# Introduction

## Numerical Methods for Deep Learning

# Learning From Data: The Core of Science - 1

Given inputs and outputs, how to choose $f$?

**Option 1** (Fundamental(?) understanding): For example, Galileo's law of motion

$$x(t) = \frac{1}{2}gt^2,$$

with unknown parameter $g$.

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$$x(t) = \frac{1}{2}gt^2,$$

with unknown parameter $g$.
To estimate $g$ observe falling object

| t | x |
|---|---|
| 0 | 0 |
| 1 | 4.9 |
| 2 | 20.1 |
| 3 | 44.1 |

Goal: Derive model from theory, calibrate it using data.

# Learning From Data: The Core of Science - 2

Given inputs and outputs, how to choose $f$?

**Option 2** (Phenomenological models): For example, Archie's law - what is the electrical resistivity of a rock and how it relates to its porosity, $\phi$ and saturation, $S_w$?

$$\rho(\phi, S_w) = a\phi^{n/2} S_w^p$$

$a, n, p$ unknown parameters

Obtaining parameters from observed data and lab experiments on rocks.

Goal: Find model that consistent with fundamental theory, without directly deriving it from theory.

# Phenomenological vs. Fundamental

**Fundamental laws** come from understanding(?) the underlying process. They are **assumed invariant** and can therefore be predictive(?).

**Phenomenological models** are data-driven. They "work" on some given data. Hard to know what their limitations are.

**But ...**

- models based on understanding can do poorly - weather, economics ...
- models based on data can sometimes do better
- how do we quantify understanding?

# Machine Learning in 3 slides - 1

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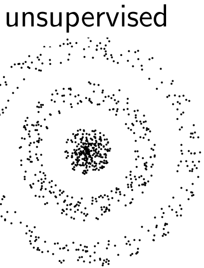
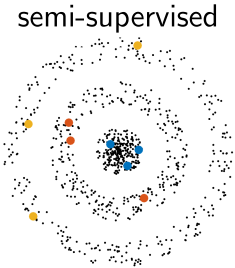
Two common tasks in machine learning:

- given data, cluster it and detect patterns in it (unsupervised learning)
- given data and labels, find a functional relation between them (supervised learning)

# Machine Learning in 3 slides - 2



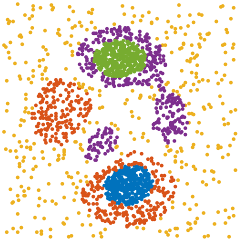

Unsupervised learning - given the data set $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_n]$ cluster the data into "similar" groups (labels).

- helps find hidden patterns
- often explorative and open-ended

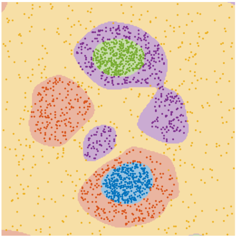
Semisupervised - label the data based on a few examples

# Machine Learning in 3 slides - 3

training data



trained model



Supervised learning - given the data set $\mathbf{Y} = [\mathbf{y}_1, \ldots, \mathbf{y}_n] \in \mathcal{Y}$ and their labels $\mathbf{C} = [\mathbf{c}_1, \ldots, \mathbf{c}_n] \in \mathcal{C}$, find the relation $f : \mathcal{Y} \rightarrow \mathcal{C}$

- models range in complexity
- older models based on support vector machines (SVM) and kernel methods
- recently, deep neural networks (DNNs) dominate

# Deep Neural Networks: History

- Neural Networks with a particular (deep) architecture
- Exist for a long time (70's and even earlier) [11, 12, 9]
- Recent revolution - computational power and lots of data [1, 10, 8]
- Can perform very well when trained with lots of data
- Applications
  - Image recognition [5, 7, 8], segmentation, natural language processing [2, 3, 6]

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  - Image recognition [5, 7, 8], segmentation, natural language processing [2, 3, 6]
- A few recent news articles:
  - Apple Is Bringing the AI Revolution to Your iPhone, WIRED 2016
  - Why Deep Learning Is Suddenly Changing Your Life, FORTUNE 2016
  - Data Scientist: Sexiest Job of the 21st Century, Harvard Business Rev '17

# Learning Objective: Demystify Deep Learning

**Artificial Intelligence / Machine Learning**

## The Dark Secret at the Heart of AI

No one really knows how the most advanced algorithms do what they do. That could be a problem.

by **Will Knight** Apr 11, 2017

Learning objectives of this minicourse:

- look under the hood of some deep learning examples
- describe deep learning mathematically (see also [4])
- expose numerical challenges / approaches to improve DL

# DNN - A Quick Overview - 1

Neural networks are data interpolator/classifier when the underlying model is unknown.

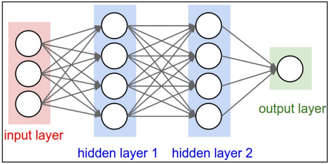
A generic way to write it is

$$\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta}).$$

- the function $f$ is the computational model
- $\mathbf{y} \in \mathbb{R}^{n_f}$ is the input data (e.g., an image)
- $\mathbf{c} \in \mathbb{R}^{n_c}$ is the output (e.g. class of the image)
- $\boldsymbol{\theta} \in \mathbb{R}^{n_p}$ are parameters of the model $f$

In supervised learning we have examples $\{(\mathbf{y}_j, \mathbf{c}_j) \ : \ j = 1, \ldots, n\}$ and the goal is to estimate or "learn" the parameters $\boldsymbol{\theta}$.

# DNN - A Quick Overview - 2



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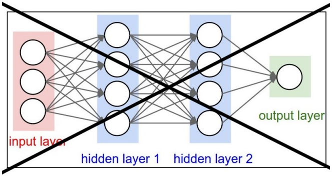


$$\begin{cases} \mathbf{y}_{l+1} &= \sigma(\mathbf{K}_l \mathbf{y}_l + \mathbf{b}_l) \\ \mathbf{y}_{l+1} &= \mathbf{y}_l + \sigma(\mathbf{K}_l \mathbf{y}_l + \mathbf{b}_l) \\ \mathbf{y}_{l+1} &= \mathbf{y}_l + \sigma\left(\mathbf{L}_l \sigma(\mathbf{K}_l \mathbf{y}_l + \mathbf{b}_l)\right) \\ & \vdots \end{cases}$$

Here:

- $l = 0, 1, 2, \ldots, N$ is the layer
- $\sigma : \mathbb{R} \to \mathbb{R}$ is the activation function
- $\mathbf{y}_0 = \mathbf{y} \in \mathbb{R}^{n_f}$ is the input data (e.g., an image)
- $\mathbf{c} \in \mathbb{R}^{n_c}$ is the output (e.g. class of the image)
- $\mathbf{L}_l, \mathbf{K}_l, \mathbf{b}_l$ are parameters of the model $f$

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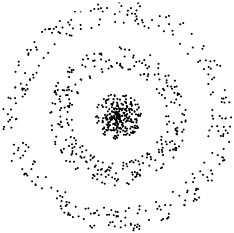
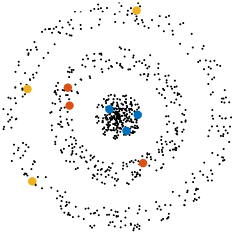
unsupervised



semi-supervised



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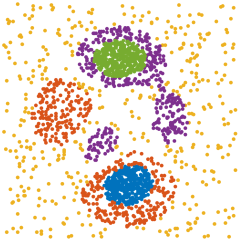


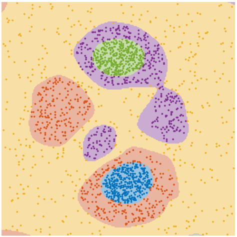


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# Generalization - 1

Suppose that we have examples $\{\mathbf{y}_j, \mathbf{c}_j\}, \quad j = 1, \ldots, n$, a model $f(\mathbf{y}, \boldsymbol{\theta})$ and some optimal parameter $\boldsymbol{\theta}^*$.
Let $\{(\mathbf{y}_j^t, \mathbf{c}_j^t) \ : \ j = 1, \ldots, s\}$ be some test set, that was not used to compute $\boldsymbol{\theta}^*$.

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For phenomenological models, there is no reason why the model should generalize, but in practice it often does.

# Generalization - 2

Why would a model generalize poorly?

$$1 \ll \|f(\mathbf{y}_j^t, \boldsymbol{\theta}^*) - \mathbf{c}_j^t\|_p$$

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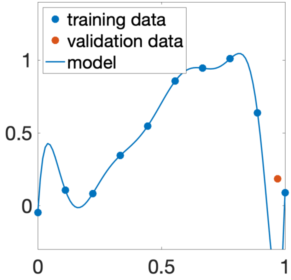


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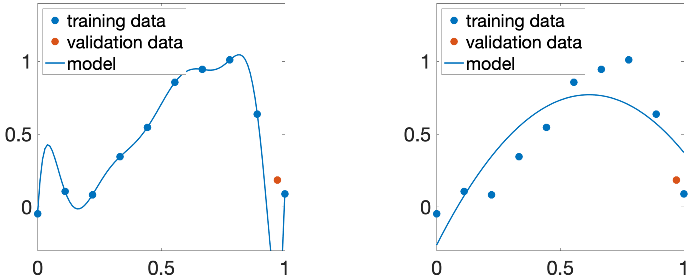


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Two common reasons:

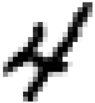
1. Our "optimal" $\boldsymbol{\theta}^*$ was optimal for the training but is less so for other data
2. The chosen computational model $f$ is poor (e.g. quadratic model for a nonlinear function).

# Example: Classification of Hand-written Digits

- Let $\mathbf{y}_j \in \mathbb{R}^{n_f}$ and let $\mathbf{c}_j \in \mathbb{R}^{n_c}$.
- The vector $\mathbf{c}$ is the probability of $\mathbf{y}$ belonging to a certain class. Clearly, $0 \le \mathbf{c}_j \le 1$ and $\sum_{j=1}^{n_c} \mathbf{c}_j = 1$.

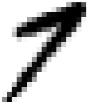
Examples (MNIST):

$\mathbf{y}_1$



$\mathbf{c}_1 = [0, 0, 0, 0, 1, 0, 0, 0, 0, 0]^\top$

$\mathbf{y}_2$



$\mathbf{c}_2 = [0, 0.3, 0, 0, 0, 0, 0, 0.7, 0, 0]^\top$

# Example: Classification of Natural Images

Image classification of natural images

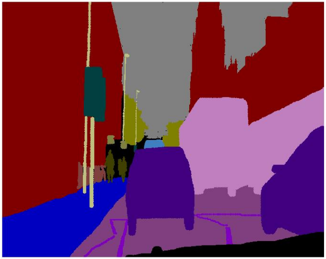
Examples (CIFAR-10):

# Example: Semantic Segmentation - 1

- let $\mathbf{y}_j \in \mathbb{R}^n$ be an RGB or grey valued image.
- let the pixels in $\mathbf{c}_j \in \{1, 2, 3, \dots\}^k$ denote the labels.

$\mathbf{y}$, input image

$\mathbf{c}$, segmentation (labeled image)



Goal: Find map $\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta})$

# Example: Semantic Segmentation - 2

Problem: Given image $\mathbf{y}$ and label $\mathbf{c}$, find a map $f(\cdot, \boldsymbol{\theta})$ such that $\mathbf{c} \approx f(\mathbf{y}, \boldsymbol{\theta})$

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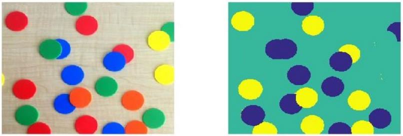
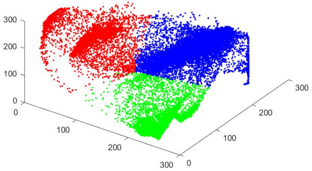
# Example: Semantic Segmentation - 3

Simpler setup

- input: $\mathbf{y}$ is the RGB value of the pixel (and its neighbors?)
- output: $\mathbf{c}$ is a labeled pixel
- goal: map $\mathbf{c} = f(\mathbf{y}, \boldsymbol{\theta})$



input image and segmentation




3D representation of RGB values

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