https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf

## Introduction to Machine Learning



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Director of the Computer Science Park 2019-



## What is machine learning?

- "Learning is any process by which a system improves performance from experience"
- Herbert Simon (Turing Award 1975, Nobel Prize in Economics 1978)

- Definition by Tom Mitchell (1998):

Machine Learning is the study of algorithms that

- improve their performance $P$
- at some task $T$
- with experience $E$

A well-defined learning task is given by $\langle P, T, E\rangle$


## Difference w.r.t. traditional programming

## Traditional Programming



## Machine Learning



No, more like gardening

- Seeds = Algorithms
- Nutrients = Data
- Gardener = You
- Plants = Programs



## When Do We Use Machine Learning?

- ML is used when:
- Human expertise does not exist (navigating on Mars, forecasting)
- Humans cant explain their expertise (recognition)
- Models must be customized (personalized medicine)
- Models are based on huge amounts of data (genomics)

$00011(1112$ $34444455>5$
 898894999 what makes $a$ « $2 »$ ?


## Some more examples of tasks that are best solved by using a learning algorithm

- Recognizing patterns:
- Facial identities or facial expressions
- Handwritten or spoken words
- Medical images
- Generating patterns:
- Generating images or motion sequences
- Recognizing anomalies:
- Unusual credit card transactions
- Unusual patterns of sensor readings in a nuclear power plant
- Forecasting:
- Future stock prices or currency exchange rates


## Some bachelor projects in machine learning

- Expression recognition
- (Dr. Luca Brunelli, now in Statwolf, data science, https://www.statwolf.com/)



## STATWOLF

## Some bachelor projects in machine learning

- Scene recognition



## Predictions

- Type of environment: indoor
- Semantic categories: office:0.61, home_office:0.13,
- SUN scene attributes: enclosedarea, nohorizon, cloth, man-made, electricindoorlighting, matte, research, sterile


## Some bachelor projects in machine learning

- creating 3D objects from 2D images

(Carlo Veronesi, Nicholas Merci, their ongoing bachelor thesis)

a particular of the 3D body


## Some bachelor projects in machine learning

- creating 3D objects from 2D images (2)

(Carlo Veronesi, Nicholas Merci, their ongoing bachelor thesis)



## Some bachelor projects in machine learning

- Birth records digitalization towards family tree estimation


Rosa


Battezzardi ib tro (???)


## Sample applications

- Web search
- Computational biology
- Finance
- E-commerce
- Space exploration
- Robotics
- Information extraction
- Social networks
- Debugging
- [Your favorite area]


## Defining the learning task

## Improve on task $T$, with respect to performance metric $P$, based on experience $E$

T: Playing checkers
P: Percentage of games won against an arbitrary opponent
E: Playing practice games against itself

T: Recognizing hand-written words
P: Percentage of words correctly classified
E : Database of human-labeled images of handwritten words

T: Driving on four-lane highways using vision sensors P: Average distance traveled before a human-judged error
E : A sequence of images and steering commands recorded while observing a human driver.

T: Categorize email messages as spam or legitimate. P: Percentage of email messages correctly classified. E: Database of emails, some with human-given labels

## Types of learning

- Supervised (inductive) learning (= regression/sup.ed classification)
- Given: training data + desired outputs (labels)
- Unsupervised learning
- Given: training data (without desired outputs)
- Semi-supervised learning
- Given: training data + a few desired outputs
- Reinforcement learning
- Rewards from sequence of actions


## Supervised Learning: Regression

- Given (x1, y1), (x2, y2), ..., (xn, yn)
- Learn a function $f(x)$ to predict $y$ given $x$
- -y is real-valued $==$ regression



## Supervised Learning: Classification

- Given (x1, y1), (x2, y2), ..., (xn, yn)
- Learn a function $f(x)$ to predict $y$ given $x$
- -y is categorical $==$ (supervised) classification

Breast Cancer (Malignant / Benign)


## Supervised Learning: Classification

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## Supervised Learning: Classification

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## Supervised Learning

- x can be multi-dimensional
- Each dimension corresponds to an attribute



## Unsupervised Learning

- Given $\times 1, \times 2, \ldots$, xn (without labels)
- Output hidden structure behind the $x$ 's
- e.g., clustering



## Unsupervised Learning




Astronomical data analysis

## Unsupervised Learning

- Genomics application: group individuals by genetic similarity


Individuals

## Unsupervised Learning

- Independent component analysis - separate a combined signal into its original sources


Input video (two people speaking together)


## Reinforcement learning

- Given a sequence of states and actions with (delayed) rewards, output a policy
- Policy is a mapping from states $\rightarrow$ actions that tells you what to do in a given state
- Examples:
- Credit assignment problem
- Game playing
- Robot in a maze
- Balance a pole on your hand


## The AgentEnvironment Interface



Agent and environment interact at discrete time steps : $t=0,1,2, \mathrm{~K}$
Agent observes state at step $t: \quad s_{t} \in S$
produces action at step $t: a_{t} \in A\left(s_{t}\right)$
gets resulting reward : $\quad r_{t+1} \in \Re$ and resulting next state : $s_{t+1}$
$\cdots-s_{t}{ }_{a_{t}} \cdot{ }^{r_{t+1}} s_{t+1}{ }_{a_{t+1}}^{r_{t+2}} s_{t+2}{ }_{a_{t+2}}^{r_{t+3}} s_{t+3}{ }_{a_{t+3}} \cdots$

## Reinforcement learning

## ML in a Nutshell

- Tens of thousands of machine learning algorithms
- Hundreds new every year
- Every machine learning algorithm has three components:
- Representation
- Evaluation
- Optimization


## Representation

- Decision trees
- Sets of rules / Logic programs
- Instances
- Graphical models (Bayes/Markov nets)
- Neural networks
- Support vector machines
- Model ensembles
- Etc.


## Evaluation

- Accuracy
- Precision and recall
- Squared error
- Likelihood
- Posterior probability
- Cost / Utility
- Margin
- Entropy
- K-L divergence
- Etc.


## Optimization

- Combinatorial optimization
- E.g.: Greedy search
- Convex optimization
- E.g.: Gradient descent
- Constrained optimization
- E.g.: Linear programming


## Types of Learning

- Supervised (inductive) learning
- Training data includes desired outputs
- Unsupervised learning
- Training data does not include desired outputs
- Semi-supervised learning
- Training data includes a few desired outputs
- Reinforcement learning
- Rewards from sequence of actions


## Inductive Learning

- Given examples of a function ( $X, F(X)$ )
- Predict function $F(X)$ for new examples $X$
- Discrete $F(X)$ : Classification
- Continuous $F(X)$ : Regression
- $F(X)=\operatorname{Probability}(X)$ : Probability estimation


## ML in Practice

- Understanding domain, prior knowledge, and goals
- Data integration, selection, cleaning, pre-processing, etc.
- Learning models
- Interpreting results
- Consolidating and deploying discovered knowledge
- Loop


## Deep Neural Networks

Thanks to: Deep Learning by Google - Take machine learning to the next level


## What is Deep Learning



Deep Learning (DL) has emerged around the ' 10 as a general tool to solve recognition problems in:

- computer vision
- speech recognition
- robotics
- discovering new medicines
- understanding natural language
- understanding documents
- ranking
- ... and many other applications!


## Overview

- History
- Preliminaries: logistic classification
- Training
- Deep networks
- Regularization
- Architectures
- Convolutional networks
- Embeddings
- Recurrent models

History


Since an early flush of optimism in the 1950s, smaller subsets of artificial intelligence - first machine learning, then deep learning, a subset of machine learning - have created ever larger disruptions.

## Everything can be optimized in Computer Science

- Given a problem to solve $P$, it can be formalized as $\{P, C, F\}$
- $P$ := the problem formulation
- $C=\left\{c_{1}, c_{1}, \ldots, c_{n}\right\}:=$ set of configurations, each one of them representing a possible solution to P
- $\mathrm{f}: \mathrm{C} \rightarrow \mathrm{R}:=$ function which provides a goodness measure of the configuration w.r.t. the problem to be solved
- Casting the problem via minimization means to maximize or minimize the function $f$ in the C space, independently on the implied meaning of $P$


## Minimization: to be used always?

- Problem $\mathrm{P}_{1}$ : sort numbers $\mathrm{x}_{1}, \mathrm{x}_{2}, \ldots, \mathrm{x}_{\mathrm{N}}$ in increasing order
- In this case, minimization could be left apart
- In facts, there is at least one algorithm (e.g., quicksort) which brings directly to the best (in sense of the function f) configuration
- Problem $P_{2}$ : foresee the stocks' trend
- Much more difficult to formalize into an algorithm
- Minimization comes to help [Yong et al. 2015]


## Inside the minimization approach

- The main goal of an optimization approach is that of exploring the configuration space C looking for the best configuration given the function $f$ (obviously avoiding the brute force way!)
- The set of configurations C give a space to explore (very often, a manifold)
- Optimizing means to explore the manifold by iterative approaches (e.g., the gradient descent family of strategies)
- The more the manifold is complex (non convex, multimodal), the more often local minima are met


## Neural Networks 1993 - Mcculocs 8 Pitss

- Optimization approaches which scale very well with data
- We are talking about artificial neurons and lavered comoutation



## Neural Networks - Neurons

NN are composed by artificial neurons (1943-McCulloch \& Pitts).
Each neuron has:

- dendrites (inputs)
- a nucleus/soma/perceptron (trancfor fıirtinn + artivatinn fıinrtinn)



## Neural Networks - Neurons (2)

The information flow is unidirectional:

- The neuron get inputs (electric potentials) from the dendrites, that weight them ( $w_{i}^{\prime} \mathrm{s}$ )
- In the nucleus, the weighted inputs are summed together (the transfer $\Sigma$ of the whole information coming from the dendrites)
- In the nucleus, the summation flows
 into an activation function, which may inhibit, diminish or amplify it
- The output of the activation function



## Neural Networks - the renaissance



## Neural Networks and Deep Learning



GPUs $\}$ Data

$\square \xrightarrow[\substack{\text { Neural } \\ \text { Networks }}]{\substack{\text { Deep } \\ \text { Netw }}}$

## Supervised Classification

- Traditional kind of problem the NN do solve

- Regression
- Ranking
o Reinforcement lea




## Preliminaries: logistic classification

## Logistic Classifier

- It assigns a score $y$ to the input $\mathbf{x}$ through a linear model (W,b)
- The score helps to identify the class label that wins


To be trained via a training procedure

## Logistic Classifier - the score is not enough

 $\mathrm{xW}+\mathrm{b}=\mathrm{y} \quad \Longrightarrow \mathrm{s}(\mathrm{y})$
$s(y)$ is the SOFTMAX
function

## Softmax function

- Converts scores into probability distributions
$\circ \mathbb{R} \rightarrow(0,1)$

- Open codomain!
- The softmax function highlights the largest values and suppress values which are signiffcantly below the maximum value $s\left(y_{i}\right)=$



## One-Hot Encoding (OHE)

## Which distance

measure?

MSE
sample

- $\rightarrow$ There is the need to evaluate the classification result
- OHE encodes labels for a C-class problem in $\mathrm{R}^{\mathrm{C}}$, indicating the che th $^{\text {th }}$ class label with 1 , the rest
$0_{0}{ }^{\text {indicating the }}(\mathrm{y})$
nee icient especially in the. Zase $C$ is very big (thousands or millions of glasses...!)ut
- $\rightarrow$ There is only one correct label for each input our


## Cross-Entropy

GOAL: computes the distance between two probability vectors

- Non sympetria functign $(\mathbf{L}, \mathbf{s})$

$$
D(\mathrm{~s}, \mathrm{~L}) \begin{cases}\rightarrow 0 & \text { high similarity } \\ \rightarrow \infty & \text { low similarity }\end{cases}
$$



- The $\log (\cdot)$ makes the training faster to converge than the other alternative MSE function $\left(5(c(v)-1)^{2}\right)$


## Résumé



$$
D(s(x W+b), L)
$$

## Training

## Gradient Descent

GOAL: search for the nearest local minimum of a function $F$

IDEA: iterate on the parameter set proportionally to the negative of the function gradient

$$
\theta_{t+1}=\theta_{t}-\alpha \nabla F\left(\theta_{t}\right), t \geq 0
$$

such that

$$
F\left(\theta_{0}\right) \geq F\left(\theta_{1}\right) \geq F\left(\theta_{2}\right) \geq \ldots
$$

## Gradient Descent

- GOAL: minimize a loss function
- Needs to compute the entire training set performance of our linear model, that consists in N inputs (which is, in general, very big)
- Needsfto Minimize a loss function, Guhichdepends $s s_{i=1}^{x} W$ (big matrix) and $\mathbf{b}$

Loss = average crossentropy


## Stochastic Gradient Descent (SGD)

- IDEA: use a random subset (batch) of the data (of a given size) to compute an approximation of the gradient of the loss function

Iterative implementation of the GD algorithm
At each step, a new batch is extracted

- Pros:

■ simple but sufficiently effective

- fast (depending on batch size)
- scale the problem with data and model size
o Cons:
■ needs more iterations to converge



## SGD trick 1: momentum

- GOAL: improve the convergence of the optimizer exploiting the accumulated knowledge from previous steps
- IDEA: add a fraction of the previous \#4pdatevector to, the curryent update vector
$M_{t}=\alpha \nabla \mathcal{L}_{t}\left(w_{i}, w_{j}\right)+\beta M_{t-1}$
$\left(w_{i}, w_{j}\right)_{t}=\left(w_{i}, w_{j}\right)_{t}-M_{t}$

faster convergence and oscillation redurtion


## SGD trick 2: learning-rate decay

- GOAL: make the optimization more robust and accurate over time
- IDEA: apply a decay function to the learning rate or reduce it when the loss functiond reaches a plateau



## SGD trick 3: z-normalization

- GOAL: avoid numerical instability

The values involved in the calculation of the gradient descent never get too big or too small
original data

zero-centered data



- IDEA: remove the mean and normalize over the variance of the $i$-th feature of the input vector $\frac{{ }^{\mathbf{x}} \mathbf{x}-E[\mathbf{x}]}{\operatorname{Var}[\mathbf{x}]}$

$$
\begin{gathered}
E[\mathbf{x}]=0 \\
\forall(i, j), \operatorname{Var}\left[\mathbf{x}_{i}\right]=\operatorname{Var}\left[\mathbf{x}_{j}\right]
\end{gathered}
$$

## z-normalization

## SGD trick 4: initialization

A random initialization of the weights and the zero-init of the biases is critical to get a good starting point for the training phase and the convergence of the $w_{i} S G D$ algorithm.

$$
\begin{aligned}
& \mathbf{b}=\left[\begin{array}{llll}
0_{1} & 0_{2} & \ldots & 0_{C}
\end{array}\right] \\
& \mu=0 \wedge \sigma \rightarrow 0 \Longrightarrow \forall(i, j), w_{i}=w_{j} \pm \epsilon
\end{aligned}
$$


equal probability of the weights (no prior)

## Gradient Descent: graphical representation (2D)



## Gradient Descent: graphical representation (3D)




## SGD: tuning

## SGD

Many hyperparameters:

- initial learning rate
- learning rate decay
- momentum
- batch size

- weight initialization


## AdaGrad

SGD modification which implicitly applies

## From MLC to NN to Deep-NN

- Multinomial Logistic Classification (MLC)
- fast: efficient computation due to the linear model
- stable: small input variations generates small output variations and the derivative of the model is constant

- What if I concatenate multiple MLCs? still a linear model...!


## From MLC to NN to Deep-NN

- GOAL: build a bigger and non linear model
- IDEA: concatenate many linear systems (MLC) and insert a non linear function between two consecutive MLCs, that is, the activation function



## Choose the (non linear) activation function



- A perceptron
- similar to sigmoid
- simplest function
- constant derivative


## ReLU: Rectified Linear Unit

$$
\operatorname{Re} L U(x)=\max (0, x)
$$





## Résumé



## Practical example (1/2)



## Practical example (2/2)

\#hidden_neurons
(H)

$$
\mathbf{x} * \mathrm{~W}_{1}+\mathbf{b}_{1}=\mathbf{y}_{1} \rightarrow \operatorname{ReLU}\left(\mathbf{y}_{1}\right) * \mathrm{~W}_{2}+\mathbf{b}_{2}=\mathbf{y}_{2}
$$

## Examples of deep networks - conclusions

