Master Recherche IAC Apprentissage Statistique, Optimisation & Applications

Anne Auger — Balazs Kégl — Michèle Sebag TAO

Nov. 28th, 2012

Contents

WHO

Anne Auger, optimizationBalazs Kégl, machine learningTAO, LAL

WHAT

1. Neural Nets

2. Stochastic Optimization

Michèle Sebag, machine learning

- 3. Reinforcement Learning
- 4. Ensemble learning

WHERE: http://tao.lri.fr/tiki-index.php?page=Courses



TAO, LRI

Fxam

Final: same as for TC2:

- Questions
- Problems

Volunteers

- Some pointers are in the slides
- ▶ Volunteer: reads material, writes one page, sends it.

Tutorials/Videolectures

- http://www.iro.umontreal.ca/~bengioy/talks/icml2012-YBtutorial.pdf
- Part 1: 1-56: Part 2: 79-133
- Group 1 (group 2) prepares Part 1 (Part 2)
- Course Dec. 12th:
 - Group 1 presents part 1; group 2 asks questions;
 - ► Group 2 presents part 2; group 1 asks questions.



Questionaire

Admin: Ouassim Ait El Hara

Debriefing

- ► What is clear/unclear
- Pre-requisites
- Work organization

This course

Bio-inspired algorithms

Classical Neural Nets History Structure

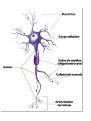
Applications

Bio-inspired algorithms



Facts

- ▶ 10¹¹ neurons
- ▶ 10⁴ connexions per neuron
- Firing time: $\sim 10^{-3}$ second 10^{-10} computers



Bio-inspired algorithms, 2

Human beings are the best!

- ► How do we do?
 - What matters is not the number of neurons

as one could think in the 80s, 90s...

- ► Massive parallelism ?
- ► Innate skills ?

= anything we can't yet explain

Is it the training process ?

Beware of bio-inspiration

- Misleading inspirations (imitate birds to build flying machines)
- Limitations of the state of the art
- Difficult for a machine <> difficult for a human

Synaptic plasticity

Hebb 1949 Conjecture

When an axon of cell A is near enough to excite a cell B and repeatedly or persistently takes part in firing it, some growth process or metabolic change takes place in one or both cells such that A's efficiency, as one of the cells firing B, is increased.

Learning rule

Cells that fire together, wire together If two neurons are simultaneously excitated, their connexion weight increases.

Remark: unsupervised learning.

This course

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Applications

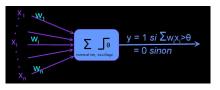
History of artificial neural nets (ANN)

- 1. Non supervised NNs and logical neurons
- 2. Supervised NNs: Perceptron and Adaline algorithms
- 3. The NN winter: theoretical limitations
- 4. Multi-layer perceptrons.

History



Mc Culloch et Pitt 1943



Ingredients

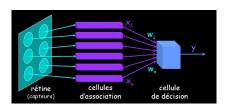
- ► Input (dendrites) x_i
- ▶ Weights *w_i*
- ▶ Threshold θ
- Output: 1 iff $\sum_i w_i x_i > \theta$

Remarks

- ▶ Neurons \rightarrow Logics \rightarrow Reasoning \rightarrow Intelligence
- ► Logical NNs: can represent any boolean function
- No differentiability.



Rosenblatt 1958



$$y = sign(\sum w_i x_i - \theta)$$
 $\mathbf{x} = (x_1, \dots, x_d) \mapsto (x_1, \dots, x_d, 1).$
 $\mathbf{w} = (w_1, \dots, w_d) \mapsto (w_1, \dots w_d, -\theta)$
 $y = sign(\langle \mathbf{w}, \mathbf{x} \rangle)$

Learning a Perceptron

Given

$$\mathcal{E} = \{(\mathbf{x}_i, y_i), \mathbf{x}_i \in \mathbb{R}^d, y_i \in \{1, -1\}, i = 1 \dots n\}$$

For $i = 1 \dots n$, do

▶ If no mistake, do nothing

no mistake
$$\Leftrightarrow \langle \mathbf{w}, \mathbf{x} \rangle$$
 same sign as $y \Leftrightarrow y \langle \mathbf{w}, \mathbf{x} \rangle > 0$

▶ If mistake

$$\mathbf{w} \leftarrow \mathbf{w} + y.\mathbf{x}_i$$

Enforcing algorithmic stability:

$$\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \alpha_t y. \mathbf{x}_\ell$$

 α_t decreases to 0 faster than 1/t.

Convergence: upper bounding the number of mistakes

Assumptions:

- ightharpoonup \mathbf{x}_i belongs to $\mathcal{B}(\mathbb{R}^d,\mathcal{C})$ $||\mathbf{x}_i|| < \mathcal{C}$
- $ightharpoonup \mathcal{E}$ is separable, i.e. exists solution \mathbf{w}^* s.t. $\forall i=1\dots n,\ y_i\ \langle \mathbf{w}^*, \mathbf{x}_i \rangle > \delta > 0$

Convergence: upper bounding the number of mistakes

Assumptions:

- lacksquare $oldsymbol{\mathsf{x}}_i$ belongs to $\mathcal{B}(\mathbbm{R}^d,\mathcal{C})$ $||oldsymbol{\mathsf{x}}_i||<\mathcal{C}$
- ${\cal E}$ is separable, i.e. exists solution ${\bf w}^*$ s.t. $\forall i=1\ldots n,\ y_i\ \langle {\bf w}^*,{\bf x}_i \rangle > \delta > 0$ with $||w^*||=1$.

Convergence: upper bounding the number of mistakes

Assumptions:

- lacksquare $f x_i$ belongs to $\mathcal{B}(\mathbb{R}^d,\mathcal{C})$ $||f x_i||<\mathcal{C}$
- ${\cal E}$ is separable, i.e. exists solution ${\bf w}^*$ s.t. $\forall i=1\ldots n,\ y_i\,\langle {\bf w}^*,{\bf x}_i\rangle>\delta>0$ with $||{\bf w}^*||=1$.

Then The perceptron makes at most $(\frac{C}{\delta})^2$ mistakes.

Bouding the number of misclassifications

Proof

Upon the k-th misclassification

for some \mathbf{x}_i

$$\begin{array}{lll} \mathbf{w}_{k+1} & = & \mathbf{w}_k + y_i \mathbf{x}_i \\ \langle \mathbf{w}_{k+1}, \mathbf{w}^* \rangle & = & \langle \mathbf{w}_k, \mathbf{w}^* \rangle + y_i \langle \mathbf{x}_i, \mathbf{w}^* \rangle \\ & \geq & \langle \mathbf{w}_k, \mathbf{w}^* \rangle + \delta \\ & \geq & \langle \mathbf{w}_{k-1}, \mathbf{w}^* \rangle + 2\delta \\ & \geq & k\delta \end{array}$$

In the meanwhile:

$$||\mathbf{w}_{k+1}||^2 = ||\mathbf{w}_k + y_i \mathbf{x}_i||^2 \le ||\mathbf{w}_k||^2 + C^2 \le kC^2$$

Therefore:

$$\sqrt{k}C > k\delta$$



Going farther...

Remark: Linear programming: Find \mathbf{w}, δ such that

Max
$$\delta$$
, subject to $\forall i = 1 \dots n, \ y_i \langle \mathbf{w}, \mathbf{x}_i \rangle > \delta$

gives the floor to Support Vector Machines...

Adaptive Linear Element

Given

$$\mathcal{E} = \{(\mathbf{x}_i, y_i), \mathbf{x}_i \in \mathbb{R}^d, y_i \in \mathbb{R}, i = 1 \dots n\}$$

Learning

Minimization of a quadratic function

$$\boldsymbol{w}^* = \textit{argmin}\{\textit{Err}(\boldsymbol{w}) = \sum (y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle)^2\}$$

Gradient algorithm

$$\mathbf{w}_i = \mathbf{w}_{i-1} + \alpha_i \nabla Err(\mathbf{w}_i)$$

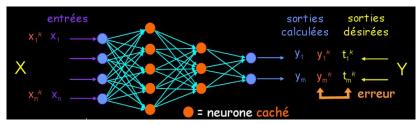
The NN winter



Limitation of linear hypotheses The XOR problem.

Minsky Papert 1969

Multi-Layer Perceptrons, Rumelhart McClelland 1986



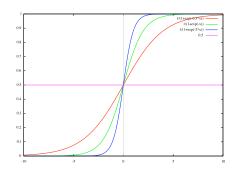
Issues

- Several layers, non linear separation, addresses the XOR problem
- A differentiable activation function

$$ouput(\mathbf{x}) = rac{1}{1 + exp\{-\langle \mathbf{w}, \mathbf{x}
angle\}}$$

The sigmoid function

- approximates step function (binary decision)
- ▶ linear close to 0
- Strong increase close to 0



Back-propagation algorithm, Rumelhart McClelland 1986; Le Cun 1986

- ightharpoonup Given (\mathbf{x}, y) a training sample uniformly randomly drawn
- ▶ Set the d entries of the network to $x_1 \dots x_d$
- ► Compute iteratively the output of each neuron until final layer: output \hat{y} ;
- ► Compare \hat{y} and y $Err(w) = (\hat{y} y)^2$
- Modify the NN weights on the last layer based on the gradient value
- ▶ Looking at the previous layer: we know what we would have liked to have as output; infer what we would have liked to have as input, i.e. as output on the previous layer. And back-propagate...
- ► Errors on each *i*-th layer are used to modify the weights used to compute the output of *i*-th layer from input of *i*-th layer.



Back-propagation of the gradient

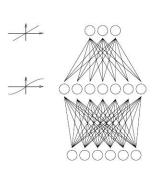
Notations

Input
$$\mathbf{x} = (x_1, \dots x_d)$$

From input to the first hidden layer $z_j^{(1)} = \sum w_{jk}x_k$
 $x_j^{(1)} = f(z_j^{(1)})$
From layer i to layer $i+1$

 $z_j^{(i+1)} = \sum w_{jk}^{(i)} x_k^{(i)}$ $x_i^{(i+1)} = f(z_i^{(i+1)})$

(f: e.g. sigmoid)



Outpu

Hidde

Inputs

Back-propagation of the gradient

 $\begin{aligned} & \mathsf{Input}(\mathbf{x},y), \ \mathbf{x} \in \mathbb{R}^d, \ y \in \{-1,1\} \\ & \mathsf{Phase} \ 1 \ \mathsf{Propagate} \ \mathsf{information} \ \mathsf{forward} \end{aligned}$

For layer $i = 1 \dots \ell$ For every neuron j on layer i $z_j^{(i)} = \sum_k w_{j,k}^{(i)} x_k^{(i-1)}$ $x_i^{(i)} = f(z_i^{(i)})$

Phase 2 Compare the target output (y) to what you get $(x_1^{(\ell)})$ NB: for simplicity one assumes here that there is a single output (the label is a scalar value).

► Error: difference between $\hat{y} = x_1^{(\ell)}$ and y. Define

$$e^{sortie} = f'(z_1^{\ell})[\hat{y} - y]$$

where f'(t) is the (scalar) derivative of f at point t.

Back-propagation of the gradient

Phase 3 retro-propagate the errors

$$e_j^{(i-1)} = f'(z_j^{(i-1)}) \sum_k w_{kj}^{(i)} e_k^{(i)}$$

Phase 4: Update weights on all layers

$$\Delta w_{ij}^{(k)} = \alpha e_i^{(k)} x_j^{(k-1)}$$

where α is the learning rate (< 1.)

This course

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Applications

Neural nets

Ingredients

- Activation function
- Connexion topology = directed graph feedforward (\equiv DAG, directed acyclic graph) or recurrent
- A (scalar, real-valued) weight on each connexion

Activation(z)

thresholded

0 if z < threshold, 1 otherwise

linear

z

sigmoid

$$1/(1+e^{-z})$$
 e^{-z^2/σ^2}

Radius-based

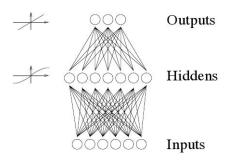
$$e^{-z^2/\sigma^2}$$

Neural nets

Ingredients

- Activation function
- ► Connexion topology = directed graph feedforward (≡ DAG, directed acyclic graph) or recurrent
- A (scalar, real-valued) weight on each connexion

Feedforward NN



(C) David McKay - Cambridge Univ. Press



Neural nets

Ingredients

- Activation function
- ► Connexion topology = directed graph feedforward (≡ DAG, directed acyclic graph) or recurrent
- ► A (scalar, real-valued) weight on each connexion

Recurrent NN

- Propagate until stabilisation
- Back-propagation does not apply
- Memory of the recurrent NN: value of hidden neurons Beware that memory fades exponentially fast
- Dynamic data (audio, video)

Structure / Connexion graph / Topology

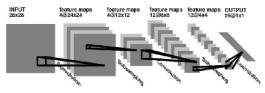
Prior knowledge

Invariance under translation, rotation,..

op

ightharpoonup ightharpoonup Complete ${\cal E}$

- consider $(op(\mathbf{x}_i), y_i)$
- or use weight sharing: convolutionnal networks



100,000 weights \rightarrow 2,600 parameters Details

http://yann.lecun.com/exdb/lenet/

Demos

http://deeplearning.net/tutorial/lenet.html

Hubel & Wiesel 1968

Visual cortex of the cat

- cells arranged in such a way that
- ... each cell observes a fraction of the visual field

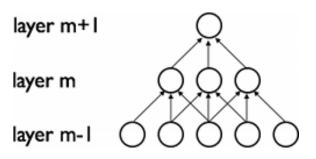
receptive field

the union of which covers the whole field

Characteristics

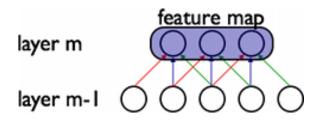
- ► Simple cells check the presence of a pattern
- More complex cells consider a larger receptive field, detect the presence of a pattern up to translation/rotation

Sparse connectivity



- Reducing the number of weights
- ▶ Layer *m*: detect local patterns
- ▶ Layer m + 1: non linear aggregation, more global field

Convolutional NN: shared weights

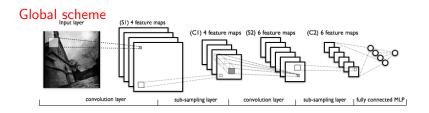


- Reducing the number of weights
- through adapting the gradient-based update: the update is averaged over all occurrences of the weight.

Max pooling: reduction and invariance

- Partitioning
- ▶ Return the max value in the subset

invariance



Properties

Good news

MLP, RBF: universal approximators

For every decent function f (= f^2 has a finite integral on every compact of \mathbb{R}^d) for every $\epsilon>0$, there exists some MLP/RBF g such that $||f-g||<\epsilon$.

Bad news

- Not a constructive proof (the solution exists, so what ?)
- ightharpoonup Everything is possible ightarrow no guarantee (overfitting).

Key issues

Model selection

- Selecting number of neurons, connexion graph
- ► Which learning criterion overfitting

More \Rightarrow Better

Algorithmic choices

a difficult optimization problem

Initialisation

w small!

- Decrease the learning rate with time
- Enforce stability through relaxation

$$\mathbf{w}_{neo} \leftarrow (1 - \alpha)\mathbf{w}_{old} + \alpha\mathbf{w}_{neo}$$

Stopping criterion

Start by normalization of data

$$X \mapsto \frac{x - average}{variance}$$



The curse of NNs

- The NIPS community has suffered of an acute convexivitis epidemic
 - ML applications seem to have trouble moving beyond logistic regression, SVMs, and exponential-family graphical models.
 - For a new ML model, convexity is viewed as a virtue
 - Convexity is sometimes a virtue
 - But it is often a limitation
 - ML theory has essentially never moved beyond convex models
 the same way control theory has not really moved beyond linear systems
 - ▶ Often, the price we pay for insisting on convexity is an unbearable increase in the size of the model, or the scaling properties of the optimization algorithm [O(n^2), O(n^3)...]

http://videolectures.net/eml07_lecun_wia/

Pointers

URL

- b course:
 http://neuron.tuke.sk/math.chtf.stuba.sk/pub/
 vlado/NN_books_texts/Krose_Smagt_neuro-intro.pdf
- ► FAQ: http://www.faqs.org/faqs/ai-faq/neural-nets/part1/preamble.html
- applets
 http://www.lri.fr/~marc/EEAAX/Neurones/tutorial/
- codes: PDP++/Emergent (www.cnbc.cmu.edu/PDP++/);
 SNNS http:
 //www-ra.informatik.uni-tuebingen.de/SgNNS/...

Also see

► NEAT & HyperNEAT Stanley, U. Texas When no examples available: e.g. robotics.

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Applications

Applications

- 1. Pattern recognition
 - ► Signs (letters, figures)
 - Faces
 - Pedestrians
- 2. Control (navigation)
- 3. Language

Intuition

Design, the royal road

- Decompose a system into building blocks
- which can be specified, implemented and tested independently.

Why looking for another option ?

Intuition

Design, the royal road

- Decompose a system into building blocks
- which can be specified, implemented and tested independently.

Why looking for another option?

- When the first option does not work or takes too long (face recognition)
- when dealing with an open world

Proof of concept

- speech & hand-writing recognition: with enough data, machine learning yields accurate recognition algorithms.
- ▶ hand-crafting → learning

Recognition of letters

```
368/796641
6757863485
2179712894
4819018894
7592668199
76186469
76186469
76186469
```

Fig. 4. Size-normalized examples from the MNIST database.

Features

- ▶ Input size *d*: +100
- ightharpoonup ightharpoonup large weight vectors :-(
- Prior knowledge: invariance through (moderate) translation, rotation of pixel data



Convolutionnal networks

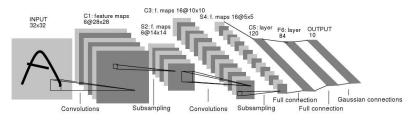


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

Lecture

http://yann.lecun.com/exdb/lenet/

➤ Y. LeCun and Y. Bengio. Convolutional networks for images, speech, and time-series. In M. A. Arbib, editor, The Handbook of Brain Theory and Neural Networks. MIT Press, 1995.

Face recognition



Viola and Jones, Robust object detection using a boosted cascade of simple features, CVPR 2001

Face recognition

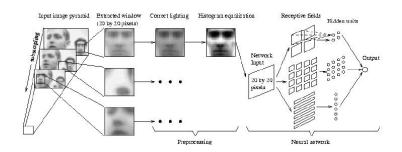
Variability

- Pose
- ► Elements: glasses, beard...
- ▶ Light
- Expression
- Orientation

Occlusions

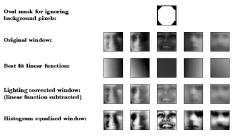
http://www.ai.mit.edu/courses/6.891/lectnotes/lect12/lect12-slides-6up.pdf

Face recognition, 2



- ▶ One equation \rightarrow 1 NN
- ▶ NN are fast

Face recognition, 3



The steps in preprocessing a window. First, a linear function is fit to the intensity values in the window, and then subtracted out, correcting for some extreme lighting conditions. Then, histogram equalization is applied, to correct for different camera gains and to improve contrast. For each of these steps, the mapping is computed based on pixels inside the oval mask, while the mapping is applied to the entire window.





Navigation, control



Lectures, Video

http://www.cs.nyu.edu/~yann/research/dave/index.html

Continuous language models

Principle

- ▶ Input: 10,000-dim boolean input
- ▶ Hidden neurons: 500 continuous neurons
- ▶ Goal: from a text window $(w_i ... w_{i+2k})$, predict
 - ▶ The grammatical tag of the central word w_{i+k}
 - ▶ The next word w_{i+2k+1}
- ightharpoonup Rk: Hidden layer: maps a text window on $m I\!R^{500}$

Bengio et al. 2001

(words)

Improving Word Embedding



Rare words are not trained properly



Sentences with similar words should be tagged in the same way:

- * The cat sat on the mat
- The feline sat on the mat





- * pull together linked words
- * push apart other pair of words

videolectures



Language Model: Think Massive

- Language Model: "is a sentence actually english or not?"

 Implicitly captures: * syntax * semantics
- Bengio & Ducharme (2001) Probability of next word given previous words. Overcomplicated we do not need probabilities here
- English sentence windows: Wikipedia ($\sim 631M$ words)

 Non-english sentence windows: middle word randomly replaced
- Multi-class margin cost:

$$\sum_{s \in \mathcal{S}} \sum_{w \in \mathcal{D}} \max \left(0, 1 - f(s, \boldsymbol{w}_{s}^{\star}) + f(s, w) \right)$$

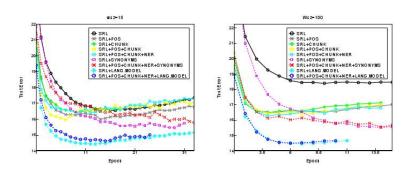
 \mathcal{S} : sentence windows \mathcal{D} : dictionary w_s^* : true middle word in s f(s,w): network score for sentence s and middle word w

Language Model: Embedding

france	jesus	xbox	reddish	scratched
454	1973	6909	11724	29869
spain	christ	playstation	yellowish	smashed
italy	god	dreamcast	greenish	ripped
russia	resurrection	psNUMBER	brownish	brushed
poland	prayer	snes	bluish	hurled
england	yahweh	wii	creamy	grabbed
denmark	josephus	nes	whitish	tossed
germany	moses	nintendo	blackish	squeezed
portugal	sin	gamecube	silvery	blasted
sweden	heaven	psp	greyish	tangled
austria	salvation	amiga	paler	slashed

Dictionary size: 30,000 words. Even rare words are well embedded.

MTL: Semantic Role Labeling



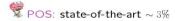
 \mathfrak{F} We get: 14.30%. State-of-the-art: 16.54% – Pradhan et al. (2004)

 $$\stackrel{\clubsuit}{$}$_{250}$\times faster than state-of-the-art. <math>\sim 0.01s$ to label a WSJ sentence.

MTL: Unified Network for NLP

Improved results with Multi-Task Learning (MTL)

	Alone	
SRL	18.40% 2.95%	14.30%
POS	2.95%	2.91%
Chunking - error rate	5.4%	4.9%
Chunking - F1-score	91.5%	93.6%



Chunking: Best system had 93.48% F1-score at CoNLL-2000 challenge http://www.cnts.ua.ac.be/conl12000/chunking. State-of-the art is 94.1%. We get 94.9% by using POS features.

Summary



We developed a deep neural network architecture for NLP



Advantages

- * General to any NLP tagging task
- * State-of-the-art performance
- * No hand designed features
- * Joint training
- * Can exploit massive unlabeled data
- * Extremely fast: 0.02s for all tags of a sentence



nconvenients

* Neural networks are a powerful tool: hard to handle



Early Impacts

- Easy to apply to other tasks or languages: extending to Japanese
- * Fast: developed a semantic search system