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Machine Learning: general concepts and applications

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Part I

Introduction to Machine Learning



- The discipline is roughly as old as computer science itself but with older roots in statistics, mathematics, and physics
- Many facets exist today, in general a collection of algorithms, methods, and analysis techniques where data plays a central role
- The ability of a computer program to aquire knowledge from data and improve performance through experience has been one of the core issues of Artificial Intelligence since ever
- Today machine learning is the fundamental reason behind the success of AI and many people talk about AI when they really mean machine learning

- Some tasks involve computing a function on data points to obtain useful predictions
 - Object recognition in images
 - Speech recognition
 - Text categorization
 - Translation (e.g. from Czech to Dutch)
 - Molecule activity prediction
 - Protein structure prediction
- Not enough domain knowledge to formalize the task and enable traditional algorithmic solutions

- In supervised learning you collect examples of instances paired with the corresponding solution, e.g.
 - This is a picture of a lemon tree
 - In this utterance the speakers says "Good morning"
 - This molecule is confirmed active against HIV
 - Dobré ráno \mapsto Goede morgen
- A machine learning algorithm will take as input many such pairs and will return a function

Supervised Learning (standard)



- (Q1) how do we define \mathcal{H} ?
- (Q2) how fo we compute $\widehat{f} = A(\mathcal{D}, \mathcal{H})$?

(Q1): Hyperplanes

- Long history, e.g., Fisher 1936, McCulloch & Pitts 1943, Berkson 1944, Rosemblatt 1957
- Heavy criticisms in 1969 by Seymour Papert and Marvin Minsky, end of early connectionism, prelude to the AI winter of the 1970s





- Also have a long history, e.g., Morgan & Sonquist 1963, Hunt 1966, Breiman et al. 1984, Quinlan 1986
- Some very effective techniques (e.g. random forests, gradient boosting, etc) still based on this idea



(Q1): Reproducing kernel Hilbert spaces

- See e.g. Mercer 1909, Kimeldorf & Wahba 1970, Cortes & Vapnik 1995
- Praised for over a decade because searching boils down to solving a convex optimization problem



(QI): Neural networks

- See e.g. Turing 1948, Fukushima 1980, Rumelhart, Hinton, & Williams 1985, Hinton et al. 2006
- Deep learning (where you actually use any differentiable computational graph) responsible for the AI explosion of this decade



(Q2): Solving the standard supervised learning problem

- Need to define a quality measure of the generated function
- Typically this is done through a loss function $L: \mathcal{X} \times \mathcal{Y} \mapsto \mathbb{R}$ where L(f(x), y) is the cost incurred when you predict f(x)and you should have predicted y
- Once we have *L* (not always obvious) the problem looks like optimization:

$$\widehat{f}_{\mathcal{H}} = \arg\min_{f\in\mathcal{H}} \mathbb{E} L(f(x), y)$$

• But unfortunately this cannot be done: the objective is not observed!

• Be happy with the "data distribution" (and regularize)

$$\begin{array}{lll} \widehat{f} &=& \arg\min_{f\in\mathcal{H}}\sum_{(x,y)\in\mathcal{D}}L(f(x),y)\\ \\ \text{Subject to} && \Omega[f] < R \end{array}$$

- *L* needs to be appropriate for the task at hand (but tractability also needs to be taken into account)
- Choice (and size) of the hypothesis space also very important
- Hyperparameter R trades complexity for overfitting
- No universally better learning algorithm (no free lunch theorem)

Many better algorithms and methods but perhaps most importantly these few things:

- Powerful hardware (2 petaFLOPS for \$400k, compare to .28 of top supercomputer Blue Gene when deep learning started, \$290 millions)
- 2. Vast software codebase
- 3. Large datasets
- 4. Really strong industrial interest