Machine Learning and Material Science

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Why do we need Machine Learning?

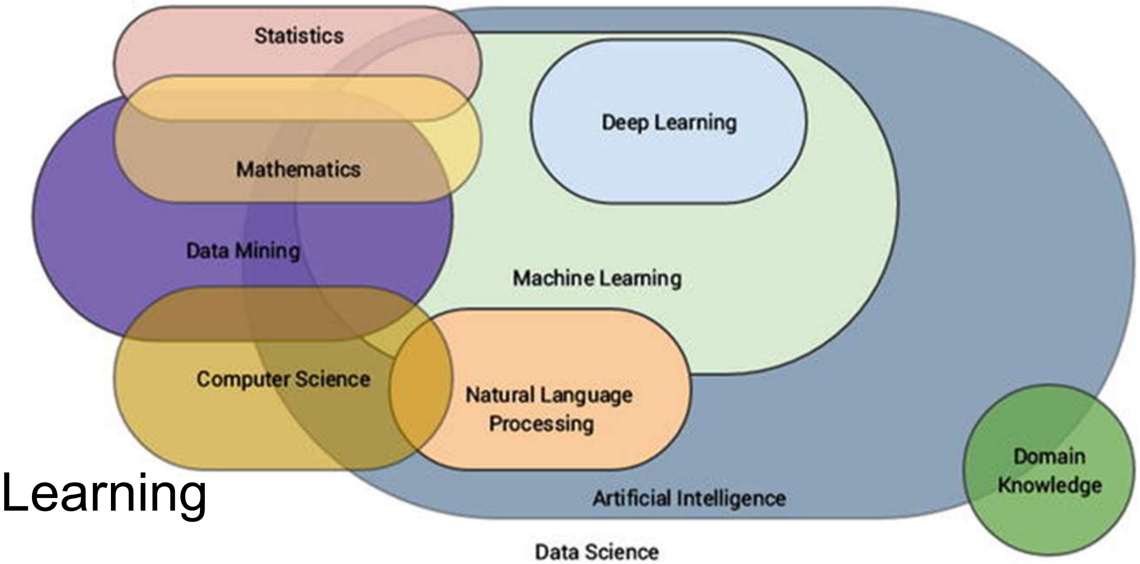
Data-rich world and computers/machines help us

Applications in day-to-day life:

- Virtual personal assistants: e.g. Siri, Alexa and Google
- Search engine results (What do you really mean / click on?)
- Social media: e.g. people you may know, face recognition
- Product recommendations (“People who bought … also bought …”)
- Online fraud detection, e.g. banks, “A person has accessed your account”)

Machine Learning: complicated/contradictory terms

Different names: “Machine Learning” – “Artificial Intelligence”



Different jobs:
- Data analyst
- Data scientist
- Specialist for Machine Learning

As always: “Learning by doing” => projects are important

Deep Learning: e.g. image processing

Data Mining: get lots of data from “sources”

Domain knowledge: have specific knowledge and learn further

Source: Bali, R., Sharma, T., & Sarkar, D. (2018)

What is Machine Learning?

'Machine Learning: Field of study that gives computers the ability to learn without being explicitly programmed.'

--- Arthur Samuel, 1959 @ IBM

'A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.'

--- Tom Mitchell, 1998

What is Machine Learning?

'A computer program is said to learn from ***experience E*** *with respect to some* ***task T*** *and some* ***performance*** *measure* ***P****, if its performance on T, as measured by P, improves with experience E.'*

--- Tom Mitchell, 1998

Task T: predict long-term creep (creep tests run month/years)

Experience E: previous creep behavior

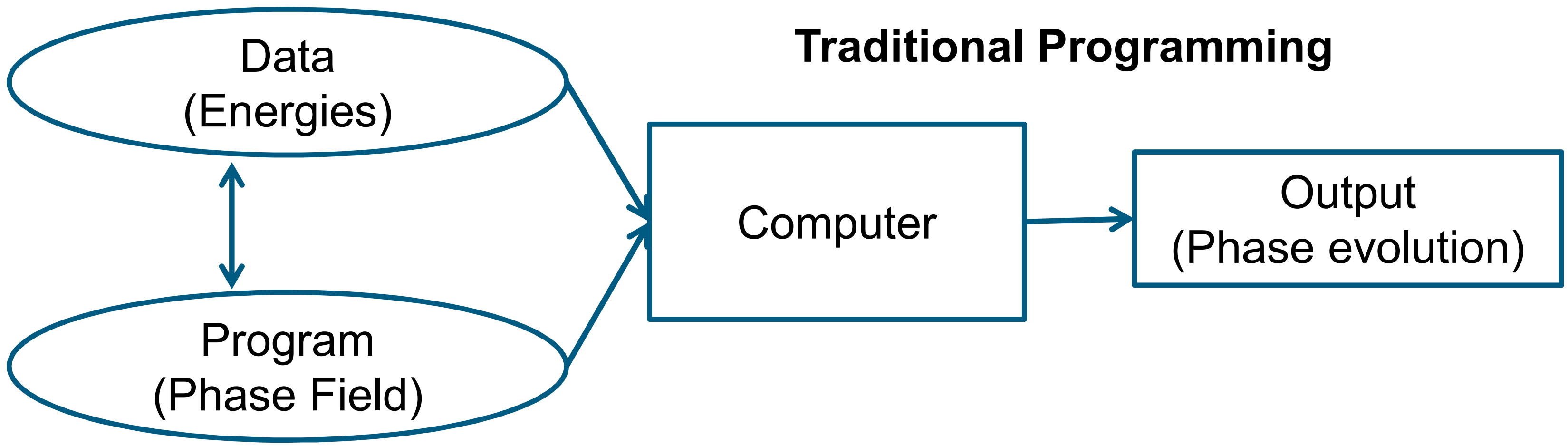
Performance P: measure how well model predicts current creep behavior

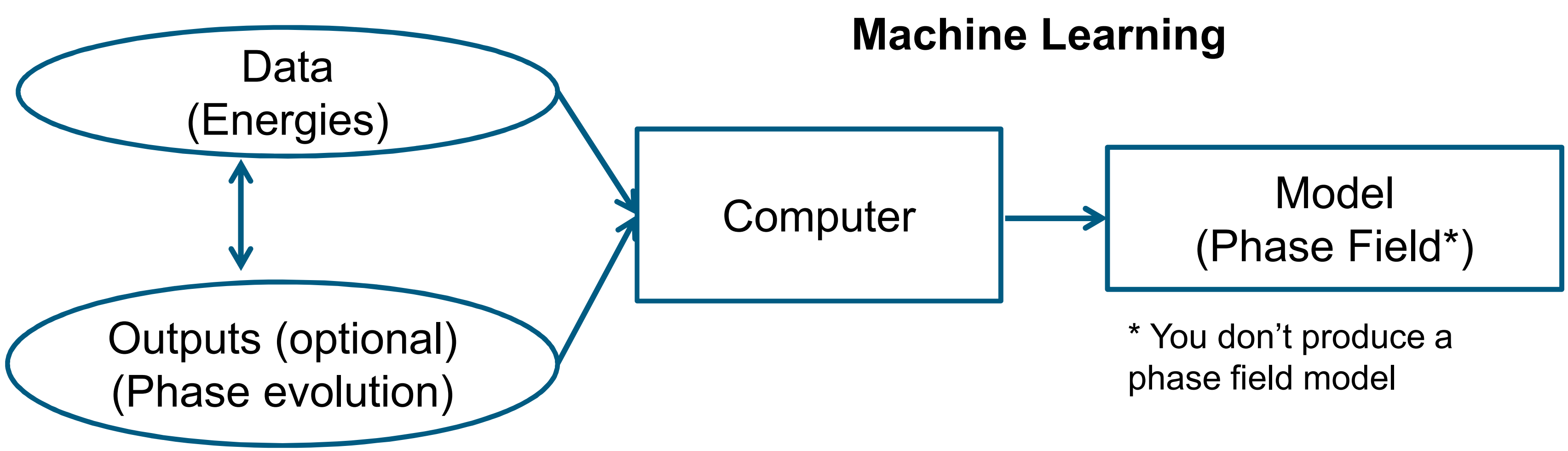
Model is successfully trained to predict creep behavior (task),

if it gets better (improves) ***performance***

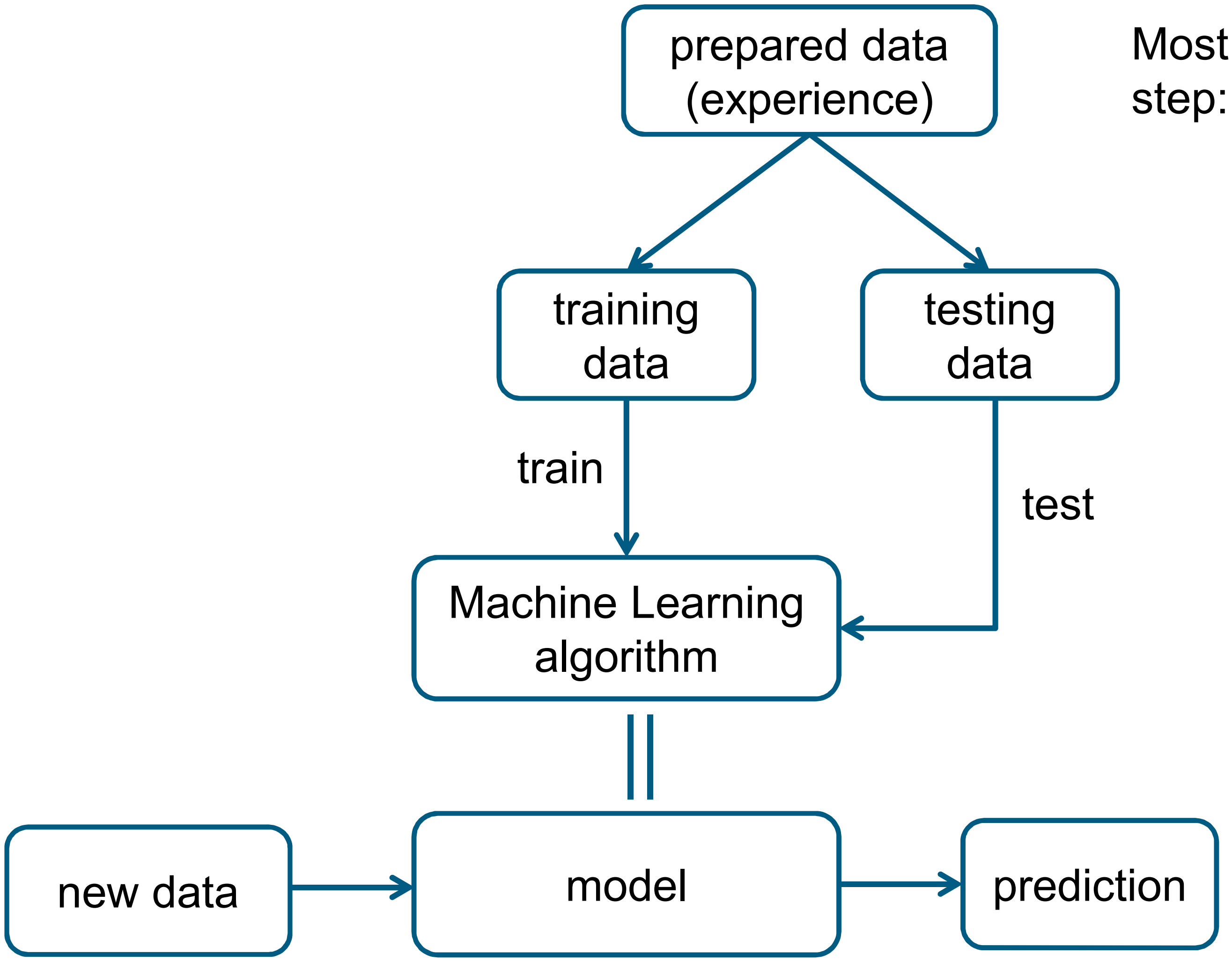
by using past information (***experience***)

Traditional programming v.s. Machine learning





Machine Learning workflow



Most time intensive step: >60%

Supervised Learning

Training Data

Input X & **Output y**

Learning algorithms to find function / model $f(X)$

Input X → $f(X)$ → Estimated output

Unsupervised Learning

Training Data

Input X

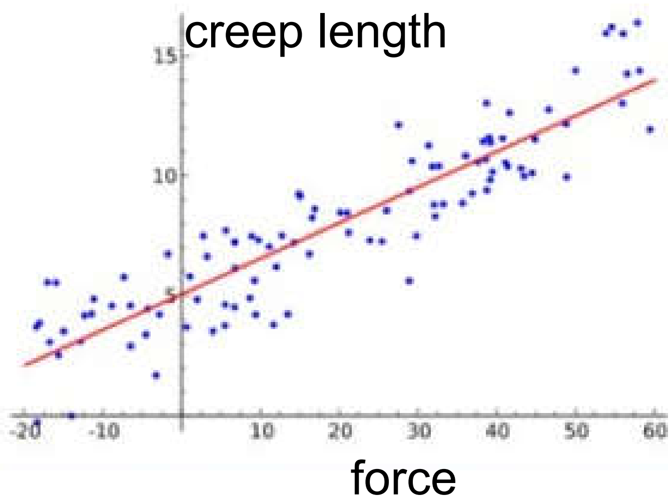
Learning algorithms

- identify patterns
- relationships

depend on input

Supervised Learning

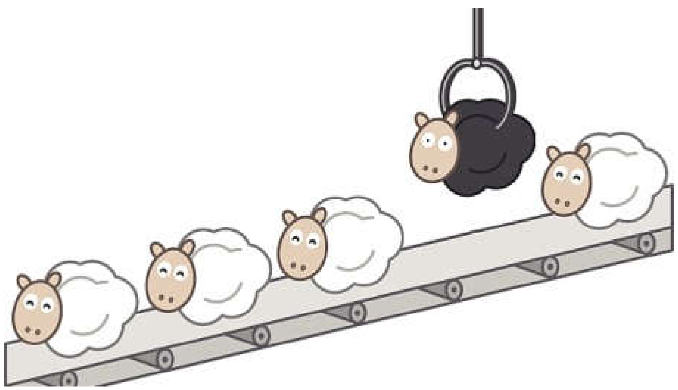
Regression: predict continuous target variable



Example: algorithm

- trained with force and creep length
- learns how to predict the creep length

Classification: group observations in set of finite labels

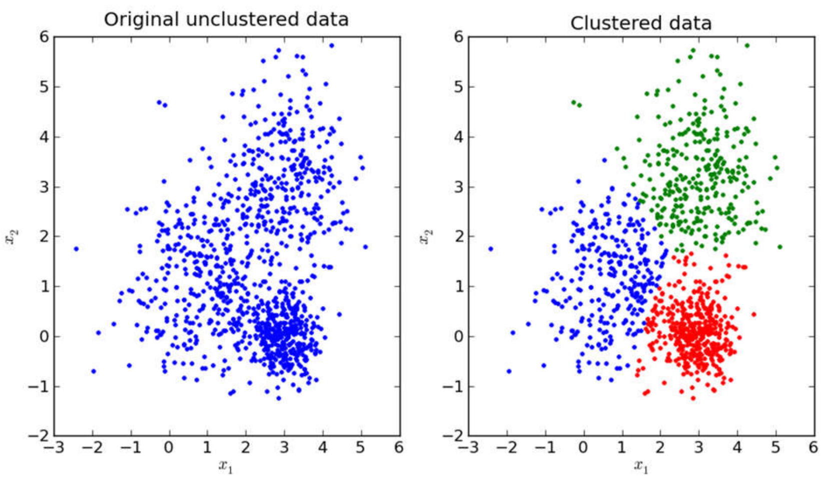


Example: algorithm

- train with labeled speed signs
- learns to identify speed signs from images

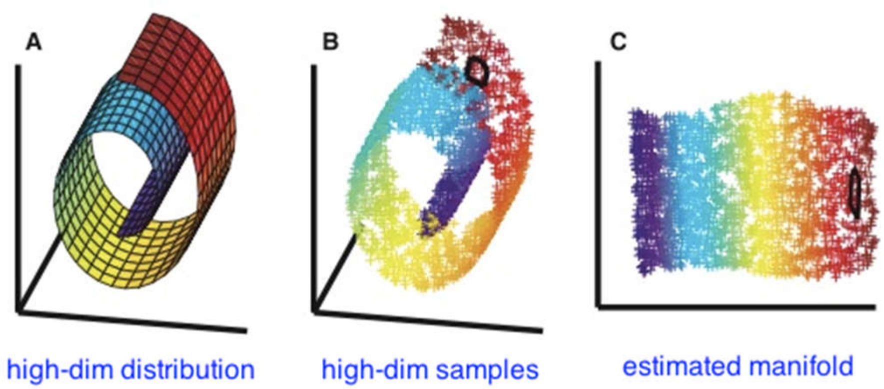
Unsupervised Learning

Cluster analysis: group / cluster data based on similarities



Example: build groups of similarity (same chemical component)

Dimensionality reduction: reduce number of variables to find principal variables



Example:

- feature selection
- extraction minimal set of variables that describe the result

Machine Learning algorithms

Supervised Learning

- Linear Regression
- Artificial Neural Network
- Convolutional Neural Networks
- Support Vector Machines
- Decision Trees
- …

Unsupervised Learning

- Combinatorial (or k-means) methods
- Hierarchical Cluster Analysis
- Principal Component Analysis
- …

Machine Learning algorithms

Supervised Learning

1. Linear regression (-> video incl. exercise)
2. Artificial Neural Network (-> video incl. exercise)
3. Convolutional Neural Networks
4. Support Vector Machine (-> video incl. exercise)
5. Decision Trees
6. …

Machine Learning Software for Python

classification, regression and clustering algorithms including support vector machines, …

Library for dataflow programming

It is a symbolic math library, and is also used for machine learning applications such as **neural network**.

Machine learning library alternative to Tensorflow

In past had many advantages over tensorflow