APL 405: Machine Learning in Mechanics

Lecture 1: Introduction

by

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What is machine learning?

Learning

“The activity or process of gaining knowledge or skill by studying, practicing, being taught, or experiencing something.”

Merriam Webster dictionary

Machine Learning

“the field of study that gives computers the ability to learn without being explicitly programmed.”

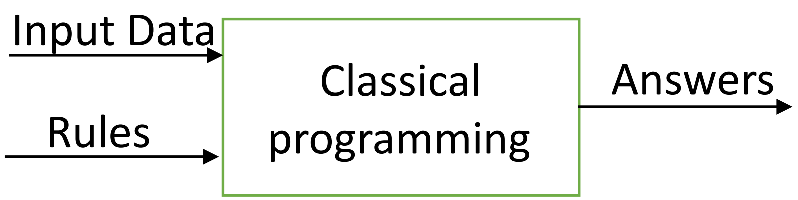
Arthur Samuel

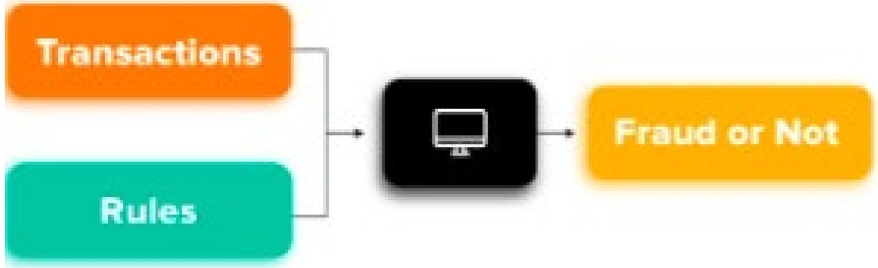
“A computer program is said to learn from *experience E* with respect to some class of *tasks T* and *performance measure P*, if its performance at tasks in T, as measured by P, improves with experience E.”

Tom Mitchell

Classical programming vs machine learning

- **Classical programming**: Program/Hard-code the rules for every task



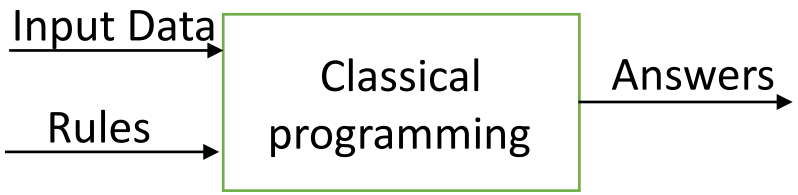


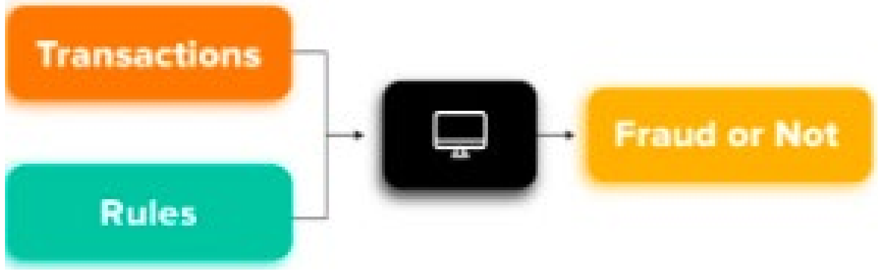
- In classical computer programming, a human designs the rules to figure out the relationship between the input data and answers and then build the rules

- However, for many tasks, it is difficult to manually design and hard-code correct rules
  - detecting spam, fraud transactions
  - recognizing people, objects
  - understanding human speech
  - detecting anomalous behaviors in mechanical systems

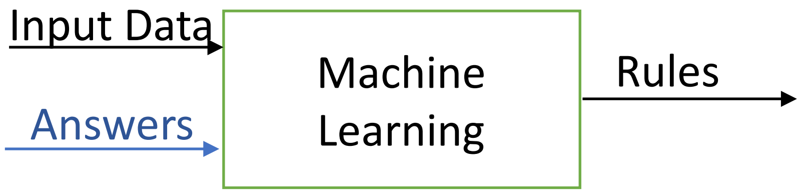
Classical programming vs machine learning

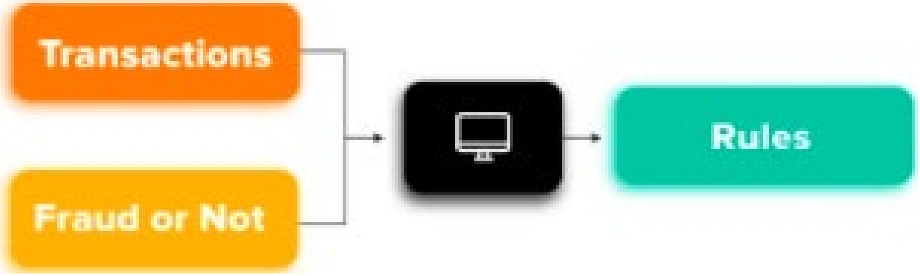
- **Classical programming**: Program/Hard-code the rules for every task





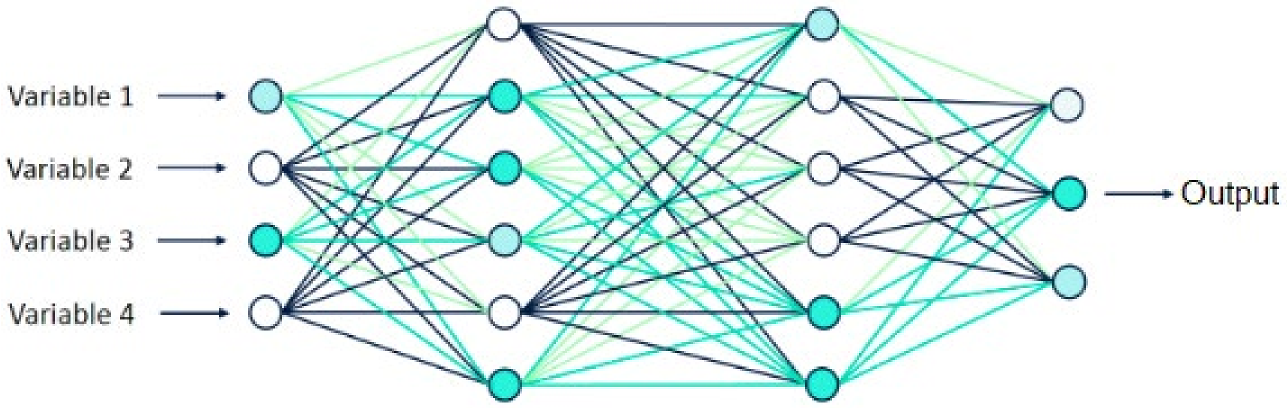
- **Machine learning approach**: An algorithm learn rules automatically from data or experience





What is machine learning?

- Machine learning is a way of generating *computer programs from examples for specific tasks*
- This generated computer program corresponds to a **mathematical model** of the data
  - It describes a relationship between *variables* (quantities involved), that correspond to the input data and the properties of interest (such as predictions, actions, etc.)
  - The model is a compact representation of the data that captures the key properties of the phenomenon we are studying

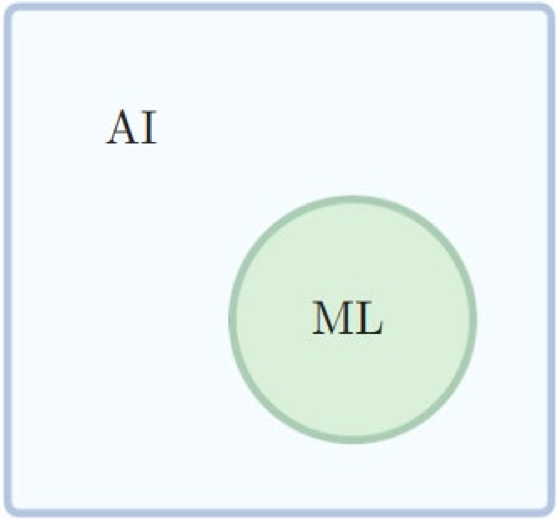


- Which model to use?
  - Guided by the machine learning engineer's insights generated when looking at the available data and the practitioner's general understanding of the problem

Machine Learning and Artificial Intelligence

- AI is the reproduction of an intelligent behavior by a machine: a combination of thinking and behaving rationally
- According to the **Turing test** (by Alan Turing), an AI agent must possess the following features:
  - Knowledge representation: to store what it knows or hears or sees
  - Automated reasoning: to use the stored information to answer questions
  - Natural language processing: to enable it to communicate successfully in a language
  - Machine learning: to detect patterns and extrapolate to unseen circumstances
  - Computer vision: to perceive objects
  - Robotics: to move and manipulate objects

- While AI and ML are very closely connected, they are not the same!
- Machine learning is a part of AI: It is the process of using mathematical models to help a computer learn without direct instruction (or hard-coding)

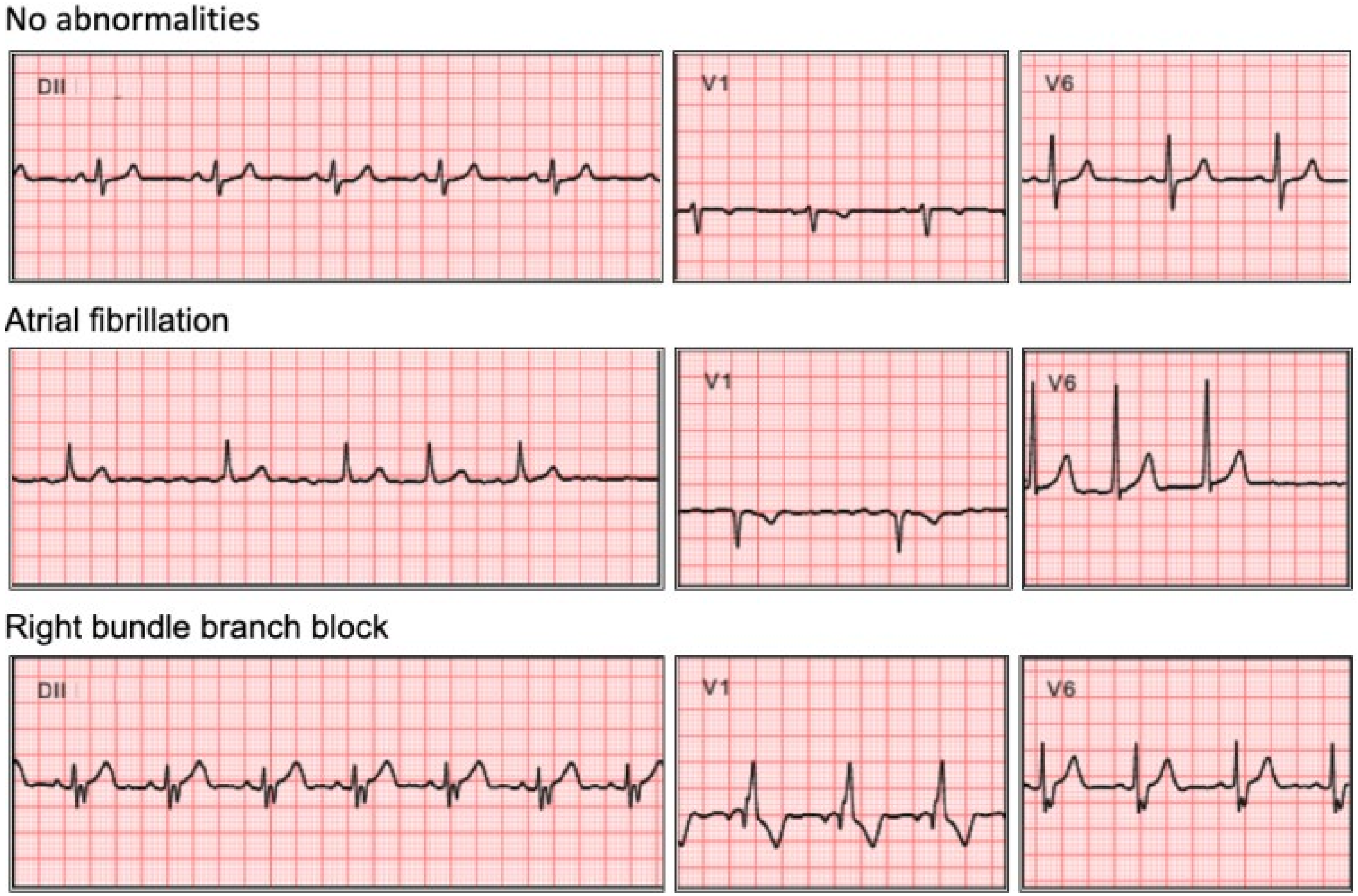


Examples of machine learning: Example 1

Automatically diagnosing heart abnormality

- Heart problems influence the electrical activity of the heart. These electrical signals can be measured using electrodes attached to the body (reported in ECG)

- ECG signal gives valuable information about the condition of the heart, which can be used to diagnose the patient and plan the treatment



Atrial fibrillation makes the heart beat without rhythm, making it hard for the heart to pump blood in a normal way

Right bundle branch block corresponds to a delay or blockage in the electrical pathways of the heart

Examples of machine learning: Example 1

Automatically diagnosing heart abnormality

- Can we construct a computer program that reads in the ECG signals, analyses the data, and returns a *prediction* regarding the normality or abnormality of the heart?

- **Challenge:** How to design a computer program that turns the raw ECG signal into a prediction about the heart condition?
  - An experienced cardiologist trying to explain his experience to a software developer (which patterns in the data to look for) would be extremely challenging!

- **Machine learning approach:** Teach the computer program through *labelled examples*.
  - Ask the cardiologist (or a group of cardiologists) to *label* a large number of recorded ECG signals with labels corresponding to the underlying heart condition.

  - A machine learning algorithm can then learn to come up with its own rules based on these examples, so that the predictions agree with the cardiologists' labels on the "training" examples

  - The hope is that, if it succeeds on the training data (where we already know the answer), then it should be possible to use the predictions made the by program on previously unseen data (where we *do not* know the answer)

Examples of machine learning : Example 1

Automatically diagnosing heart abnormality

- Ribeiro et. al. developed a machine learning model for ECG prediction
- 23,00,000 ECG records (each of 7-10 s, sampled at 300-600Hz) were used evaluate the electrical activity of the heart of 17,00,000 patients
- The dataset comes with associated labels for **six different** classes according to the status of the heart, i.e., no abnormalities, atrial fibrillation, RBBB, etc.
- Based on this data, a machine learning model (specifically, a deep neural network) was trained to automatically classify a new ECG recording without requiring a human doctor to be involved
- To evaluate how the trained model performs in practice, cardiologists with experience in ECG examined and classified
- The average performance was then compared
- The result was that the algorithm achieved better or the same result when compared to the human performance on classifying six types of abnormalities

Ribeiro, Antônio H., et al. "Automatic diagnosis of the 12-lead ECG using a deep neural network." *Nature communications* 11.1 (2020): 1-9.

Examples of machine learning : Example 1

Various concepts central to machine learning can be understood from this ECG example

1. Data is an important ingredient in machine learning

2. In the ECG example, each data point consists of an **input** (e.g. ECG signal) and an associated **output** (e.g. label corresponding to the heart condition). Such type of data with both input and output is called *labelled* data

3. “Training” a model with labelled data (both inputs and outputs) points is referred to as ***supervised learning***
   - Think of the learning as being supervised by the domain expert, and the learning objective is to obtain a computer program that can mimic the labelling done by the expert

4. The ECG example represents a ***classification*** problem
   - Classification is a supervised machine learning task which amounts to predicting a certain class, for each data point
   - Another type of supervised learning problem is **regression**, where the output is a numerical value

5. In the first phase, a chunk of data is used to train the machine learning model → **Training** data

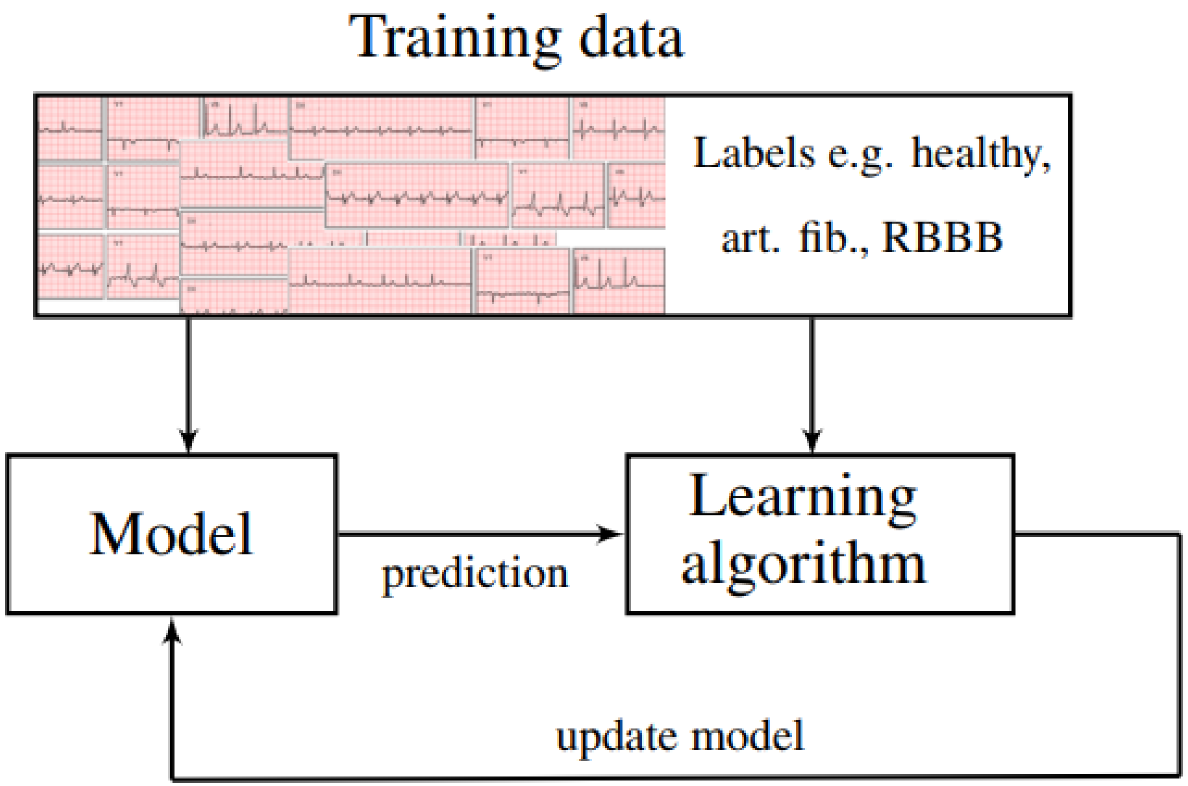
6. The ultimate goal of the trained ML model is to obtain accurate predictions in future. We say that the predictions made by the model must *generalise beyond the training data*

7. In 2nd phase, new unseen unlabelled data (only inputs) are fed to the computer program to predict the labels

Examples of machine learning : Example 1

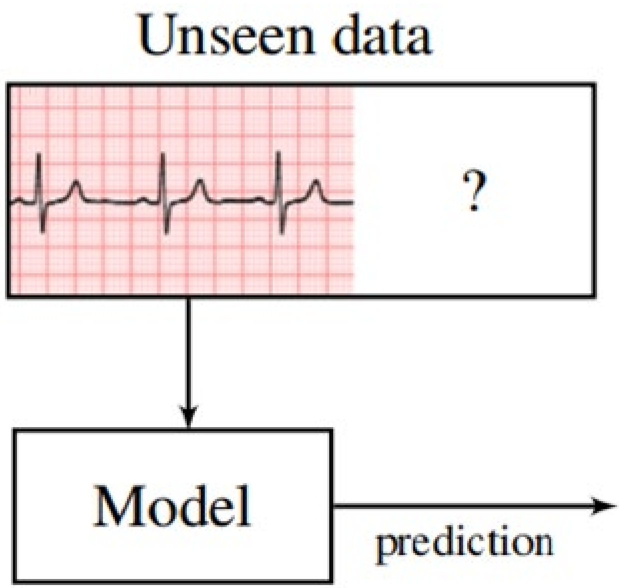
Automatically diagnosing heart abnormality

Training phase



The parameters of the model are tuned by the learning algorithm such that the model best describes the available training data

Testing phase



The learned model is used on new, previously unseen data (**test** data), where we hope to obtain a correct classification

Examples of supervised machine learning

- **Supervised learning - classification**: ECG ML model predicted a certain class

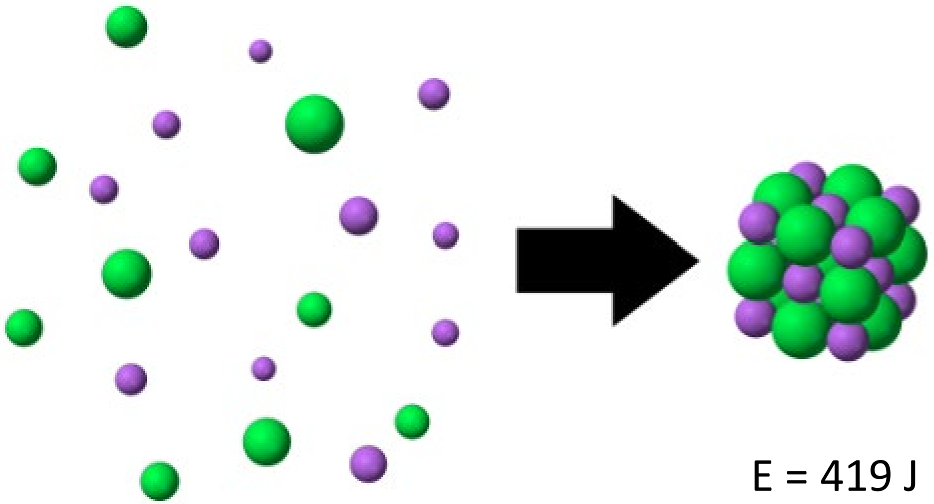
→ Normal or Abnormal?

Examples of machine learning : Example 2

Predicting formation energy of crystals

- **Motivation**:

  A basic property of interest when trying to discover or synthesize a hypothetical material is the *formation energy* of a crystal. The formation energy can be thought of as the energy that nature needs to spend to form the crystal from the individual elements. A crystal with lower formation energy is more stably synthesized



- **Challenge**: DFT is very accurate but computationally very expensive, even on modern supercomputers. Hence, only a small fraction of all potentially interesting materials can been analysed

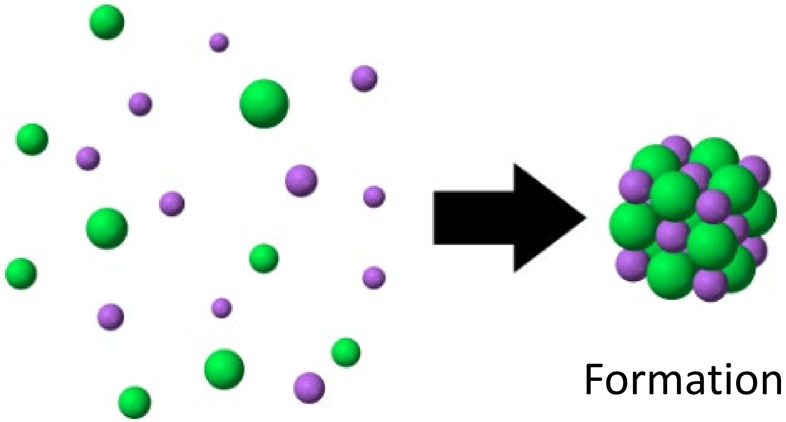
- **Machine learning approach:** Train an ML model that mimics the DFT but is computationally fast
  - Input → Description of the positions and atoms in the candidate crystal
  - Output → Formation energy of the candidate crystal computed using DFT
  - Faber et. al. (2016) used kernel ridge regression to predict the formation energy of 2 million crystals

Examples of supervised machine learning

- **Supervised learning - classification**: ECG ML model predicted a certain class

→ Normal or Abnormal?

- **Supervised learning - regression**: Material discovery model predicted a numerical value (formation energy of crystal)



Formation energy, E

Regression and classification are the two types of prediction problems that we will learn in this course

Different types of machine learning

Supervised	Unsupervised	Semi-supervised	Reinforcement
Teacher provides answer	No teacher, find patterns!		Teacher provides rewards
			
▪ Labeled data ▪ Direct feedback ▪ Predict outcome	▪ No labels ▪ No feedback ▪ Find hidden structure	▪ Some labelled data ▪ A lot of unlabeled data	▪ Decision process ▪ Rewards ▪ Learn series of actions
• Classification • Regression	• Clustering • Dimensionality reduction • Outlier detection		• Gaming • Control