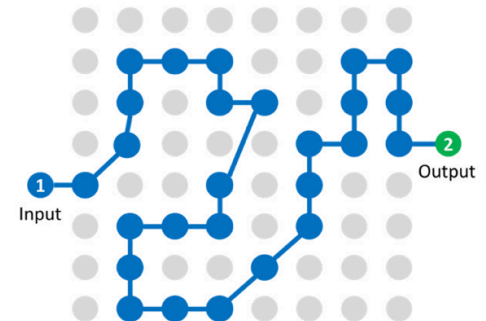

Traditional Programming

Artificial Intelligence (AI)

Reference : INTRODUCTION TO ARTIFICIAL INTELLIGENCE (AI) TECHNOLOGY https://cdn-dynmedia-1.microsoft.com/is/content/microsoftcorp/microsoft/final/en-us/microsoft-brand/documents/2024-wttc-introduction-to-ai.pdf

Artificial Intelligence (AI)

- Where are we with AI?

  - Big Data

Volume
Big Data involves massive quantities of information

Velocity
The speed at which new data is bring produced is incredibly fast

Variety
Big Data comes from a diverse variety of sources and in many formats, such as text, images, video and audio

Veracity
Big Data is sometimes inaccurate. Ensuring the quality, accuracy and reliability of big data can be challenging, due to the many diverse data sources and formats

Reference : INTRODUCTION TO ARTIFICIAL INTELLIGENCE (AI) TECHNOLOGY https://cdn-dynmedia-1.microsoft.com/is/content/microsoftcorp/microsoft/final/en-us/microsoft-brand/documents/2024-wttc-introduction-to-ai.pdf

Artificial Intelligence (AI)

- Where are we with AI?

  - Compute
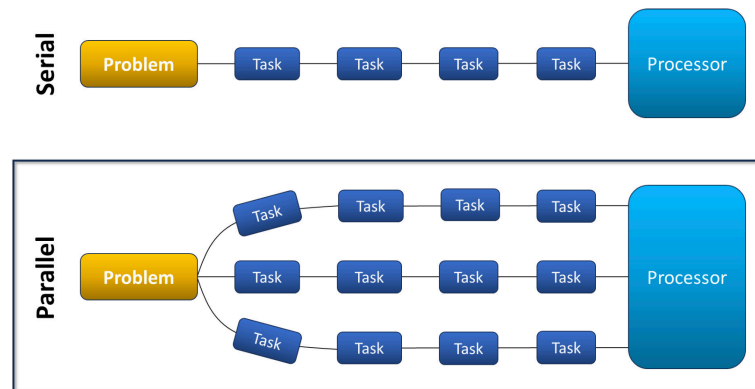
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Artificial Intelligence (AI)
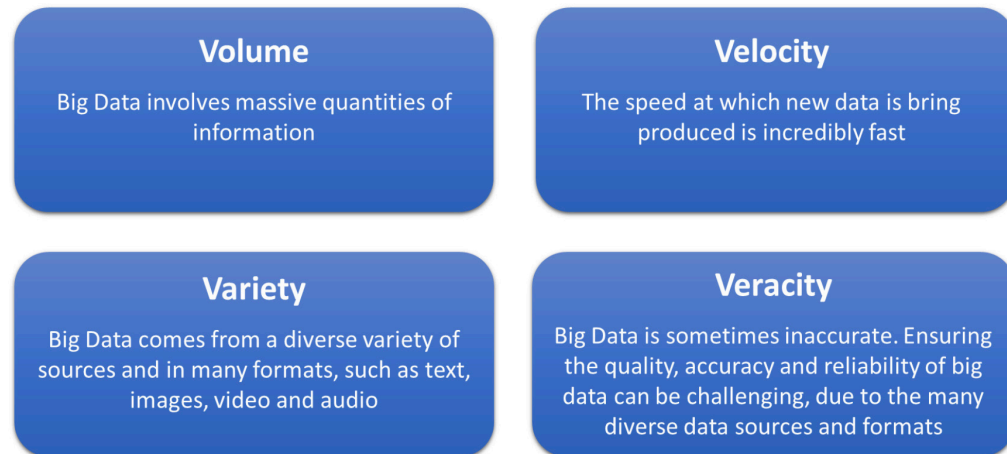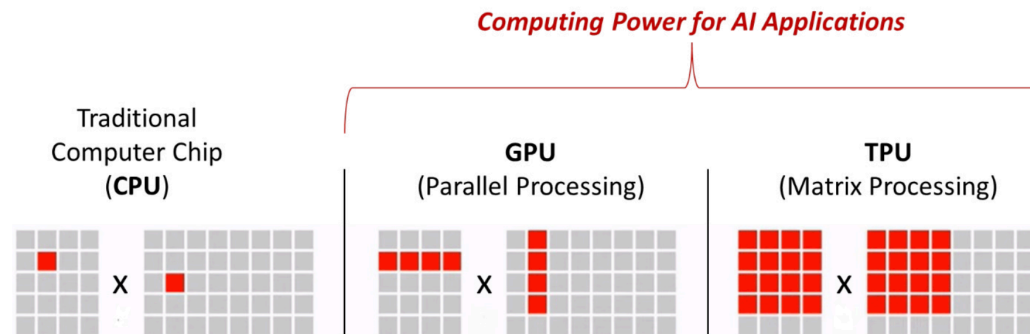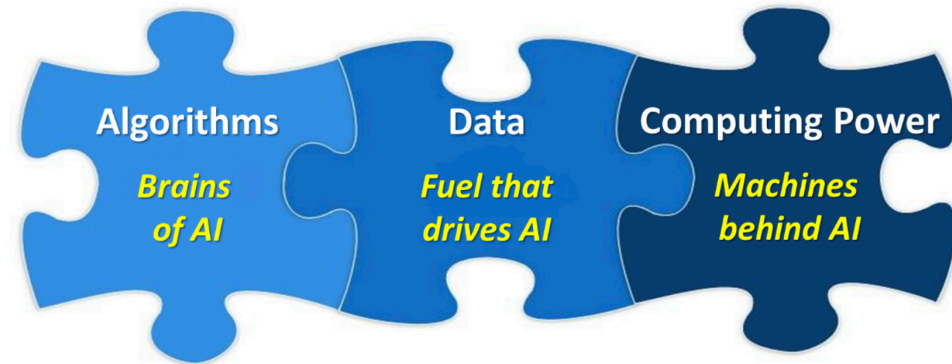
- Where are we with AI?

  - Algorithm

  - Data

  - Compute

Algorithms tell computers what to do. Data tells computers what to learn.
Computing power gives machines the power to learn and make decisions

Core Elements of Artificial Intelligence

Algorithms + Data + Compute

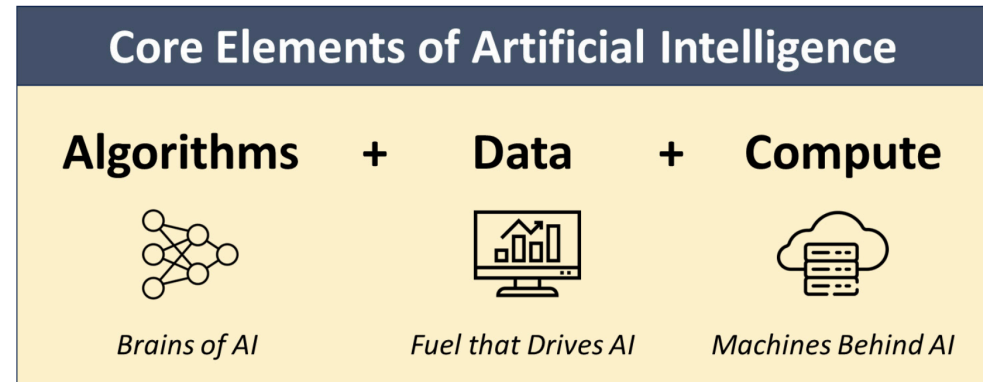Brains of AI   Fuel that Drives AI   Machines Behind AI

Reference : INTRODUCTION TO ARTIFICIAL INTELLIGENCE (AI) TECHNOLOGY https://cdn-dynmedia-1.microsoft.com/is/content/microsoftcorp/microsoft/final/en-us/microsoft-brand/documents/2024-wttc-introduction-to-ai.pdf

Artificial Intelligence (AI)

- Types of AI ?

Types of Artificial Intelligence

AI systems can be **classified by**….

1 The way an AI system **learns**

| Machine Learning | or | Deep Learning |

or

2 An AI system's **capabilities**

| Artificial Narrow Intelligence (ANI) | or | Artificial General Intelligence (AGI) | or | Artificial Super Intelligence (ASI) |

or

3 An AI system's **functionality**

| Expert System | or | Predictive AI | or | Generative AI |