Deep Learning in Practice

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. . . and guests!

Overview

- Course summary and organization
- Chapters overview

Context

- Deep learning: impressive results in the machine learning literature
- yet difficult to train, and still poorly understood;
  results = black-boxes missing explanations.
- Huge societal impact of ML today (assistance in medicine, hiring process, bank loans...)
  $\Longrightarrow$ explain their decisions, offer guarantees?
- Real world problems: usually do not fit standard academic assumptions (data quantity and quality, expert knowledge availability...).
- This course: aims at providing theoretical insights and tools to address these practical aspects, based on mathematical concepts and practical exercises.

Organisation and evaluation

- Most courses: a lesson + practical exercises (to hand in within 2 weeks, and evaluated)
- Extras: a few guest talks

Schedule

8 classes of 3 hours, at CentraleSupelec (just next to ENS Paris-Saclay), January-March 2023; check the webpage for more up-to-date schedule.

Webpage & subscription:

https://www.lri.fr/~gcharpia/deeppractice/

Prerequisite

- The introduction to Deep Learning course by Vincent Lepetit (1st semester), or any similar course
- Notions in differential calculus, Bayesian statistics, analysis, information theory

Links with other Deep Learning courses

- Introduction to Deep Learning (V. Lepetit) : prerequisite

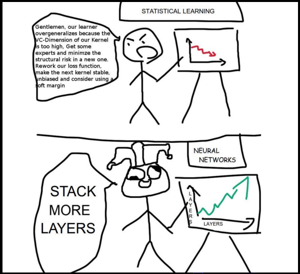
- Fondements Théoriques du deep learning (F. Malgouyres & al)
- Modélisation en neurosciences et ailleurs (J-P Nadal)
- Apprentissage Profond pour la Restauration et la Synthese d'Images (A. Almansa & al)
- Deep learning for medical imaging (O. Colliot & M. Vakalopoulou)
- Object recognition and computer vision (Willow team & al)
- etc. (NLP, graphs...)

- Our course: theoretical understanding and tools to make NN work in practice with a focus on architecture design, explainability, societal impact, real datasets and tasks (e.g. small data, limited computational power vs. scaling up, RL...).
  $\Longrightarrow$ negligible overlap

Outline

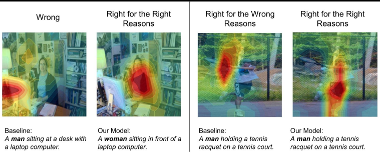
Deep learning vs. classical ML and optimization

- **Going Deep or not?**
  - Examples of successes and failures of deep learning vs. classical techniques (random forests)
  - Approximation theorems vs. generalization [3, 4]
  - Why deep: ex. of depth vs. layer size compromises (explicit bounds)
- **Gap between classical Machine Learning and Deep Learning**
  - Forgotten Machine Learning basics (Minimum Description Length principle, regularizers, objective function different from evaluation criterion) and incidental palliatives (drop-out, early stopping, noise)
- **Hyper-parameters and training basics**
  - + list of practical tricks



Interpretability

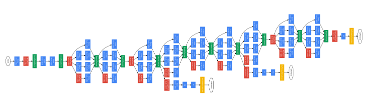
- **At stake:** the example of medical diagnosis, and societal issues with black-box algorithms [5]



- **Interpretability of neural networks**
  - Analyzing the black-box
    - at the neuron level: filter visualisation, impact analysis
    - at the layer level: layer statistics...
    - at the net level: low-dimensional representation (t-SNE) + IB
    - by sub-task design: "explainable AI"
  - Adversarial examples & remedies
- **Issues with datasets**
  - Biases in datasets : 4 definitions of fairness
    - Getting invariant to undesirable dataset biases (e.g. gender in CVs / job offers matching)
    - Ensuring errors are uniform over the dataset
  - Differential privacy (database client protection)
- Visualization tools: grad-CAM

Architectures

- Architectures as priors on function space
  - Change of design paradigm
  - Random initialization
- Architecture zoo
  - Reminder (CNN, auto-encoder, LSTM, adversarial...)
  - Dealing with scale & resolution (fully-convolutional, U-nets, pyramidal approaches...)
  - Dealing with depth (ResNet, auxiliary losses) and mixing blocks (Inception)
  - Attention mechanisms
  - GraphCNN



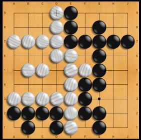
- Problem modeling: molecular dataset using graph-NN

Small data, weak supervision and robustness

- **Small data**
  - Data augmentation / synthetic data
  - Multi-tasking
  - Transfer learning
- **Few labeled examples: forms of weak supervision**
  - Semi-supervision
  - Weak supervision
  - Self-supervision
  - Active learning
- **Noisy data**
  - Denoising auto-encoder
  - Classification with noisy labels
  - Regression with noisy labels
- **Exploiting known invariances or priors**
  - Permutation invariance: "deep sets" [8], applied to people genetics
  - Choosing physically meaningful metrics, e.g. optimal transport (Sinkhorn approximation)[9]
- Transfer learning

Guest talks (to be confirmed)

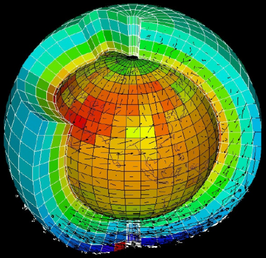
- **Deep Reinforcement Learning** by Olivier Teytaud (Facebook FAIR)
  - Crash-course about deep RL. . .
  - . . . until alpha-0!
  - and more topics (evolutionary optimization...)



- **Presentation of Therapixel** by Yaroslav Nikulin
  - start-up in medical imaging (DL to detect breast cancer in scans)

Incorporating physical knowledge / Learning physics

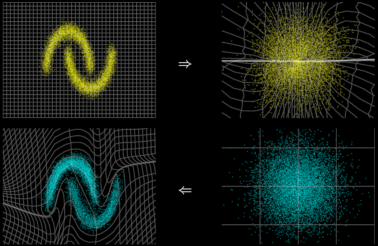
- Course by Michele Alessandro Bucci and Lionel Mathelin (Safran/LISN)
  - Data assimilation
  - Learning a PDE (equation not known)
  - Incorporating invariances/symmetries of the problem
  - Knowing an equation that the solution has to satisfy: solving PDEs!
  - Deep for physic dynamics : learning and controlling the dynamics



- Learning a dynamical system

Generative models + Modeling tasks and losses

- **Generative models**
  - GAN, VAE (Variational Auto-Encoder), and Normalizing Flows
- **Modeling tasks and losses**
  - KL, optimal transport, MMD...
- GAN vs. VAE vs. NF



Guarantees? Generalization and formal proofs + Auto-DL

- **Guarantees?**
  - Generalization: double gradient descent and Neural Tangent Kernel
  - formal proofs of (very small) neural networks
- **Auto-DeepLearning** by Isabelle Guyon's group
  - Overview of recent approaches for automatic hyper-parameter tuning (architecture, learning rate, etc.): classical blackbox optimisation, Reinforcement Learning approaches, constrained computational time budget, self-adaptive architectures...
  - Presentation of the Auto-ML & Auto-DL challenges

To attend the course

- go see the website and **subscribe to the course**
  `https://www.lri.fr/~gcharpia/deeppractice/`
- install PyTorch, Jupyter and matplotlib
- See you... on Tuesday 24th of January

Biographies

- Guillaume Charpiat is an INRIA researcher in the TAU team (INRIA Saclay/LISN/Paris-Sud). He has worked mainly in computer vision, optimization and machine learning, and now focuses on deep learning. He conducts studies on neural networks both in theory (self-adaptive architectures, formal proofs) and in applications (remote sensing, people genetics, molecular dynamics simulation, brain imagery, weather forecast...).
- Matthieu Nastorg, Francesco Pezzicoli and Cyriaque Rousselot are PhD students in the TAU team, working on deep learning for physical systems (PDEs), on equivariant graph-NN for the glass problem, and on causality, respectively.

Bibliography

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