DESCRIPTIF DU SUJET ET
ARGUMENTAIRE DU DIRECTEUR DE THESE

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Si codirecteur de thèse, date d'obtention de l'HDR : Il s'agfit d'une thèse en co-tutelle avec l'Hongrie, il n'y a pas d'équivalent d'HDR en Hongrie.

Intitulé du sujet de thèse (en français) : Fondements théoriques de l'apprentissage des équations différentielles neuronales robustes.

Résumé du sujet de thèse (Décrire en français les objectifs visés en 1500 caractères maximum)
Le but de ce projet est d'apporter des garanties théoriques pour l'apprentissage d'équations différentielles neuronales robustes. Les équations différentielles neuronales représentent une généralisation des réseaux neuronaux profonds, qui évitent plusieurs inconvénients de ce dernier. Par exemple, elles ont la tendance d'être plus robustes, elles sont capables de prendre en compte des contraintes physiques, de modéliser des processus variables dans le temps et peuvent nécessiter moins de ressources de calcul. Dans cette thèse, nous souhaitons formuler des garanties formelles (mathématiques) sur l'exactitude et la robustesse des équations différentielles neuronales apprises à partir des données. Par robustesse, nous entendons que les modèles appris ne sont pas sensibles aux petites perturbations. Par exactitude, nous entendons que les prédictions générées par le modèle sont suffisamment précises, même lorsqu'elles sont appliquées aux nouvelles données.

DESCRIPTIF DU SUJET (en 3 pages minimum)

The thesis will be done in collaboration with Informatics Laboratory, HUN-REN Institute for Computer Science and Control (SZTAKI), Hungary. SZTAKI is expected to provide 50\% of the funding and the student is expected to spend half of its time at SZTAKI.

1) Le sujet de recherche choisi et son contexte scientifique et économique :
In recent years Artificial Intelligence (AI) has undergone a rapid development and has proliferated into several aspects of everyday life. Despite its success, its adoption is slowed down by questions of safety, reliability, trustworthiness and computation costs. More precisely, AI algorithms represent black-boxes, with very little guarantees on their safety or correctness. In turn, this generates mistrust towards these algorithms and it makes companies hesitant to use them is safety-critical applications (autonomous vehicles, medical devices, etc.). In addition, many of the off the shelf AI algorithms do not take into account physical constraints of the devices they are supposed to be deployed, and they require serious computational resources. For all these reasons, creating Embedded AI applications remains a challenge.
One possible solution proposed by the scientific community is the use of Neural Ordinary Differential Equations (Neural ODEs) [1]. Neural ODEs are dynamical models blending neural networks and dynamical systems. Intuitively, Neural ODEs represent a deep neural network with an inifnite number of layers, where the indices of layers are viewed as time instances. That is, Neural ODEs can be thought of as limits of deep neural networks as the depth tends to infinity.

Neural ODEs have gained popularity in recent years mainly because of their attractive properties, e.g., ability to take into account physical constraints, to model irregularly sampled time-series, provide classifiers which are robust to adversarial attacks, predict long range dependencies, ability to serve as generative models (images, etc.) Despite many advances, there are important gaps in learning theory of such systems. One such gap is lack of formal guarantees for the generalization error, i.e., the consistency of the learning algorithm.

In this thesis we aim at filling these gaps by formalising neural ODEs and providing theoretical guarantees for learning robust neural ODEs.

Scientific methodology

To this end, we plan to combine ideas from control theory on stability and robustness of dynamical systems and their learning with approaches from statistical machine learning. Learning dynamical systems from data is the subject of system identification [2], which is a subfield of control theory. System identification provides a rich literature on the theoretical properties of such learning algorithms. However, the existing literature focuses on classes of dynamical systems relevant for control theory, and hence cannot be applied directly to general neural ODEs. Combining knowledge from system identification and machine learning, we aim at solving the following research problems

1a) Robustness. Intuitively, robustness of a model means that small perturbations in inputs (or the distribution of inputs) will not result in a significant change of the label predicted by the model. One may argue that non-robust models are of limited use for prediction. In this thesis we plan to concentrate on robust neural ODEs. The notion of robustness is central to control theory, and it has been extensively studied there. In particular, formalisations of various versions of robustness are known such as input-to-output stability, L_p gains, input convergence, etc. Furthermore, various computationally effective conditions for checking robustness exist.

We plan to apply these notions to neural ODEs. The challenge is that most of the results are geared towards classes of dynamical systems which are used for designing controllers. The class of neural ODEs is more general than the popular classes of dynamical systems studied in control. Moreover, neural ODEs are used primarily for prediction and not for control. Hence, it will be necessary to extend and adapt these results to neural ODEs.

1b) Provide theoretical guarantees for statistical consistency of learning robust neural ODEs.

We would like to show that if a large enough number of data points is used for learning, then the generalization error of neural ODEs learned from these data will converge to some lower bound representing the intrinsic error of modeling the underlying phenomenon by neural ODEs.

1c) Provide analytic finite sample bounds, in particular PAC and PAC-Bayesian [3] bounds, for neural ODEs.

The goal is to relate the generalization loss (prediction error on unseen data) with the prediction error on the training data (empirical loss). More precisely, we would like to derive upper bounds on the generalization gap (the difference between the generalization loss and the empirical loss). The upper bound depends on the number of data points (samples) , hence often they are referred to as finite sample bounds.

Finite sample bounds are ideally such that they converge to zero with the increase of the number of data points, hence, they also provide statistical consistency for learning algorithms. However, they are much more powerful than proofs of statistical consistency, as they allow estimating the generalization loss for a given number of data points. In contrast, statistical consistency only indicates that for a large enough number of data points the generalization loss will be close to the smallest possible one for the given model class. Finite sample bounds can be specific for a certain learning algorithm, or can hold true for all models. The latter bounds are known as PAC (Probably Approximately Correct). PAC bounds are bounds on the worst case generalisation gap for a class of models. They hold in a probabilistic sense, i.e., with a certain probability. PAC bounds allow to characterize the predictive power for models obtained via any learning algorithm, but they tend to be conservative. PAC-Bayesian bounds are modifications of PAC bounds which consider the average (according to some distribution on models) of the dgeneralization gap. They are less conservative than PAC bounds, but they are useful for analyzing only those learning algorithms which have a Bayesian interpretation, i.e., the model learned by the algorithm can be viewed as a mean or a random sample of a data dependent posterior density on the models. That is, data used to modify our hypothesis on likelihood of each model : models which are less consistent with the data are assign lower probability. The resulting probability distribution is known as posterior.

We plan to derive finite sample bounds, with a special emphasis on PAC and PAC-Bayesian bounds for neural ODEs. To this end, we plan to extend existing work [4], [5]

State of the art

Machine learning and control theory are two closely related subjects with common roots. Recently, the two topics started to converge again: control theorists are becoming increasingly interested in using machine learning techniques, while researchers in machine learning start looking at control problems and at possibilities to use results from control theory for machine learning.

Despite this synergy, there is little prior work on applying ideas from control theory for proving consistency and error bounds for neural ODEs. Regarding robustness of neural ODEs, there were a few attempts to formalize the notion of robustness, however, these formalizations are not yet satisfactory and they do not propose computationally efficient parameterizations of robust neural ODEs. Over the last few years, PAC- and PAC-Bayesian analyses have been conducted to explain the generalization performance of deep neural networks, but most of the studies are limited to feed-forward neural networks, which are not suited for modelling dynamical systems in general, and for neural ODEs in particular.

There are some prior work on PAC bounds for some classes of neural ODEs, see [6] for references, but the resulting bounds have several disadvantages: they apply only to independently sampled multiple time-series and the bounds tend to grow exponentially with time. These disadvantages make them difficult to use for several learning tasks of interest, in particular, for learning models of physical systems. Moreover, the cited work does not address the role of robustness in generalization power.

CV of the supervisors

Mihaly Petreczky received the Ph.D. degree from Vrije Universiteit in Amsterdam, The Netherlands in 2006 and the HDR degree from Université Lille in 2023. In the past, he was a postdoc at Johns Hopkins University, USA (2006 - 2007), Eindhoven University of Technology, The Netherlands (2007-2009) and assistant professor at Maastricht University, The Netherlands (2009 – 2011) and at Ecole des Mines de Douai, France (2011 - 2015). He is currently a CNRS researcher at Centre de Recherche en Informatique, Signal et Automatique de Lille (CRIStAL), UMR CNRS 9189, France. His research interests include data-driven modelling of cyber-physical systems for control and its synergy with machine learning and statistics. In particular, he is interested in theoretically sound algorithms for learning models of cyber-physical systems and simplifying existing models. He co-authored 26 journal papers, some of them in high-impact journals, IEEE Trans. Automatic Control (7), Automatica (9), Systems \& Control Lett. (4), SIAM J. Control (1), ESAIM COCV (2), Int. Journal of Nonlinear and Robust Control (2), NAHS (2), 3 book chapters, over 40 peer reviewed conference papers, leading conferences AAAI, CDC, ACC, ECC, IFAC World Congress, HSCC, ADHS, MTNS,NOLCOS.

He is the scientific coordinator of *CIFRE* 'Motion dynamics modeling for fall of humans or two-wheeled vehicles (motorcycles/bicycles) : Combining domain knowledge-based and data driven models', Autoliv, and the *CNRS IEA* research project 'Stability of learning algorithms for deep and recurrent neural networks by using geometry and control theory via understanding the role of overparameterization' with SZTAKI,

In the past, he was the scientific coordinator of the research contract « Reliable AI for cyber-physical systems using control theory' » *Confiance.ia,* IRT System-X, the regional project *CPER Data* « Machine learning meets Control », *CNRS PEPS Blanc 2019*, « PAC-Bayesian theory for recurrent neural networks: a control theoretic approac », regional project *ARCIR* « Estimation distribu\ée de systèmes dynamiques en réseaux' » 2013-2017. He is an active member of the *GDR MACS* action on IA and Control, an associate editor of Systems & Control Letters, and a member of *GRAIHSYM.*

Andras Benczur is the head of Informatics Laboratory of 20 doctoral students, post-docs and developers hosting in addition a Theory of Computing and a Natural Language Technology groups. Andras received his Ph.D. at the Massachusetts Institute of Technology in 1997, since then his interest turned to Information Retrieval and Web Search. He was representing SZTAKI as principal investigator in several EU and national R\&D projects. He received a major permanent grant of the President of the Hungarian Academy of Sciences for Big Data research in 2012.

received his Ph.D. in 1997 in applied mathematics from the Massachusetts Institute of Technology. At present, he is senior researcher at the Institute for Computer Science and Control, Hungarian Research Network, and the scientific director of the Artificial Intelligence National Laboratory Hungary, a consortium of 11 institutions and over 200 researchers. His research revolves primarily around data mining, machine learning and web search, and he has represented his current institution as a principal investigator for multiple European Union and national R\&D projects.

Ying Tang received the M.S. Degree in Systems and Control Theory from the Institut Polytechnique de Grenoble, France, in 2012. She received the Ph.D. in Automatic Control from Grenoble Alpes University (Gipsa-lab), France in 2015. From 2015 to 2017 she was post-doc at CRAN, Nancy, France. Since September 2017 she is Assistant Professor at Lille University. Her research interests are in stability,analysis and parameter estimation of nonlinear systems with applications to traffic control problems and neural models.

Balint Daroczy. From 2007 he worked on industrial and research projects related to machine learning, visual and text processing and multimodal search engines at the Institute for Computer Science and Control (SZTAKI), Eötvös Loránd Research Network (formerly part of the Hungarian Academy of Sciences) in Budapest. From 2010 he started to teach data mining and machine learning related courses at the Budapest University of Technology and Economics (BME). Beside teaching he was supervising 8 BSc and 10 MSc theses and he currently co-supervises a PhD student at the Mathematical doctoral school at Eötvös Loránd University. He defended my PhD thesis at Eötvös Loránd University, Budapest, Hungary (title: "Machine learning methods for multimedia information retrieval", supervisor András Benczúr, PhD) in February 2017 with summa cum laude. In 2018 he received MTA Premium Postdoctoral Grant from the Hungarian Academy of Sciences for his research project ``Manifolds and deep structures'' and as a continuation he worked as a postdoctoral researcher funded by the grant at SZTAKI. Between November 2020 and October 2022 he joined professor Julien Hendrickx group at INMA at Université catholique de Louvain, Louvain-la-Neuve,
Belgium as a postdoctoral researcher in the MIS “Learning from Pairwise Comparisons” of the F.R.S.-FNRS project. From November 2022 he will be full time research fellow at SZTAKI and continue his research project.

2) L’état du sujet dans le laboratoire d’accueil.

The supervision team has already published preliminary results on the topic [7], [8], [10] in leading conferences in control and machine learning . In particular, Mihaly Petreczky and his collaborators have a track record in system identification, and they successfully made the first steps towards PAC-Bayesian error bounds for learning dynamical systems [4], [5] and neural ODEs [6], [8]. Andras Benczur is a senior researcher in the field of machine learning and network science.
Balint Daroczy has extensive experience in theoretical properties of statistical learning algorithms and neural networks. The Hungarian team has a track record on gradient-based learning algorithms and neural ODEs [6], [7].
Ying Tang has extensive experience on stability analysis and estimation of various classes of dynamical systems, which contain relevant classes of neural ODEs [9].
The supervisory team has a history of collaboration [6], [7] ont the topic of the project.
In addition, the team secured funding on topics related to the thesis: the CPER Data project 'Machine learning meets control' 2018-2020, the CNRS PEPS Blanc 2019 project 'PAC-Bayesian theory for recurrent neural networks, and to the recently granted project 'Reliable AI for cyber-physical systems using control theory', which is a joint project with IRT System-X, and which is financed by the industrial initiative 'confiance.ia', and CNRS IEA 'Stability of learning algorithms for deep and recurrent neural networks by using geometry and control theory via understanding the role of overparameterization'.
This indicates that the supervision team will be able to ensure that the prospective student achieves the stated goals. Mihaly Petreczky co-supervised several students in the past, and he has earned his HDR degree in January 2023. Both Ying Tang and Balint Daroczy are actively involved in the co-supervision of PhD students.

3) Les objectifs visés, les résultats escomptés.

The objective of the thesis is to develop new knoweldge on theoretical foundations for learning Neural ODE models. As a consequence, the expected results will be mainly scientific publications. This being said, we also expect to be able to derive new machine learning algorithms, which may lead to new software products and patents, possibly startups. In addition, as the proposed thesis is an international one, another EU member state, it can be a starting point for a EU Horizon project.

4) Le programme de travail avec les livrables et l’échéancier prévisionnel.

The work will be organised in the following work packages.
WP1: Bibliography and state-of-the-art (0 - 6 month) The prospective PhD student will be expected to study the relevant literature and prepare a summary of the state of the art of the subject.
WP2: Statistical consistency of learning neural ODEs (12 - 28 month) The goal of this work package is to prove statistical consistency of learning algorithms for neural ODEs. This work package is likely to use the preliminary results [10]. It can also be viewed as a preliminary step to WP3.
WP3: Finite sample PAC(PAC-Bayesian) error bounds for neural ODEs (12-28 month) The purpose of this work package is to develop finite sample bounds for neural ODEs. In particular, we plan to focus PAC and PAC-Bayesian error bounds for learning neural ODEs. This package can use the existing results [4]–[6], [8].

Note that the PAC(-Bayesian) error bounds can also be used to show statistical consistency of learning algorithms, hence helping WP2.

WP4: Writing up the thesis and preparing the defence (27-36 month)

This work package is devoted to writing the thesis and preparing its defense.

WP5: Dissemination (12-36 month) The PhD student is expected to publish his/her results in leading journals and conference proceedings in control (IEEE Trans. Automatic Control, Automatica, CDC, ACC) and machine learning (AAAI, NIPS, ICML, ECML, J. Machine Learning Research, Neurocomputing) and to present these papers in the leading conferences of both control theory and machine learning.

5) Les collaborations prévues (préciser le cadre, la nature des collaborations, l'ancrage régional, national, international, la transdisciplinarité éventuellement)**.**

The proposed thesis involves international collaboration, as it is co-financed by SZTAKI, Hungary and it will be carried out in collaboration with SZTAKI. The proposed thesis is also multi-disciplinary, as it combines two distinct fields, namely, control theory and artificial intelligence (machine learning). The main advisor, Mihaly Petreczky, is member of UMR 9189 CRIStAL, one of the leading research units of the region in the field of control theory and machine learning.

6) Une liste de 10 publications maximum portant directement sur le sujet en soulignant celles du laboratoire.

[1] S. Massaroli, M. Poli, J. Park, A. Yamashita, and H. Asama, 'Dissecting neural odes', *Adv. Neural Inf. Process. Syst.*, vol. 33, pp. 3952–3963, 2020.

[2] L. Ljung, *System Identification: Theory for the user (2nd Ed.)*. PTR Prentice Hall., Upper Saddle River, USA, 1999.

[3] B. Guedj, 'A Primer on PAC-Bayesian Learning', *ArXiv Prepr. ArXiv190105353*, 2019.

[4] Deividas Eringis, John leth, Rafal Wisniewski, Zheng-Hua Tan, Mihaly Petreczky. PAC-Bayes Generalisation Bounds for Dynamical Systems Including Stable RNNs. In AAAI 2024

[5] Deividas Eringis, John leth, Rafal Wisniewski, Zheng-Hua Tan, Mihaly Petreczky. PAC-Bayesian Error Bound, via R'enyi Divergence, for a Class of Linear Time-Invariant State-Space Models. In ICML 2024

[6] Daniel Racz, Martin Gonzalez, Mihaly Petreczky, Andras Benczur, and Balint Daroczy. "A finite-sample generalization bound for stable LPV systems." *arXiv preprint arXiv:2405.10054* (2024).

[7] D. Rácz, M. Petreczky, A. Csertán, and B. Daróczy, 'Optimization dependent generalization bound for ReLU networks based on sensitivity in the tangent bundle', in NeurIPS *OPT 2023: Optimization for Machine Learning*, 2023. [Online]. Available: https://openreview.net/forum?id=5wsQaTjEAa

[8] M. Gonzalez, T. Defourneau, H. Hajri, and M. Petreczky, 'Realization Theory of Recurrent Neural ODEs using Polynomial System Embeddings', *Syst. Control Lett.*, vol. 173, p. 105468, 2023, doi: https://doi.org/10.1016/j.sysconle.2023.105468.

[9] Y. Tang, C. Prieur, and A. Girard, 'Stability analysis of a singularly perturbed coupled ODE-PDE system', in *2015 54th IEEE Conference on Decision and Control (CDC)*, 2015, pp. 4591–4596. doi: 10.1109/CDC.2015.7402936.

[10] P. B. Cox, R. Toth, and M. Petreczky, 'Towards efficient maximum likelihood estimation of LPV-SS models', *Automatica*, vol. 97, pp. 392–403, Nov. 2018, doi: 10.1016/j.automatica.2018.08.021.

ARGUMENTAIRE DU DIRECTEUR DE THESE

En quoi le sujet répond à l'un au moins des critères de priorisation de la Région ? cf. Délibération de lancement de l'appel à projets Allocations **n° 2023.01809 du 30 novembre 2023 :**
https://guide-aides.hautsdefrance.fr/dispositif491

The topic of PhD project fits well the topic <<Intelligence artificielle embarquée>> of the region . Indeed, the major motivation for using neural ODEs , namely robustness by design, the ability to integrate physical constraints, and the relative small size compared to its performance, are all essential for embedded AI. Furthermore, the specific topic of the PhD project, namely providing theoretical guarantees for robustness and correctness, in order to ensure reliability and safety of AI systems, is one of the major challenges in embedded AI. Indeed, embedded AI is likely to be used in safety-critical applications, where reliability and safety is a major concern.

En quoi le sujet participe à la structuration de la recherche en Région ?
Indiquer si le sujet contribue ou non à un programme régional en cours ou envisagé, notamment un projet retenu au CPER 2021-2017, si le sujet est lié à l'arrivée d'un chercheur en région, à la création d'une nouvelle équipe, à un rapprochement d'équipes, à un projet collaboratif etc.
The topic of the PhD thesis belongs to machine learning/AI, and as such the proposed topic fits well the work package WP1 'bases théoriques et scientifiques de l'IA' of CPER Cornelia.
The PhD project involves international collaboration with SZTAKI, the most prestigious research institute in computer science and control in Hungary. SZTAKI also provides 50\% of funding, hence the proposed project is both international and co-funded by a third party. International and co-funded projects enjoy a high priority with the region.
The main advisor from CRIStAL, Mihaly Petreczky has recently earned his HDR degree (2023) and he is not a main advisor of any PhD student at this point. This project would allow him to make the first step towards independent supervision of PhD students, and to do so on a topic which is important for CRIStAL and the region, and with international partners who contribute financally to the project.

En quoi le sujet s'inscrit dans les priorités du cofinanceur sollicité ? Pour les sujets en lien avec un partenariat public-privé ou un partenariat entre plusieurs laboratoires publics, quelles sont les modalités du partenariat ?
nature, moyens, propriété, partage et diffusion des résultats, encadrement et localisation du doctorant…

SZTAKI is the leading Hungarian research institution in computer science, in particular, artificial intelligence. The proposed project fits well the overall strategy of SZTAKI, due to its focus on machine learning and its internation nature. SZTAKI is expected to provide 50\% of the funding and the PHD student is expected to spend half of its time at SZTAKI.

En quoi le sujet pourrait être valorisé dans un cadre national, européen, international (Conférences, publications) ?

The topic of the thesis can be seen as a building block for building Trustworthy and Reliable AI. The latter problem is recognized as a major challenge both on international level, e.g., Artificial Intellegince Act of EU, the French national program Conifance.ia, of which the main advisor has been an active participant. This challenge is also recognized by the research community, see for example the dedicated conference tracks of AAAI 2024 on Safe, Robust and Reliable AI. The outcomes of the proposed project can be used for developing safe, robust and trustworthy AI, which is relevant for national, EU and international level.
In addition, as the project involves collaboration with an EU member state, it can give rise to a EU Horizon project proposal.

Furthermore, we plan to publish the obtained results in leading journals (IEEE TAC, Automatica, System & Control Letters, JMRL, TMLR) and conferences (CDC, ICML, NeurIPS, AAAI, AISTATS).

Quelles sont les perspectives de valorisation, de transfert et d'innovation sur le territoire des Hauts-de-France ?
Le projet contribue-t-il à la Stratégie Recherche Innovation de la région (S3) ? Si oui, pour quel Domaine d'Activité Stratégique ? D'une façon plus générale, quelles sont les retombées socio-économiques pour le territoire régional ?
https://delibinternet.hautsdefrance.fr/Docs/CommissionPermanente/2022/03/17/DELIBERATION/2022.00573_annexe.PDF

The proposed project contributes to S3 of the region, as it contributes to the topic « Intelligence artificielle embarquée », axis <<Science des données et intelligence artificielle>> and the application domain <<Automatisation des systèmes mobiles et de la logistique>>, due to the relevance of the project for reliability of AI algorithms and their integration with physical systems.
More generally, the outcomes of the project will contribute to the economy of the region by training experts in the very promising field of Trustworthy and Reliable AI for physical systems. Moreover, the project may lead to further EU Horizon projects, which may give a boost to the innovation ecosystem of the region. Finally, the project may give rise to a startup, which would create high skill employment in the region.

Le sujet peut-il ou non contribuer à Rev3 Transformons les Hauts-de-France *cf Feuille de route Rev3*
https://delibinternet.hautsdefrance.fr/Docs/CommissionPermanente/2022/06/23/DELIBERATION/2022.01210_annexe.PDF
Feuille de route Economie circulaire

https://delibinternet.hautsdefrance.fr/Docs/CommissionPermanente/2020/11/19/DELIBERATION/2020.02126_annexe.PDF
Référentiel Rev3 enseignement supérieur et recherche
https://rev3.hautsdefrance.fr/thematique/recherche-regionale-innovation-et-entreprises/

The project, via creating new knowledge relevant for local companies, and possibly by creating startups, will contribute to the increase of collaboration between research labs and SMEs of the region.

Le sujet peut-il contribuer à développer la bioéconomie en région ? *cf. master plan délibération n° 2018.1233 bioéconomie* https://www.hautsdefrance.fr/categorie/dossiers/bioeconomie/

The project is not related to bio-economy.

Le sujet peut-il contribuer à développer une autre politique régionale (exemple : innovation pédagogique, transports, handicap…).

Fait à Villeneuve d'Ascq

Le 11/12/2023
Mihaly PETRECZKY

Prénom, Nom du Directeur de Thèse
Signature

M. Petreczky