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

Introduction to Machine Learning



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...what we want is a machine that can learn from experience.

66

Alan Turing, 1947



Voshua Bengio

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 <*P*, *T*, *E*>



Difference w.r.t. traditional programming

Traditional Programming





Magic?

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 can't explain their expertise (recognition)
 - Models must be customized (personalized medicine)
 - Models are based on huge amounts of data (genomics)

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> A case of handwritten recognition: 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

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





Scene recognition





- 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

 creating 3D objects from 2D images



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





a particular of the 3D body

 creating 3D objects from 2D images (2)



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



2D image

3D generated images

 Birth records digitalization towards family tree estimation



Rosa



Battezzardi ib tro (???)

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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



Data from G. Witt. Journal of Statistics Education, Volume 21, Number 1 (2013)

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



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Supervised Learning

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



- Clump Thickness
- Uniformity of Cell Size
- Uniformity of Cell Shape

...

- Given x1, x2, ..., xn (without labels)
- Output hidden structure behind the x's
- e.g., clustering





Organize computing clusters





Market segmentation



Astronomical data analysis

• Genomics application: group individuals by genetic similarity



Genes

Individuals

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



Input video (two people speaking together)



Video source: Team Coco, https://www.youtube.com/watch?v=UT7h4nRcWjU

Reinforcement learning

- Given a sequence of states and actions with (delayed) rewards, output a policy
 - Policy is a mapping from states → 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 Agent-Environment Interface



Agent and environment interact at discrete time steps : t = 0, 1, 2, KAgent observes state at step t: $s_t \in S$ produces action at step t: $a_t \in A(s_t)$ gets resulting reward : $r_{t+1} \in \Re$ and resulting next state : s_{t+1}

$$\frac{r_{t+1}}{a_t} \underbrace{s_{t+1}}_{a_{t+1}} \underbrace{s_{t+2}}_{a_{t+2}} \underbrace{s_{t+3}}_{a_{t+2}} \underbrace{s_{t+3}}_{a_{t+3}} \underbrace{s_{t+3}} \underbrace{s_{t+3}} \underbrace{s_{t+3}}$$

Reinforcement learning



https://www.youtube.com/watch?v=4cgWya-wjgY

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)* = 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 <u>tool to</u> <u>solve recognition problems</u> 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
 - o Embeddings
 - o Recurrent models

History

ARTIFICIAL INTELLIGENCE



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 = {c₁,c₁,...,c_n} := set of configurations, each one of them representing a possible solution to P
 - f:C→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 P₁: *sort numbers* x₁,x₂,...,x_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 P₂: foresee the stocks' trend
 - Much more difficult to formalize into an algorithm
 - Minimization comes to help [Yong et al. 2015]

[Yong et al. 2015] Hu, Yong, et al. "Application of evolutionary computation for rule discovery in stock algorithmic trading: A literature review." *Applied Soft Computing* 36 (2015): 534-551.

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 [1943 - McCulloch & Pitts]

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



Neural Networks - Neurons

NN are composed by artificial neurons (1943 - McCulloch & Pitts).

Each neuron has:

- *dendrites* (inputs)
- a nucleus/soma/perceptron (transfer function + activation function)





Neural Networks - Neurons (2)

The information flow is **unidirectional**:

- The neuron get inputs (electric potentials) from the *dendrites*, that weight them (w_i's)
- In the *nucleus*, the weighted inputs are summed together (the **transfer** Σ 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



http://people.csail.mit.edu/torralba/research/drawCNN/drawNet.html

Neural Networks and Deep Learning



Supervised Classification

- Traditional kind of problem the NN do solve
 - o Regression
 - o Ranking
 - o Reinforcement Lea











Labels {'a', 'b', 'c', 'd', 'e'}

Preliminaries: logistic classification

Logistic Classifier



x = input or feature vector; F = number of features; W = weights matrix;
 C = number of classes b = biases; y = output or logits/scores vector

Logistic Classifier - the score is not enough



Softmax function

- Converts scores into probability distributions
 - $\circ \mathbb{R}
 ightarrow (0,1)$
 - Open codomain!





One-Hot Encoding (OHE)

- → There is only one correct label for each input sample
- → There is the need to evaluate the classification result
- OHE encodes labels for a C-class problem in R^c, indicating the c₁th class label with 1, the rest

results

Which distance measure? MSE Cross-1.0 0.0 g.t. labels

Cross-Entropy

<u>GOAL</u>: computes the distance between two probability vectors

• Non symmetric function \mathbf{L}, \mathbf{s}

$$D(\mathbf{s}, \mathbf{L}) \stackrel{\frown}{=} 0 \quad \text{high similarity}$$
$$\stackrel{\frown}{\to} \infty \quad \text{low similarity}$$

 The log(·) makes the training faster to converge than the other alternative MSE function (Σ(s(y)-l)²)

$$D(\mathbf{s}, \mathbf{L}) = -\sum_{j=1}^{c} L_{i} \log s_{i} = 0.36$$

Résumé



Multinomial Logistic Classification

 $D(s(\mathbf{xW+b}), \mathbf{L})$



Gradient Descent

<u>GOAL</u>: search for the nearest local minimum of a function F

<u>IDEA</u>: iterate on the parameter set proportionally to the negative of the function gradient

$$\theta_{t+1} = \theta_t - \alpha \nabla F(\theta_t), t \ge 0$$

such that

$$F(\theta_0) \ge F(\theta_1) \ge F(\theta_2) \ge \dots$$

Gradient Descent

- <u>GOAL</u>: 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)
- Needs to Minimize a loss function, Which depends on W (big matrix) and 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

o 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

... but tricks to ameliorate SGD are present!

W

 $\mathcal{L}(w_i, w_j)$

W

SGD trick 1: momentum

- <u>GOAL</u>: improve the convergence of the optimizer exploiting the accumulated knowledge from previous steps
- IDEA: add a fraction of the previous MpdateWector to the current update vector $M_t = \alpha \nabla \mathcal{L}_t(w_i, w_j) + \beta M_{t-1}$ $(w_i, w_j)_t = (w_i, w_j)_t - M_t$

M = momentum; **B**: friction value (usually 0.9)



SGD trick 2: learning-rate decay

tim

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



SGD trick 3: z-normalization

• <u>GOAL</u>: avoid numerical instability

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

• <u>IDEA</u>: remove the mean and normalize over the variance of the *i*-th feature of the input vector $\mathbf{x} - E[\mathbf{x}]$ $Var[\mathbf{x}]$

z-normalization



 $E[\mathbf{x}] = 0$ $\forall (i, j), Var[\mathbf{x}_i] = Var[\mathbf{x}_j]$

http://cs231n.github.io/

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 SGD algorithm. $w_i = \mathcal{N}(\mu = 0, \sigma \to 0)$

$$\mathbf{b} = \begin{bmatrix} 0_1 & 0_2 & \dots & 0_C \end{bmatrix}$$

$$\mu = 0 \land \sigma \to 0 \implies \forall (i, j), w_i = w_j \pm \epsilon$$

$$\mathbf{c}$$
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

Momentum and learning rate decay. It uses SGD: H. Robinds and S. Monro, "A stochastic approximation method," Annals of Mathematical Statistics, vol. 22, pp. 400–407, 1951. **AdaGrife: WerhipEntrannet & Singer**, "Adaptive subgradient methods for online leaning and stochastic optimization," in COLT, 2010.



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





but...
x
$$W_1$$
 n_1^{t} **b**₁ $\underset{s}{\overset{es}{=}}$ **y**₁ W_2 $\overset{re}{=}$ **b**₂ $\underset{s}{\overset{ns}{=}}$ **y**₂ $\underset{s}{\overset{ns}{=}}$ **x** W_3 + **b**₃ = **y**₃
• What if I concatenate multiple MLCs?
still a linear model...!

From MLC to NN to Deep-NN

• <u>GOAL</u>: build a bigger and non linear Which function? model ^{sigmoid} ReLU • <u>IDEA</u>: concatenate many linear systems tanh (MLC) and insert a *non linear function* between two consecutive MLCs, that is, the activation function \mathbf{b}_1 \rightarrow \rightarrow **b**₂ W_1 **Y**₁ W_2 $\rightarrow s(\mathbf{y}_2)$ + = ? = Χ +**Y**₂

Choose the (non linear) activation function


ReLU: Rectified Linear Unit



Résumé



H = number of "neurons" in the hidden layer

Practical example (1/2)



Practical example (2/2)



Examples of deep networks - conclusions