Activity Report 2018

Team TAU

TAckling the Underspecified

Inria teams are typically groups of researchers working on the definition of a common project, and objectives, with the goal to arrive at the creation of a project-team. Such project-teams may include other partners (universities or research institutions).

RESEARCH CENTER
Saclay - Île-de-France

THEME
Optimization, machine learning and statistical methods

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Keywords:

Computer Science and Digital Science:

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A8.2. - Optimization
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Other Research Topics and Application Domains:

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2. Overall Objectives

2.1. Presentation

The last two years have been a turning point for the team. Of course, since its creation in 2003, TAO activities had constantly but slowly evolved, as old problems were being solved, and new applications arose. But recent abrupt progresses in Machine Learning (and in particular in Deep Learning) have greatly accelerated these changes also within the team. It so happened that this change of slope also coincided with some more practical changes in TAO ecosystem: following Inria 12-years rule, the team definitely ended in December 2016. The new team TAU (for **TA**ckling the **U**nderspecified) has been proposed, and the creation process is on-going. At the same time important staff changes took place, that also justify even sharper changes in the team focus. During the year 2018, the second year of this new era for the (remaining) members of the team, our research topics have now stabilized around a final version of the TAU project.

Following the dramatic changes in TAU staff during the years 2016-2017 (see the 2017 activity report of the team for the details), the research around continuous optimization has definitely faded out in TAU (while the research axis on hyperparameter tuning has focused on Machine Learning algorithms), the Energy application domain has slightly changed direction under Isabelle Guyon's supervision (Section 4.2), after the completion of the work started by Olivier Teytaud, and a few new directions have emerged, though yet too young to have given any visible fruit, around the robustness of ML systems (Section 3.1.2). The other research topics have been continued, as described below.

2.2. Context and overall goal of the project

Building upon the expertise in machine learning (ML) and optimization of the TAO team, the TAU project will tackle some **under-specified challenges behind the New Artificial Intelligence wave**. The simultaneous advent of massive data and massive computational power, blurring the boundaries between data, structure, knowledge and common sense, seemingly makes it possible to fulfill all promises of the good old AI, now or soon.

This makes NewAI under-specified in three respects. A first dimension regards the relationships between AIs and human beings. The necessary conditions for AIs to be accepted by mankind and/or contribute to the common good are yet to be formally defined; it is hard to believe that a general and computable definition of "ethical behavior" can be set once for all. Some of these necessary conditions (explainable and causal modeling; unbiased data and models; model certification) can nevertheless be cast as ambitious and realistic goals for public research.

A second dimension regards the relationships between AI, data and knowledge. In closed worlds AIs can manage and acquire sufficient data to reach human-level performances from scratch [81]. In open worlds however, prior knowledge is used in various ways to overcome the lack of direct interactions with the world, e.g. through i) exploiting domain-dependent data invariances in intension or in extension (ranging from convolution to domain augmentation); ii) taking advantage of the low-rank structure (generative learning) or known properties (equivariant learning) of the observed data; iii) leveraging diverse domains and datasets, assumedly related to each other (domain adaptation; multi-task learning). A general and open question is how available prior knowledge can be best leveraged by an AI, all the more so as domains with small to medium-size data are considered.

A third dimension regards the intrinsic limitations of AI in terms of information theory. Long established theories, e.g. rooted in Occam's razor, currently hardly account for the practical leaps of deep learning, where the solution dimension outnumbers the input dimension. Beyond trials-and-errors, a long-term goal is to characterize the learning landscape w.r.t. order parameters to be defined, and *a priori* estimate the regions of problem instances where it is likely/possible/unlikely to learn accurate models.

The above under-specified AI issues define three core research pillars (Section 3), examining three interdependent aspects of AI:

I. The first pillar aims to answer the question of what it means to be a good AI and how to build them. More specifically, our goal is to advance the state of the art concerning robust learning (re adversarial attacks), causal modeling (aimed to support explanations and prescriptions), and unbiased models in the sense of prescribed neutrality constraints (including the assessment and repair of the data).

II. The second pillar tackles the "innate *vs* acquired" question: how to best combine available human knowledge, and agnostic machine learning. TAU will examine this question focusing on domains with spatial and temporal multi-scale structure, as pervasive in natural sciences (where domain knowledge is expressed using PDEs, or through powerful compact representations as in signal processing), taking advantage of the pluri-disciplinary expertise and scientific collaborations of the TAU members.

III. The third pillar aims to understand the learning landscape. In the short term, it tackles the so-called Auto-☆ issue of automatically selecting and configuring an algorithm portfolio for a problem instance. This issue governs the knowledge transfer from research labs to industry [92], [91], all the more so as massive computational resources are at stake. In the medium term, our goal is to integrate the hyper-parameters and model structure in the learning criteria, using information theory and/or bilevel programming [93]. In the long-term, our goal is to establish a phase diagram of the learning landscape, through i) determining order parameters; ii) relating the different regions defined along these order parameters, to the quality of the optimal solution, and the probability of finding a good approximation thereof. These goals are aligned with the unique scientific expertise of TAU in statistical physics and in information theory, and benefit from our decade-long expertise in Auto-☆.
The above research pillars will take inspiration and be validated with three applicative topics (Section 4):

1.Energy management encompasses a variety of scientific problems related to research pillars I. (fair learning, privacy-compliant modelling, safety-related guarantees) and II. (spatio-temporal multi-scale modelling, distributional learning). It is also a strategic application for the planet, where TAU benefits from the TAO expertise and the long established relationships with Artelys (ILab Metis) and RTE.

2.Computational Social Sciences offer questions and methodological lessons about how to address these questions in a common decency spirit, along research pillar I. On-going studies at TAU include the learning and randomized assessment of prescriptive models for Human Resources (hiring and vocational studies; quality of life at work and economic performance) and nutrition habits (in relation with social networks and health), where i) learned models must be unbiased although data are undoubtedly biased; ii) prior knowledge must be accounted for and the interpretation of the learned models is mandatory; iii) causal modelling is key as models are deployed for *prescription* and self-fulfilling prophecies must be avoided at all costs [131].

3.Optimal data-driven design considers several physical/simulated phenomenons, ranging from high-energy physics to space weather, from population biology to medical imaging, from signal processing to certification of autonomous vehicle controllers, with: i) medium-size data; ii) extensive prior knowledge, notably concerning the symmetries and properties of the sought models; iii) computationally expensive simulators. All three characteristics are relevant to pillars II and III.

3. Research Program

3.1. Toward Good AI

As discussed by [134], the topic of ethical AI was non-existent until 2010, was laughed at in 2016, and became a hot topic in 2017 as the AI disruptivity with respect to the fabric of life (travel, education, entertainment, social networks, politics, to name a few) became unescapable [131], together with its expected impacts on the nature and amount of jobs. As of now, it seems that the risk of a new AI Winter might arise from legal[1] and societal[2] issues. While privacy is now recognized as a civil right in Europe, it is feared that the GAFAM, BATX

[1] For instance, the (fictitious) plea challenge proposed to law students in Oct. 2018 considered a chain reaction pileup occurred among autonomous and humanly operated vehicles on a highway.

[2] For instance related to information bubbles and nudge [98], [148].

and others can already capture a sufficient fraction of human preferences and their dynamics to achieve their commercial and other goals, and build a Brave New Big Brother (BNBB, a system that is openly beneficial to many, covertly nudging, and possibly dictatorial).

The ambition of TAU is to mitigate the BNBB risk along several intricated dimensions, and build i) causal and explainable models; ii) fair data and models; iii) provably robust models.

3.1.1. Causal modeling and biases

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PhD: Diviyan Kalainathan
Collaboration: Olivier Goudet (TAU then Univ. Angers), David Lopez-Paz (Facebook)

The extraction of causal models, a long goal of AI [132], [112], [133], became a strategic issue as the usage of learned models gradually shifted from *prediction* to *prescription* in the last years. This evolution, following Auguste Comte's vision of science (*Savoir pour prévoir, afin de pouvoir*) indeed reflects the exuberant optimism about AI: Knowledge enables Prediction; Prediction enables Control. However, although predictive models can be based on correlations, prescriptions can only be based on causal models[3].

Among the research applications concerned with causal modeling, predictive modeling or collaborative filtering at TAU are all projects described in section 4.1 (see also Section 3.4), studying the relationships between: i) the educational background of persons and the job openings (FUI project JobAgile and DataIA project Vadore); ii) the quality of life at work and the economic performance indicators of the enterprises (ISN Lidex project Amiqap) [114] ; iii) the nutritional items bought by households (at the level of granularity of the barcode) and their health status, as approximated from their body-mass-index (IRS UPSaclay Nutriperso); iv) the actual offer of restaurants and their scores on online rating systems. In these projects, a wealth of data is available (though hardly sufficient for applications ii), iii and iv))) and there is little doubt that these data reflect the imbalances and biases of the world as is, ranging from gender to racial to economical prejudices. Preventing the learned models from perpetuating such biases is essential to deliver an AI endowed with common decency.

In some cases, the bias is known; for instance, the cohorts in the Nutriperso study are more well-off than the average French population, and the Kantar database includes explicit weights to address this bias through importance sampling. In other cases, the bias is only guessed; for instance, the companies for which Secafi data are available hardly correspond to a uniform sample as these data have been gathered upon the request of the company trade union.

3.1.2. Robustness of Learned Models

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Collaboration: Zakarian Chihani (CEA); Hiba Hage, Philippe Reynaud, and Yves Tourbier (Renault)

Due to their outstanding performances, deep neural networks and more generally machine learning-based decision making systems, referred to as MLs in the following, have been raising hopes in the recent years to achieve breakthroughs in critical systems, ranging from autonomous vehicles to defense. The main pitfall for such applications lies in the lack of guarantees for MLs robustness.

[3] One can predict that it rains based on the presence of umbrellas in the street; but one cannot induce rainfall by going out with an umbrella. Likewise, the presence of books/tablets at home and the good scores of children at school are correlated; but offering books/tablets to all children might fail to improve their scores *per se*, if both good scores and books are explained by a so-called confounder variable, like the presence of adults versed in books/tablets at home.

Specifically, MLs are used when the mainstream software design process does not apply, that is, when no formal specification of the target software behavior is available and/or when the system is embedded in an open unpredictable world. The extensive body of knowledge developed to deliver guarantees about mainstream software − ranging from formal verification, model checking and abstract interpretation to testing, simulation and monitoring − thus does not directly apply either. Another weakness of MLs regards their dependency to the amount and quality of the training data, as their performances are sensitive to slight perturbations of the data distribution. Such perturbations can occur naturally due to domain or concept drift (e.g. due to a change in light intensity or a scratch on a camera lens); they can also result from intentional malicious attacks, a.k.a adversarial examples [149].

These downsides, currently preventing the dissemination of MLs in safety-critical systems (SCS), call for a considerable amount of research, in order to understand when and to which extent an MLs can be certified to provide the desired level of guarantees.

Julien Girard's PhD (CEA scholarship), started in Oct. 2018, co-supervised by Guillaume Charpiat and Zakaria Chihani (CEA), is devoted to the extension of abstract interpretation to deep neural nets, and the formal characterization of the transition kernel from input to output space achieved by a DNN (robustness by design, coupled with formally assessing the coverage of the training set). This approach is tightly related to the inspection and opening of black-box models, aimed to characterize the patterns in the input instances responsible for a decision – another step toward explainability.

On the other hand, experimental validation of MLs, akin statistical testing, also faces three limitations: i) real-world examples are notoriously insufficient to ensure a good coverage in general; ii) for this reason, simulated examples are extensively used; but their use raises the *reality gap* issue [123] of the distance between real and simulated worlds; iii) independently, the real-world is naturally subject to domain shift (e.g. due to the technical improvement and/or aging of sensors). Our collaborations with Renault tackle such issues in the context of the autonomous vehicle (see Section 7.1.3).

3.2. Hybridizing numerical modeling and learning systems

Participants: Guillaume Charpiat, Cécile Germain, Isabelle Guyon, Marc Schoenauer, Michèle Sebag
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In sciences and engineering, human knowledge is commonly expressed in closed form, through equations or mechanistic models characterizing how a natural or social phenomenon, or a physical device, will behave/evolve depending on its environment and external stimuli, under some assumptions and up to some approximations. The field of numerical engineering, and the simulators based on such mechanistic models, are at the core of most approaches to understand and analyze the world, from solid mechanics to computational fluid dynamics, from chemistry to molecular biology, from astronomy to population dynamics, from epidemiology and information propagation in social networks to economy and finance.

Most generally, numerical engineering supports the simulation, and when appropriate the optimization and control[4] of the phenomenons under study, although several sources of discrepancy might adversely affect the results, ranging from the underlying assumptions and simplifying hypotheses in the models, to systematic experiment errors to statistical measurement errors (not to mention numerical issues). This knowledge and know-how are materialized in millions of lines of code, capitalizing the expertise of academic and industrial labs. These softwares have been steadily extended over decades, modeling new and more fine-grained effects through layered extensions, making them increasingly harder to maintain, extend and master. Another difficulty is that complex systems most often resort to hybrid (pluridisciplinary) models, as they involve many components interacting along several time and space scales, hampering their numerical simulation.

[4] Note that the causal nature of mechanistic models is established from prior knowledge and experimentations.

At the other extreme, machine learning offers the opportunity to model phenomenons from scratch, using any available data gathered through experiments or simulations. Recent successes of machine learning in computer vision, natural language processing and games to name a few, have demonstrated the power of such agnostic approaches and their efficiency in terms of prediction [118], inverse problem solving [161], and sequential decision making [154], [81], despite their lack of any "semantic" understanding of the universe. Even before these successes, Anderson's claim was that *the data deluge [might make] the scientific method obsolete* [69], as if a reasonable option might be to throw away the existing equational or software bodies of knowledge, and let Machine Learning rediscover all models from scratch. Such a claim is hampered among others by the fact that not all domains offer a wealth of data, as any academic involved in an industrial collaboration around data has discovered.

Another approach will be considered in TAU, investigating how existing mechanistic models and related simulators can be partnered with ML algorithms: i) to achieve the same goals with the same methods with a gain of accuracy or time; ii) to achieve new goals; iii) to achieve the same goals with new methods.

Toward more robust numerical engineering: In domains where satisfying mechanistic models and simulators are available, ML can contribute to improve their accuracy or usability. A first direction is to refine or extend the models and simulators to better fit the empirical evidence. The goal is to finely account for the different biases and uncertainties attached to the available knowledge and data, distinguishing the different types of *known unknowns*. Such *known unknowns* include the model hyper-parameters (coefficients), the systematic errors due to e.g., experiment imperfections, and the statistical errors due to e.g., measurement errors. A second approach is based on learning a surrogate model for the phenomenon under study that incorporate domain knowledge from the mechanistic model (or its simulation). See Section 7.5 for case studies.

A related direction, typically when considering black-box simulators, aims to learn a model of the error, or equivalently, a post-processor of the software. The discrepancy between simulated and empirical results, referred to as *reality gap* [123], can be tackled in terms of domain adaptation [74], [97]. Specifically, the source domain here corresponds to the simulated phenomenon, offering a wealth of inexpensive data, and the target domain corresponds to the actual phenomenon, with rare and expensive data; the goal is to devise accurate target models using the source data and models.

Extending numerical engineering: ML, using both experimental and numerical data, can also be used to tackle new goals, that are beyond the current state-of-the-art of standard approaches. Inverse problems are such goals, identifying the parameters or the initial conditions of phenomenons for which the model is not differentiable, or amenable to the adjoint state method.

A slightly different kind of inverse problem is that of recovering the ground truth when only noisy data is available. This problem can be formulated as a search for the simplest model explaining the data. The question then becomes to formulate and efficiently exploit such a simplicity criterion.

Another goal can be to model the distribution of given quantiles for some system: The challenge is to exploit available data to train a generative model, aimed at sampling the target quantiles.

Examples tackled in TAU are detailed in Section 7.5. Note that the "Cracking the Glass Problem", described in Section 7.2.3 is yet another instance of a similar problem.

Data-driven numerical engineering : Finally, ML can also be used to sidestep numerical engineering limitations in terms of scalability, or to build a simulator emulating the resolution of the (unknown) mechanistic model from data, or to revisit the formal background.

When the mechanistic model is known and sufficiently accurate, it can be used to train a deep network on an arbitrary set of (space,time) samples, resulting in a meshless numerical approximation of the model [145], supporting by construction *differentiable programming* [120].

When no mechanistic model is sufficiently efficient, the model must be identified from the data only. Genetic programming has been used to identify systems of ODEs [142], through the identification of invariant quantities from data, as well as for the direct identification of control commands of nonlinear complex systems, including some chaotic systems [85]. Another recent approach uses two deep neural networks, one for the state of the system, the other for the equation itself [135]. The critical issues for both approaches include the scalability, and the explainability of the resulting models. Such line of research will benefit from TAU unique mixed expertise in Genetic Programming and Deep Learning.

Finally, in the realm of signal processing (SP), the question is whether and how deep networks can be used to revisit mainstream feature extraction based on Fourier decomposition, wavelet and scattering transforms [77]. E. Bartenlian's PhD (started Oct. 2018), co-supervised by M. Sebag and F. Pascal (Centrale-Supélec), focusing on musical audio-to-score translation [144], inspects the effects of supervised training, taking advantage from the fact that convolution masks can be initialized and analyzed in terms of frequency.

3.3. Learning to learn

According to Ali Rahimi's test of times award speech at NIPS 17, the current ML algorithms *have become a form of alchemy*. Competitive testing and empirical breakthroughs gradually become mandatory for a contribution to be acknowledged; an increasing part of the community adopts trials and errors as main scientific methodology, and theory is lagging behind practice. This style of progress is typical of technological and engineering revolutions for some; others ask for consolidated and well-understood theoretical advances, saving the time wasted in trying to build upon hardly reproducible results.

Basically, while practical achievements have often passed the expectations, there exist caveats along three dimensions. Firstly, excellent performances do not imply that the model has captured what was to learn, as shown by the phenomenon of adversarial examples. Following Ian Goodfellow, some well-performing models might be compared to *Clever Hans*, the horse that was able to solve mathematical exercizes using non verbal cues from its teacher [111]; it is the purpose of Pillar I. to alleviate the *Clever Hans* trap (section 3.1).
Secondly, some major advances, e.g. related to the celebrated adversarial learning [101], [97], establish proofs of concept more than a sound methodology, where the reproducibility is limited due to i) the computational power required for training (often beyond reach of academic labs); ii) the numerical instabilities (witnessed as random seeds happen to be found in the codes); iii) the insufficiently documented experimental settings. What works, why and when is still a matter of speculation, although better understanding the limitations of the current state of the art is acknowledged to be a priority. After Ali Rahimi again, *simple experiments, simple theorems are the building blocks that help us understand more complicated systems*. Along this line, [128] propose toy examples to demonstrate and understand the defaults of convergence of gradient descent adversarial learning.
Thirdly, and most importantly, the reported achievements rely on carefully tuned learning architectures and hyper-parameters. The sensitivity of the results to the selection and calibration of algorithms has been identified since the end 80s as a key ML bottleneck, and the field of automatic algorithm selection and calibration, referred to as AutoML or Auto-☆ in the following, is at the ML forefront.

TAU aims to contribute to the ML evolution toward a more mature stage along three dimensions. In the short term, the research done in Auto-☆ will be pursued (section 3.3.1). In the medium term, an information theoretic perspective will be adopted to capture the data structure and to calibrate the learning algorithm *depending on the nature and amount of the available data*. In the longer term, our goal is to leverage the methodologies forged in statistical physics to understand and control the trajectories of complex learning systems (section 3.3.3).

*3.3.1. Auto-**

Participants: Isabelle Guyon, Marc Schoenauer, Michèle Sebag
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The so-called Auto-☆ task, concerned with selecting a (quasi) optimal algorithm and its hyper-parameters depending on the problem instance at hand, remained a key issue in ML for the last three decades [75], as well as in optimization at large [110], including combinatorial optimization and constraint satisfaction [117], [100] and continuous optimization [71]. This issue, tackled by several European projects along the decades, governs the knowledge transfer to industry, due to the shortage of data scientists. It becomes even more crucial as models are more complex and their training requires more computational resources. This has motivated several international challenges devoted to Auto-ML [45] (see also Section 3.4), including the on-going AutoDL [37] (see also Section 7.6).

Several approaches have been used to tackle Auto-☆ in the literature, and TAU has been particularly active in the first two. Meta-learning aims to build a surrogate performance model, estimating the performance of an algorithm configuration on *any* problem instance characterized from its meta-feature values [138], [100], [72], [71] [11]. Collaborative filtering, considering that a problem instance "likes better" an algorithm configuration yielding a better performance, learns to recommend good algorithms to problem instances [147], [130]. Bayesian optimization proceeds by alternatively building a surrogate model of algorithm performances on *the* problem instance at hand, and tackling it [92]. This last approach currently is the prominent one; as shown in [130], the meta-features developed for AutoML are hardly relevant, hampering both meta-learning and collaborative filtering.

Beyond these, current research directions in TAU include the design of more efficient features, as well as the design of an original approach based on MCTS algorithm (see Section 7.2.1).

3.3.2. Information theory: adjusting model complexity and data fitting

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Collaboration: Yann Ollivier (Facebook)

In the 60s, Kolmogorov and Solomonoff provided a well-grounded theory for building (probabilistic) models best explaining the available data [139], [103], that is, the shortest programs able to generate these data. Such programs can then be used to generate further data or to answer specific questions (interpreted as missing values in the data). Deep learning, from this viewpoint, efficiently explores a space of computation graphs, described from its hyperparameters (network structure) and parameters (weights). Network training amounts to optimizing these parameters, namely, navigating the space of computational graphs to find a network, as simple as possible, that explain the past observations well.

This vision is at the core of variational auto-encoders [116], directly optimizing a bound on the Kolmogorov complexity of the dataset. More generally variational methods provide quantitative criteria to identify superfluous elements (edges, units) in a neural network, that can potentially be used for structural optimization of the network (Leonard Blier's PhD, started Oct. 2018).

The same principles apply to unsupervised learning, aimed to find the maximum amount of structure hidden in the data, quantified using this information-theoretic criterion.

The known invariances in the data can be exploited to guide the model design (e.g. as translation invariance leads to convolutional structures, or LSTM is shown to enforce the invariance to time affine transformations of the data sequence [150]). Scattering transforms exploit similar principles [77]. A general theory of how to detect *unknown* invariances in the data, however, is currently lacking.

The view of information theory and Kolmogorov complexity suggests that key program operations (composition, recursivity, use of predefined routines) should intervene when searching for a good computation graph. One possible framework for exploring the space of computation graphs with such operations is that of genetic programming [70]. It is interesting to see that evolutionary computation appeared in the last two years among the best candidates to explore the space of deep learning structures [137], [122]. Other approaches might proceed by combining simple models into more powerful ones, e.g. using "Context Tree Weighting" [158] or switch distributions [88]. Another option is to formulate neural architecture design as a reinforcement learning problem [73]; the value of the building blocks (predefined routines) might be defined using e.g., Monte-Carlo

Tree Search. A key difficulty is the computational cost of retraining neural nets from scratch upon modifying their architecture; an option might be to use neutral initializations to support warm-restart.

3.3.3. Analyzing and Learning Complex Systems

Participants: Cyril Furtlehner, Aurélien Decelle, François Landes, Michèle Sebag
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Collaboration: Enrico Camporeale (CWI); Jacopo Rocchi (LPTMS Paris Sud), the Simons team: Rahul Chako (post-doc), Andrea Liu (UPenn), David Reichman (Columbia), Giulio Biroli (ENS), Olivier Dauchot (ESPCI).

Methods and criteria from statistical physics have been widely used in ML. In early days, the capacity of Hopfield networks (associative memories defined by the attractors of an energy function) was investigated by using the replica formalism [68]. Restricted Boltzmann machines likewise define a generative model built upon an energy function trained from the data. Along the same lines, Variational Auto-Encoders can be interpreted as systems relating the free energy of the distribution, the information about the data and the entropy (the degree of ignorance about the micro-states of the system) [157]. A key promise of the statistical physics perspective and the Bayesian view of deep learning is to harness the tremendous growth of the model size (billions of weights in recent machine translation netwowrks), and make them sustainable through e.g. weight quantization [125], posterior drop-out [129], and probabilistic binary networks [126]. Such "informational cooling" of a trained deep network can reduce its size by several orders of magnitude while preserving its performance.

Statistical physics is among the key expertises of TAU, originally only represented by Cyril Furtlehner, later strenghtened by Aurélien Decelle's and François Landes' arrivals in 2014 and 2018. On-going studies are conducted along several directions.

Generative models are most often expressed in terms of a Gibbs distributions $P[S] = \exp(-E[S])$, where energy E involves a sum of building blocks, modelling the interactions among variables. This formalization makes it natural to use mean-field methods of statistical physics and associated inference algorithms to both train and exploit such models. The difficulty is to find a good trade-off between the richness of the structure and the efficiency of mean-field approaches. One direction of research pursued in TAU, [94] in the context of traffic forecasting, is to account for the presence of cycles in the interaction graph, to adapt inference algorithms to such graphs with cycles, while constraining graphs to remain compatible with mean-field inference.

Another direction, explored in TAO in the recent years, is based on the definition and exploitation of self-consistency properties, enforcing principled divide-and-conquer resolutions. In the particular case of the message-passing Affinity Propagation algorithm for instance [159], self-consistency imposes the invariance of the solution when handled at different scales, thus enabling to characterize the critical value of the penalty and other hyper-parameters in closed form (in the case of simple data distributions) or empirically otherwise [95].

A more recent research direction examines the quantity of information in a (deep) neural net along the random matrix theory framework [80]. It is addressed in Giancarlo Fissore's PhD, and is detailed in Section 7.2.3.

A collaboration with L. Zbederova's group at Ecole Normale Supérieure is just starting, thanks to François Landes' arrival, based on the study of some information-theoretic indicators for some class of Neural Network. It is, too, described in more details in Section 7.2.3.

Finally, we note the recent surge in using ML to address fundamental physics problems: from turbulence to high-energy physics and soft matter as well (with glasses at its core). TAU's dual expertise in Deep Networks and in statistical physics places it in an ideal position to significantly contribute to this domain and shape the methods that will be used by the physics community in the future. François Landes' recent arrival in the team makes TAU a unique place for such interdisciplinary research, thanks to his collaborators from the Simons Collaboration *Cracking the Glass Problem* (gathering 13 statistical physics teams at the international level). This project is detailed in Section 7.2.3.

3.4. Organisation of Challenges

Participants: Cécile Germain, Isabelle Guyon, Marc Schoenauer, Michèle Sebag
Challenges have been an important drive for Machine Learning research for many years, and TAO members have played important roles in the organization of many such challenges: Michèle Sebag was head of the challenge programme in the Pascal European Network of Excellence (2005-2013); Isabelle Guyon, as mentioned, was the PI of many challenges ranging from causation challenges [104], to AutoML [105]. The Higgs challenge [65], most attended ever Kaggle challenge, was jointly organized by TAO (C. Germain), LAL-IN2P3 (D. Rousseau and B. Kegl) and I. Guyon (not yet at TAO), in collaboration with CERN and Imperial College.

TAU was also particularly implicated with the ChaLearn Looking At People (LAP) challenge series in Computer Vision, in collaboration with the University of Barcelona [90] including the Job Candidate Screening Coopetition [89]; the Real Versus Fake Expressed Emotion Challenge (ICCV 2017) [155]; the Large-scale Continuous Gesture Recognition Challenge (ICCV 2017) [155]; the Large-scale Isolated Gesture Recognition Challenge (ICCV 2017) [155].

Other challenges have been organized in 2018, or are planned for the near future, detailed in Section 7.6. In particular, many of them now run on the Codalab platform, managed by TAU and maintained at LRI.

4. Application Domains

4.1. Computational Social Sciences

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag, Paola Tubaro
Collaboration: Jean-Pierre Nadal (EHESS); Marco Cuturi, Bruno Crépon (ENSAE); Thierry Weil (Mines); Jean-Luc Bazet (RITM)

Computational Social Sciences (CSS) studies social and economic phenomena, ranging from technological innovation to politics, from media to social networks, from human resources to education, from inequalities to health. It combines perspectives from different scientific disciplines, building upon the tradition of computer simulation and modeling of complex social systems [99] on the one hand, and data science on the other hand, fueled by the capacity to collect and analyze massive amounts of digital data.

The emerging field of CSS raises formidable challenges along three dimensions. Firstly, the definition of the research questions, the formulation of hypotheses and the validation of the results require a tight pluridisciplinary interaction and dialogue between researchers from different backgrounds. Secondly, the development of CSS is a touchstone for ethical AI. On the one hand, CSS gains ground in major, data-rich private companies; on the other hand, public researchers around the world are engaging in an effort to use it for the benefit of society as a whole [119]. The key technical difficulties related to data and model biases, and to self-fulfilling prophecies have been discussed in section 3.1. Thirdly, CSS does not only regard scientists: it is essential that the civil society participate in the science of society [146].

TAO was involved in CSS for the last five years, and its activities have been strengthened thanks to P. Tubaro's and I. Guyon's expertises respectively in sociology and economics, and in causal modeling. Details are given in Section 7.3.

4.2. Energy Management

Participants: Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhD: Victor Berger, Benjamin Donnot, Balthazar Donon, Herilalaina Rakotoarison
Collaboration: Antoine Marot, Patrick Panciatici (RTE), Vincent Renault (Artelys), Olivier Teytaud (Facebook)

Energy Management has been an application domain of choice for TAO since the end 2000s, with main partners SME Artelys (METIS Ilab Inria; ADEME project POST; ADEME project NEXT) and RTE (See.4C European challenge; two CIFRE PhDs). The goals concern i) optimal planning over several spatio-temporal scales, from investments on continental Europe/North Africa grid at the decade scale (POST), to daily planning of local or regional power networks (NEXT); ii) monitoring and control of the French grid enforcing the prevention of power breaks (RTE); iii) improvement of house-made numerical methods using data-intense learning (as described in Section 3.2) in all aspects of IFPEN activities, from geological problems in oil prospection (IF**P**EN) to the optimal placement of eolians in eolian fields (IFP**EN**).
Optimal planning over long periods of time amounts to optimal sequential decision under high uncertainties, ranging from stochastic uncertainties (weather, market prices, demand prediction) handled based on massive data, to non-stochastic uncertainties (e.g., political decisions about the nuclear policy) handled through defining and selecting a tractable number of scenarios. Note that non-anticipativity constraints forbid the use of dynamic programming-related methods; this led to propose the *Direct Value Search* method [79] at the end of the POST project. A further recent work in the same direction [21] proposes and theoretically studies the *Direct Model Predictive Control* approach, a hybrid model which merges the properties of two different dynamic optimization methods, Model Predictive Control and Stochastic Dual Dynamic Programming, has robust convergence properties, and experimentally competes with both methods alone.

The daily maintainance of power grids requires the building of approximate predictive models on the top of any given network topology. Deep Networks are natural candidates for such modelling, considering the size of the French grid ($\sim$ 10000 nodes), but the representation of the topology is a challenge when, e.g. the RTE goal is to quickly ensure the "n-1" security constraint (the network should remain safe even if any of the 10000 nodes fails). Existing simulators are too slow to be used in real time, and the size of actual grids makes it intractable to train surrogate models for all possible (n-1) topologies (see Section 7.4 for more details).

Even when efficient simulators do exist, they need to be calibrated (adjusting their hyper-parameters with real data), and complemented by uncertainty propagation models. Such adaptations and extensions are at the core of the NEXT project; hyper-parameter tuning is also a challenge regarding the development plans of the local grids, that heavily rely on graph optimization algorithms.
Furthermore, predictive models of local grids are based on the estimated consumption of end-customers: Linky meters provide coarse grain information only due to privacy issues, and very few samples of fine-grained consumption are available (from volunteer customers). A first task is to transfer knowledge from small data to the whole domain of application. A second task is to directly predict the peak of consumption based on the user cluster profiles and their representativity (see Section 7.4.2).

Another research direction formulates security maintenance as a reinforcement problem, taking inspiration from the recent successes of Deep Reinforcement Learning. This direction is being investigated in Balthazar Donon's RTE CIFRE PhD with RTE (started Oct. 2018).

4.3. Data-driven Numerical Modeling

Participants: Guillaume Charpiat, Cécile Germain, Isabelle Guyon, Flora Jay, Marc Schoenauer, Michèle Sebag
PhD and Post-doc: Victor Estrade, Loris Felardo, Adrian Pol, Théophile Sanchez
Collaboration: D. Rousseau (LAL), M. Pierini (CERN)

As said (section 3.2), in domains where both first principle-based models and equations, and empirical or simulated data are available, their combined usage can support more accurate modelling and prediction, and when appropriate, optimization, control and design. This section describes such applications, with the goal of improving the time-to-design chain through fast interactions between the simulation, optimization, control and design stages. The expected advances regard: i) the quality of the models or simulators (through data assimilation, e.g. coupling first principles and data, or repairing/extending closed-form models); ii) the exploitation of data derived from different distributions and/or related phenomenons; and, most interestingly, iii) the task of optimal design and the assessment of the resulting designs.

The proposed approaches are based on generative and adversarial modelling [116], [102], extending both the generator and the discriminator modules to take advantage of the domain knowledge.

A first challenge regards the design of the model space, and the architecture used to enforce the known domain properties (symmetries, invariance operators, temporal structures). When appropriate, data from different distributions (e.g. simulated vs real-world data) will be reconciled, for instance taking inspiration from real-valued non-volume preserving transformations [84] in order to preserve the natural interpretation.
Another challenge regards the validation of the models and solutions of the optimal design problems. The more flexible the models, the more intensive the validation must be, as reminded by Leon Bottou. Along this way, generative models will be used to support the design of "what if" scenarios, to enhance anomaly detection and monitoring via refined likelihood criteria.

5. Highlights of the Year

5.1. Highlights of the Year

5.1.1. Awards

- *GECCO 2018 10-years impact award*, awarded to the paper published in GECCO 2008 that had the greatest impact, seen from 10 years later, for the paper

  Adaptive operator selection with dynamic multi-armed bandits, by Luis DaCosta, Alvaro Fialho, Marc Schoenauer, and Michèle Sebag, in Maarten Keijzer (Ed), Proc. ACM-GECCO, pp 913-920, 2008.
- Nacim Belkhir, Winner ACM-GECCO 2018 **BBComp single-objective** and **expensive single-objective** tracks. Nacim completed his PhD in TAU in 2017 [71], co-supervised by Marc Schoenauer, Johann Dréo and Pierre Savéant (Thalès TRT).

5.1.2. Visibility

- Marc Schoenauer, member of the core team responsible for the *Villani mission* regarding the French strategy on Artifical Intelligence. The mission started Sept. 2017 and the final report was delivered on March 29. 2018.
- Michèle Sebag, elected member of French Académie des Technologies, Apr. 2018.
- Michèle Sebag, chevalière de la Légion d'Honneur, Dec. 2018.

6. New Software and Platforms

6.1. io.datascience

Input Output Data Science
KEYWORDS: Open data - Semantic Web - FAIR (Findable, Accessible, Interoperable, and Reusable)
FUNCTIONAL DESCRIPTION: io.datascience (Input Output Data Science) is the instance of the Linked Wiki platform developed specifically in Paris-Saclay University as part of its Center for Data Science.

The goal of io.datascience: to facilitate the sharing and use of scientific data. The technological concept of io.datascience: the exploitation of semantic web advances, and in particular wiki technologies.

(Findable, Accessible, Interoperable, and Reusable) (Wilkinson, M., and The FAIR Guiding Principles for Scientific Data Management and Stewardship, Nature Scientific Data 2016) io.datascience is both a data sharing platform and a framework for further development. It realizes a practical implementation of FAIR (Findable, Accessible, Interoperable, and Reusable - Wilkinson, M., Nature Scientific Data 2016) principles through a user-centric approach.

- Partners: Border Cloud - Paris Saclay Center for Data Science - Université Paris-Sud
- Contact: Cécile Germain-Renaud
- Publications: Data acquisition for analytical platforms: Automating scientific workflows and building an open database platform for chemical anlysis metadata - A platform for scientific data sharing - TFT, Tests For Triplestores - Une autocomplétion générique de SPARQL dans un contexte multi-services - Certifying the interoperability of RDF database systems - Transforming Wikipedia into an Ontology-based Information Retrieval Search Engine for Local Experts using a Third-Party Taxonomy - The Grid Observatory 3.0 - Towards reproducible research and open collaborations using semantic technologies
- URL: https://io.datascience-paris-saclay.fr/

6.2. Codalab

KEYWORDS: Benchmarking - Competition
FUNCTIONAL DESCRIPTION: Challenges in machine learning and data science are competitions running over several weeks or months to resolve problems using provided datasets or simulated environments. Challenges can be thought of as crowdsourcing, benchmarking, and communication tools. They have been used for decades to test and compare competing solutions in machine learning in a fair and controlled way, to eliminate “inventor-evaluator" bias, and to stimulate the scientific community while promoting reproducible science. See our slide presentation.

As of december 2017 there are 145 public competitions on Codalab and over 10000 users. Some of the areas in which Codalab is used include Computer vision and medical image analysis, natural language processing, time series prediction, causality, and automatic machine learning. Codalab was selected for the million Euro challenge See.4C that was awarded a H2020 EU grant for its organization.

TAU is going to continue expanding Codalab to accommodate new needs. One of our current focus is to support use of challenges for teaching (i.e. include a grading system as part of Codalab) and support for hooking up data simulation engines in the backend of Codalab to enable Reinforcement Learning challenges and simulate interactions of machines with an environment. For the third year, we are using Codalab for student projects. M2 AIC students create mini data science challenges in teams of 6 students. L2 math and informatics students then solve them as part of their mini projects. We are collaborating with RPI (New York, USA) to use this platform as part of a curriculum of medical students. Our PhD. students are involved in co-organizing challenges to expose the research community at large with the topic of their PhD. This helps them formalizing a task with rigor and allows them to disseminate their research.

- Partner: Microsoft
- Contact: Isabelle Guyon
- URL: http://competitions.codalab.org

6.3. Cartolabe

KEYWORD: Information visualization
FUNCTIONAL DESCRIPTION: The goal of Cartolabe is to build a visual map representing the scientific activity of an institution/university/domain from published articles and reports. Using the HAL Database, Cartolabe provides the user with a map of the thematics, authors and articles . ML techniques are used for dimensionality reduction, cluster and topics identification, visualisation techniques are used for a scalable 2D representation of the results.

NEWS OF THE YEAR: Improvement of the graphical interface

- Partners: LRI - Laboratoire de Recherche en Informatique - CNRS
- Contact: Philippe Caillou
- URL: http://www.cartolabe.fr/

7. New Results

7.1. Toward Good AI

7.1.1. Causal Modeling

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag;
Post-docs and PhDs: Olivier Goudet, Diviyan Kalainathan
Collaboration: David Lopez-Paz (Facebook).

The search for **causal models** relies on quite a few hardly testable assumptions, e.g. causal sufficiency [152]; it is a data hungry task as it has the identification of independent and conditionally independent pairs of variables at its core. A new approach investigated through the Cause-Effects Pairs (CEP) Challenge [107] formulates causality search as a supervised learning problem, considering the joint distributions of pairs of variables (e.g. (Age, Salary)) labelled with the proper causation relationship between both variables (e.g. Age "causes" Salary) and learning algorithms apt to learn from distributions have been proposed [109]. An edited book is in preparation [64].

In D. Kalainathan's PhD and O. Goudet's postdoc, the search for causal models has been tackled in the framework of generative networks [44], trained to minimize the Maximum Mean Discrepancy loss; the resulting Causal Generative Neural Network improves on the state of the art on the CEP Challenge. However, due to the shortage of real-world variable pairs for which the causation type is known, the CEP challenge has been enriched using artificial pairs (e.g. considering variations on pairs of entities involved in biological regulatory networks), biasing the causation training process. On-going studies investigate how the use of such artificial pairs (the so-called Mother Distribution) to train a causation model aimed at real pairs can be cast as a domain adaptation problem [97], [78].

An attempt to circumvent the need for a large dataset of variable pairs, sampled for the Mother Distribution, we proposed the Structural Agnostic Model approach [57]. Working directly on the observational data, this global approach implements a variant of the popular adversarial game [97] between a discriminator, attempting to distinguish actual samples from fake ones, obtained by generating each variable, given real values from all others. A sparsity L_1 penalty forces all generators to consider only a small subset of their inpu variables, yielding a sparse causal graph. SAM obtains state-of-the-art performances on synthetic data.

An innovative usage of causal models is for educational training in sensitive domains, such as medicine, along the following line. Given a causal generative model, artificial data can be generated using a marginal distribution of causes; such data will enable students to test their diagnosis inference (with no misleading spurious correlations in principle), while forbidding to reverse-engineer the artificial data and guess the original data. Some motivating applications for causal modeling are described in section 4.1.

7.1.2. Explainability

Participants: Isabelle Guyon, François Landes, Marc Schoenauer, Michèle Sebag.

Causal modeling is one particular method to tackle explainability, and TAU has been involved in other initiatives toward explainable AI systems. Following the LAP (Looking At People) challenges, Isabelle Guyon and co-organizers have edited a book [29] that presents a snapshot of explainable and interpretable models in the context of computer vision and machine learning. Along the same line, they propose an introduction and a complete survey of the state-of-the-art of the explainability and interpretability mechanisms in the context first impressions analysis [56].

The team is also involved in the proposal for the IPL HyAIAI (Hybrid Approaches for Interpretable AI), coordinated by the LACODAM team (Rennes) dedicated to the design of hybrid approaches that combine state of the art numeric models (e.g., deep neural networks) with explainable symbolic models, in order to be able to integrate high level (domain) constraints in ML models, to give model designers information on ill-performing parts of the model, and to provide understandable explanations on its results.

Finally, a completely original approach to DNN explainability might arise from the study of structural glasses (7.2.3), with a parallel to CNNs with rotational invariances, that could become an excellent non-trivial example for developing explainability protocols.

7.1.3. Experimental Validation of the Autonomous Vehicle

Participants: Guillaume Charpiat, Marc Schoenauer; **PhD and Engineers**: Marc Nabhan, Nizham Makhoud, Raphaël Jaiswal
Collaboration: Hiba Hage, Philippe Reynaud, and Yves Tourbier (Renault)

As said (Section 3.1.2, TAU is considering two directions of research related to the certification of MLs. The first direction, toward experimental validation, focuses on the coverage of the datasets (more particularly here, used to train an autonomous vehicle controller), and is the subject of this section, while the second one, related to formal approaches, has just started with the beginning of Julien Girard's PhD and has not yet lead to results.

Statistical guarantees (e.g., less than 10^{-8} failure per hour of operation) are obtained by empirical tests, involving millions of kilometers of driving in all possible road, weather and traffic conditions as well as intensive simulations, the only way to full control of the driving conditions. The validation process thus involves 3 steps: i) making sure that all parts of the space of possible scenarios are covered by experiments/tests with sufficiently fine grain; ii) identify failures zones in the space of scenarios; iii) fix the controller flaws that resulted in these failures.

TAU is collaborating with Renault on steps i) (topic of a one-year POC) and ii) (Marc Nabhan's CIFRE PhD). In both cases, the current target scenario is the insertion of a car on a motorway, the "drosophila" of autonomous car scenarios.

Note that another approach toward experimental robustness is investigated in Nizam Makdoud's PhD (CIFRE Thalès), started in March 2018, where Reinforcement Learning is used to find ways to fool some security system.

Clustering of scenarios A first one-year Proof of Concept (ending Oct. 2018) has demonstrated the feasibility and the usefulness of scenario clustering, assuming the availability of data describing the scenarios, i.e., the trajectories of all vehicles involved. Publicly available datasets (e.g., NGSIM were used in a first step. The difficulties met are the following. Firstly, trajectories are varying-length time series, requiring the use of recurrent NNs or LSTMs. Secondly, a scenario is invariant under permutations of the different vehicles involved; neural architectures are taking inspiration from *social LSTMs* [67]. Lastly, most recorded real-world scenarios are uninteresting (all vehicles drive on in their lanes).

The results of this POC have been duly delivered to Renault, but will remain internal at this point. The follow-up collaboration will explore metrics (in the latent space, or learned via Siamese networks), to complete the clustering in a semi-supervised setting (exploiting human feedback to select "typical" scenarios).

Detection of controller flaws Marc Nabhan's PhD (CIFRE Renault) is concerned with the identification of the conditions of failures of the autonomous car controller. Only simulations are considered here, with one scenario being defined as a parameter setting of the in-house simulator SCANeR. The goal is the detection of as many failures as possible, running as few simulations as possible.

A key difficulty, beside that of getting actual data, is the very low probability of failure.On-going work builds upon TAU expertise in active learning using Monte-Carlo Tree Search [140] and evolutionary optimization, in particular taking inspiration from Novelty Search [121] to focus the exploration on unexplored regions of the scenario space, as well as portfolio optimization and instance-based algorithm selection (see Section 3.3.1).

7.2. Learning to Learn

*7.2.1. Auto-**

Participants: Guillaume Charpiat, Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhDs: Léonard Blier, François Gonard, Zhengying Liu, Herilalaina Rakotoarison, Lisheng Sun, Pierre Wolinski
Collaboration: Vincent Renault (SME Artelys); Olivier Bousquet (Google Zurich), Yann Ollivier (Facebook)

TAU is an active player in the Auto-☆ field, having organized the sixth COSEAL workshop in Paris in September 2018. Furthermore, Auto-☆ studies at TAU investigate several directions.

As discussed in Section 3.3, the most widely used approach is based on meta-features describing datasets, and builds upon past work in the team, such as Nacim Belkhir's PhD defended in 2017 [71], who won a GECCO competition in 2018 (Section 5.1.1), and François Gonard's PhD [11], defended in May 2018: an empirical performance model is built from the meta-features, and used to choose the best algorithm and its parameter configuration for unknown datasets. One key difficulty is to design useful meta-features: taking inspiration from equivariant learning [136] and learning from distributions [124], on-going work aims to learn such meta-features, based on the OpenML archive [153]. This extensive archive reports on the test predictive accuracy obtained by a few hundred algorithm configurations over a few thousand datasets.

Also mentioned in Section 3.3, another popular approach for algorithm selection is collaborative filtering. Active learning was used on top of the CofiRank algorithm for matrix factorization [156], improving the results and the time to solution of the recommendation algorithm [62].

An original approach to Auto-☆, explored in Herilalaina Rakotoarison's PhD, extends and adapts Monte-Carlo Tree Search to explore the structured space of pre-processing + learning algorithm configurations, and gradually determine the best pipeline [40]; the resulting algorithm yields promising results comparatively to AutoSklearn. A difficulty consists in managing the exploration together with the resource allocation (considering subsampled datasets and/or limited computational resources in the early MCTS stages, akin [91]).

Most real-world domains evolve with time, and an important issue in real-world applications is that of life-long learning, as static models can rapidly become obsolete. An extension of AutoSklearn was proposed, part of Lisheng Sun's PhD, that detects concept drifts and corrects the current model accordingly [38].

Two on-going works focus on the specific adjustment of hyper-parameters for neural nets, deriving rules for the network architecture (Pierre Wolinski's PhD), or (Leonard Blier's PhD) attaching fixed learning rates to each neuron and calibrating the learning rate distribution in such a way that neurons are sequentially active, learning in an optimally agile manner during a given learning phase, and being stable in later phases.

A last direction of investigation concerns the design of challenges, that contribute to the collective advance of research in the Auto-☆ direction. The team has been very active in the series of AutoML challenges [42], and continuously contributes to the organization of new challenges (Section 7.6).

7.2.2. Deep Learning: Practical Theoretical Insights

Participants: Guillaume Charpiat, Marc Schoenauer, Michèle Sebag
PhDs: Léonard Blier, Corentin Tallec
Collaboration: Yann Ollivier (Facebook AI Research, Paris), the Altschuler and Wu lab. (UCSF, USA)

Even though a full mathematical understanding of deep learning is not available today, theoretical insights from information theory or from dynamical systems can bring significant improvements to practical deep learning algorithms or offer strong explanations for the success of some architectures compared to others.

In [32] we fully derive the LSTM structure from first axiomatic principles, using an axiom of *robustness to temporal deformation (warpings) in the data*. The LSTM architecture, introduced in the 90's, has become the currently dominant architecture for modeling temporal sequences (such as text) in deep learning. But the LSTM architecture itself is quite complex and appears very much ad hoc at first sight. We prove that LSTMs necessarily arise if one wants the model to be able to handle time warpings in the data (such as arbitrary accelerations or decelerations in the signal). In fact, LSTM-like structures are the only way to provide robustness to such deformations: their complex equations can be derived axiomatically.

In [28] (long oral presentation at ICML) we tackle the problem of mode loss in generative models via information theory. The problem is to find generative models to produce more samples similar to samples in a dataset (eg, realistic images). The standard GAN approach is to couple a generative network and an adversary network whose job is to tell the differences between generated and genuine images. This suffers from mode loss: the generator focuses on doing some images well, rather than covering a full variety of images. Instead we propose to have the discriminator predict the proportion of true and fake images in a set of images, via an information theory criterion. This makes the discriminator work at the level of the *overall distribution* of images from the generator rather than individual images. By working on sets of images, the discriminator can detect statistical imbalances between different types of images created by the generator, thus reducing mode loss. An adapted architecture is derived for this, provably able to detect (in principle) all permutation-invariant statistics in a set of images.

In [43] we tackle the problem of recurrent network training via the theory of dynamical systems. Recurrent networks deal with temporal data sequences exhibiting temporal dependencies. Then backpropagation becomes backpropagation through time: for every new data point, training must rewind the network's computations backward in time on all past data to update the model parameters. This is unrealistic in any real-time application where the data arrive online. Two years ago we presented a fully online solution avoiding this "time rewind" step, based on real-time, noisy but unbiased approximations of model gradients. Our previous solution was mathematically well motivated but extremely complex to implement for standard models such as LSTMs. We now have a simpler variant which can be implemented easily in a black-box fashion on top of any recurrent model, and which is just as well-justified mathematically. The price to pay is more variance. In the long run, this could quite extend the applicability range of recurrent model to real-time situations.

In [31][5], we introduce a multi-domain adversarial learning algorithm in the semi-supervised setting. We extend the single source H-divergence theory for domain adaptation to the case of multiple domains, and obtain bounds on the average- and worst-domain risk in multi-domain learning. This leads to a new loss to accommodate semi-supervised multi-domain learning and domain adaptation. We obtain state-of-the-art results on two standard image benchmarks, and propose as a new benchmark a novel bioimage dataset, CELL, in the domain of automated microscopy data, where cultured cells are imaged after being exposed to known and unknown chemical perturbations, and in which each dataset displays significant experimental bias.

7.2.3. Analyzing and Learning Complex Systems

Participants: Cyril Furtlehner, Aurélien Decelle, François Landes
PhDs: Giancarlo Fissore
Collaboration: Jacopo Rocchi (LPTMS Paris Sud), the Simons team: Rahul Chako (post-doc), Andrea Liu (UPenn), David Reichman (Columbia), Giulio Biroli (ENS), Olivier Dauchot (ESPCI).
The information content of a trained restricted Boltzmann machine (RBM) for instance can be analyzed by comparing the singular values/vectors of its weight matrix, referred to as data modes, to that of a random RBM (typically following a Marchenko-Pastur distribution) [83]. The general strategy here is to replace the analysis of the learning process of a single instance by that of a well chosen statistical ensemble of models. In G. Fissore's PhD, the learning trajectory of an RBM is shown to start with a linear phase recovering the dominant modes of the data, followed by a non-linear regime where the interaction among the modes is characterized [15]. While the mean-field analysis conducted in closed form requires simplifying assumptions, it suggests some simple heuristics to speed up the convergence and to simplify the models. Ongoing works

[5] to be presented at ICLR 2019

concern extensions of these considerations to settings with missing input on the practical side and to the analysis of exactly solvable RBM - i.e. non-linear RBM for which the contrastive divergence can be computed in closed forms - on the theoretical side. Additionnally, we are collaborating with J. Rocchi, working at the LPTMS (Univ. Paris Sud), to investigate the landscape of RBMs learned from different initial conditions and to characterized it as a function of the number of parameters (hidden nodes) of the system.

A long standing application of our aforementioned mean-field inference methods based on probabilistic modelling concerns road traffic forecasting. In [49] we wrap up some of the techniques developed in these past works and perform, thanks to PTV-SISTeMA comprehensive experimental tests on various real world Urban traffic dataset in order to illustrate in various conditions the effectiveness of our method. As a by-product we show to some extent how to disentangle the model bias from errors caused by corrupted data and shed some light on the nature of the data themselves.

An emerging research topic, that we started to investigate thanks to exchanges with Lenka Zdeborova's group [96], is to revisit the Information Bottleneck framework [151] and analyze on non-toy NNs the gradual distillation of the mutual information (MI) along the NN layers, minimizing the MI with the input while preserving the MI with the sought output (the labels). More generally, information theory concepts could also be used to analyze the behavior of the network, for instance to detect adversarial attacks through unusual neural activity mapping.

As mentioned earlier, the use of ML to address fundamental physics problems is quickly growing. One example is the domain of glasses (how the structure of glasses is related to their dynamics), which is one of the major problems in modern theoretical physics. The idea is to let ML models automatically find the hidden structures (features) that control the flowing or non-flowing state of matter, discriminating liquid from solid states. These models could then help identifying "computational order parameters", that would advance the understanding of physical phenomena, on the one hand, and support the development of more complex models, on the other hand. Furthermore, this problem is new to the ML community and could provide an original non-trivial example for engineering, testing and benchmarking explainability protocols.

7.3. Computational Social Sciences

Computational Social Sciences (CSS) is making significant progress in the study of social and economic phenomena thank to the combination of social science theories and new insight from data science. But while the simultaneous advent of massive data and massive computational power has opened exciting new avenues, it has also raised new questions and challenges.

Almost ten years after the first enthusiasms for "big data" in social science, P. Tubaro has undertaken a reflective effort to look back at progress made so far and at directions for the near future. She edited a special issue of *Revue Française de Sociologie* on the effects of data both on society itself and on the scientific disciplines that engage with it [46], of which she co-authored the introduction [13].

Meanwhile, four data-based studies are being conducted in TAU, about labor (hiring, working on Internet, quality of life and economic performance), about nutrition (health, food, and socio-demographic issues), around Cartolabe, a platform for scientific information system and visual querying and around GAMA, a multi-agent based simulation platform.

7.3.1. Labor Studies

Participants: Philippe Caillou, Isabelle Guyon, Michèle Sebag, Paola Tubaro
Post-docs; PhDs: Olivier Goudet; François Gonard, Diviyan Kalainathan, Thomas Schmitt
Collaboration: Jean-Pierre Nadal (EHESS); Marco Cuturi, Bruno Crépon (ENSAE); Antonio Casilli (Telecom); Thierry Weil (Mines); Jean-Luc Bazet (RITM)

A first area of activity of TAU in Computational Social Sciences is the study of labor, from the functioning of the job market, to the rise of new, atypical forms of work in the networked society of internet platforms, and the quality of life at work.

Job markets Our first study in the domain of job markets (Th. Schmitt's and F. Gonard's PhDs [12], [11]) tackled the matching of job ads and CVs. This study, funded by the Lidex *Institut de la Société Numérique* (ISN) at Univ. Paris-Saclay, was conducted in collaboration with EHESS, on data provided by the hiring Web agency Qapa (for blue-collars and temporary jobs) and by Association Bernard Gregory (for scientists in industry). Among other difficulties, this study revealed that for both qualified and unqualified job sectors, job seekers and recruiters do not speak the same language [143]. This first study will be continued and extended along two directions: counterfactual analysis (*What would be my options if I had this additional skill ?* DATAIA project Vadore, coll. ENSAE and Pôle Emploi), and the recommendation of vocational training (BPI-PIA contract JobAgile, coll. EHESS and Qapa). Both projects start end 2018.

The platform economy and digital labor Another topic concerns the digital economy and the transformations of labor that accompany the current developments of AI. P. Tubaro has researched the so-called "sharing economy" and ideals of social change associated to the economic model of the platform [33]. However, the platform economy is also disrupting traditional industries. CNRS's MITI office has funded a research on the effects of online services for the restaurant sector (such as La Fourchette, Trip Advisor, Yelp) on working conditions and quality of service. This project involves P. Tubaro, P. Caillou and partners at Telecom ParisTech and Paris Dauphine University.

Ongoing research is exploring online platform labor and its linkages to the development of AI. In collaboration with A.A. Casilli (Telecom ParisTech), P. Tubaro has received funding to conduct research on this topic from the Union Force Ouvrière (OPLa project), from France Stratégie (a Prime Minister's service), and from MSH Paris-Saclay (DiPLab project). A recent grant from DARES (French Ministry of Labor) will enable exploring labor changes in B2B platforms (with O. Chagny of IRES, a unions-funded think-tank).

Quality of life at work. A study, funded by ISN, examined the relationship between the quality of life at work (QLW), and the economic performance of companies [113]. The management and economics literature has already established a correlation between QLW and economic performance [76]. The question that we are currently addressing regards the direction of causality: do profitable companies pay more attention to the QLW ? Or do companies paying attention to QLW tend to be more profitable ? This project (coll. RITM Univ. Paris-Sud, SES Telecom ParisTech, Ecole des Mines, La Fabrique de l'Industrie) combines data at the individual level (DARES, Ministère du Travail) and at the company level (Secafi); cutting-edge causality algorithms are applied to address the question, and handle confounder variables such as the sector of activity.

7.3.2. Health, food, and socio-demographic issues

Participants: Philippe Caillou, Michèle Sebag, Paola Tubaro
Post-docs; PhDs: Nayat Sanchez-Pi
Collaboration: Louis-Georges Soler, Olivier Allais (INRA)

Another area of activity concerns the relationships between eating practices, socio-demographic features and health.

The Nutriperso project (IRS Univ. Paris-Saclay, coll. INRA, CEA, CNRS, INSERM, Telecom ParisTech and Univ. Paris-Sud) aims to: i) determine the impact of food items on health (e.g., related to T2 diabetes); ii) identify alternative food items, admissible in terms of taste and budget, and better in terms of health; iii) emit personalized food recommendations (noting that general recommendations such as *Eat 5 fruit and vegetable per day* are hardly effective on the targeted populations. Based on the Kantar database, reporting the food habits of 20,000 households over 20 years, our challenge is to analyze the food purchases at an unprecedented fine-grained scale (at the barcode level), and to investigate the relationship between diets, socio-demographic features, and body mass index (BMI). The challenge also regards the direction of causality; while some diets are strongly correlated to high BMI, the question is to determine whether, e.g., sugar-free sodas are a cause, or a consequence of obesity, or both.

Previous research in this area included the study of eating disorders and their relationship to people's social network and usages of technology [18].

7.3.3. Scientific Information System and Visual Querying

Participants: Philippe Caillou, Michèle Sebag
Engineer: Anne-Catherine Letournel, Jonas Renault
Collaboration: Jean-Daniel Fekete (AVIZ, Inria Saclay)

A third area of activity concerns the 2D visualisation and querying of the scientific expertise in an institute/university, based on their scientific production, given as a set of articles (authors, title, abstract). The Cartolabe project started as an Inria ADT (coll. TAO and AVIZ, 2015-2017). It received a grant from CNRS (coll. TAU, AVIZ and HCC-LRI, 2018-2019). Further extension proposals, in collaboration with the department of bibliometry from Univ. Paris-Saclay, are under submission at the time of writing.

This project was initially devised as an open-source platform, aimed to answer burning questions, as the growth of academic organization prevents anyone from having a precise knowledge of who does what in the organization: Who is expert in a topic (described as a bag of words)? How are topics related? What are the rising topics? (see also Section 6.3)

Its development and the interaction with the beta-user scientists using it, increasingly raises new questions at the crossroad of human-centered computing, data visualization and machine learning: How to deal with poly-thematic researchers? How to take advantage of the fact that researchers have ideas about their relevant scientific neighborhood, and learn person-dependent metric?

7.3.4. Multi-Agent based simulation framework for social science

Participants: Philippe Caillou
Collaboration: Patrick Taillandier (INRA), Alexis Drogoul and Nicolas Marilleau (IRD), Arnaud Grignard (MediaLab, MIT), Benoit Gaudou (Université Toulouse 1)

Since 2008, P. Caillou contributes to the development of the GAMA platform, a multi-agent based simulation framework. Its evolution is driven by the research projects using it, which makes it very well suited for social sciences studies and simulations.

The 1.8 version of the platform[20] brings new capabilities required for social science research, such as High Performance Computing to explore the simulation, Co-Modeling to link projects, advanced agent architectures to model complex behaviors and advanced visualization to display nice 3D representations for exploration and presentations.

7.4. Energy Management

7.4.1. Power Grids Daily Management

Participants: Isabelle Guyon, Marc Schoenauer
PhDs: Benjamin Donnot, Balthazar Donon, Herilalaina Rakotoarison
Collaboration: Antoine Marot, Patrick Panciatici (RTE), Olivier Teytaud (Facebook)

In the context of the Power Grid safety (Benjamin Donnot's CIFRE PhD with RTE, to be defended in February 2019), the goal is to assess in real time the so-called "(n-1)" safety (see Section 4.2) of possible recovery actions after some problem occurred somewhere on the grid. However, the simulator that allows to compute the power flows in the whole network is far too slow to simulate in real time all n-1 possible failures. A simplified simulator is also available, but its accuracy is too poor to give any good result. Deep surrogate models can be trained off-line, based on the results of the slow simulator, with high0enough accuracy, but training as many models as possible failures (i.e., n-1), obviously doesn't scale up: the topology of the grid must be an input of the learned model, allowing to instantly compute the power flows at least for grid configurations close to the usual running state of the grid. A standard approach is the one-hot encoding of the topology, where n additional boolean inputs are added to the neural network, encoding the presence or absence of each line. An original "guided dropout" approach was proposed [24], in which the topology directly acts on the connections of the deep network: a missing line suppresses some connections. However, whereas the standard dropout method disconnect random connections for every batch, in order to improve the generalization capacity of the network, the "guided dropout" method removes some connections based on the actual topology of the network. THis approach is experimentaly validated against the above-mentionned approaches on small subsets of the French grid (up to 308 lines). Interestingly, and rather suprisingly, even though only examples with a single disconnected line are used in the training set, the learned model is able of some additive generalization, and predictions are also accurate enough in the case 2 lines are disconnected. The guided dropout approach was later robustified [23] by learning to rapidly rank higher order contingencies including all pairs of disconnected lines, in order to prioritize the cases where the slow simulator is run: Another neural network is trained to rank all (n-1) and (n-2) contingencies in decreasing order of presumed severity.

7.4.2. Local Grids Optimization, and the Modeling of Worst-case Scenarios

Participants: Isabelle Guyon, Marc Schoenauer, Michèle Sebag
PhDs: Victor Berger, Herilalaina Rakotoarison; **Post-doc**: Berna Batu
Collaboration: Vincent Renaut (Artelys)

One of the goals of the ADEME Next project, in collaboration with SME Artelys (see also Section 4.2), is the sizing and capacity design of regional power grids. Though smaller than the national grid, regional and urban grids nevertheless raise scaling issues, in particular because many more fine-grained information must be taken into account for their design and predictive growth.

Provided accurate predictions of consumption (see below), off-the-shelf graph optimization algorithms can be used. Berna Batu is gathering different approaches, while Herilalaina Rakotoarison's PhD is concerned with the automatic tuning of their parameters (see Section 7.2.1, and his original approach, at the moment applied to standard benchmarks [40], as well as to Artelys' home optimizer at large Knitro, and compared to the state-of-the-art in parameter tuning (confidential deliverable).

In order to get accurate consumption predictions, V. Berger's PhD tackles the identification of the peak of energy consumption, defined as the level of consumption that is reached during at least a given duration with a given probability, depending on consumers (profiles and contracts) and weather conditions. The peak identification problem is currently tackled using Monte-Carlo simulations based on consumer profile- and weather-dependent individual models, at a high computational cost. The challenge is to exploit individual models to train a generative model, aimed to sampling the collective consumption distribution in the quantiles with highest peak consumption.

7.5. Data-driven Numerical Modelling

7.5.1. High Energy Physics

Participants: Cécile Germain, Isabelle Guyon
PhD: Victor Estrade, Adrian Pol
Collaboration: D. Rousseau (LAL), M. Pierini (CERN)

The role and limits of simulation in discovery is the subject of V. Estrade's PhD, specifically uncertainty quantification and calibration, that is how to handle the systematic errors, arising from the differences ("known unknowns") between simulation and reality, coming from uncertainty in the so-called nuisance parameters. In the specific context of HEP analysis, where relatively numerous labelled data are available, the problem is at the crosspoint of domain adaptation and representation learning. We have investigated how to directly enforce the invariance w.r.t. the nuisance in the sought embedding through the learning criterion (tangent back-propagation) or an adversarial approach (pivotal representation). The results [25] contrast the superior performance of incorporating a priori knowledge on a well separated classes problem (MNIST data) with a real case setting in HEP, in relation with the Higgs Boson Machine Learning challenge [66]. More indirect approaches based on either incorporating variance reduction for the parameter of interest or constraining the representation in a variational auto-encoder farmework are currently considered.

Anomaly detection is the subject of A. Pol PhD. Reliable data quality monitoring is a key asset in delivering collision data suitable for physics analysis in any modern large-scale high energy physics experiment. [60] focuses on supervised and semi-supervised methods addressing the identification of anomalies in the data collected by the CMS muon detectors. The combination of DNN classifiers capable of detecting the known anomalous behaviors, and convolutional autoencoders addressing unforeseen failure modes has shown unprecedented efficiency, compared either to production solution or classical anomaly detection (one-class or I-Forest). The result has been included in the production suite of the CMS experiment at CERN.

The highly visible TrackML challenge is described in section 7.6.

7.5.2. Remote Sensing Imagery

Participants: Guillaume Charpiat
Collaboration: Yuliya Tarabalka, Armand Zampieri, Nicolas Girard, Pierre Alliez (Titane team, Inria Sophia-Antipolis)

The analysis of satellite or aerial images has been a long-time ongoing topic of research, but the remote sensing community moved only very recently to a principled vision of the tasks in a machine learning perspective, with sufficiently large benchmarks for validation. The main topics are the segmentation of (possibly multispectral) remote sensing images into objects of interests, such as buildings, roads, forests, etc., and the detection of changes between two images of the same place taken at different moments. The main differences with classical computer vision is that images are large (covering whole countries, typically cut into 5000×5000 pixels tiles), containing many small, potentially similar objects (and not one big object per image), that every pixel needs to be annotated (w.r.t. assigning a single label to a full image), and that the ground truth is often not reliable (spatially mis-registered, missing new constructions).

This year, deep learning techniques took over classical approaches in most labs, adapting neural network architectures to the specifics of the tasks. This is due notably to the creation of several large scale benchmarks (including one by us [127] and, soon after, larger ones by GAFAM). A still ongoing issue is the ability to generalize across datasets (as urban and rural areas look different in different parts of the world, or even within the same country, e.g. roof types in France).

The task of segmenting satellite images comes together with the one of their registration with cadastral maps. Indeed, the ground truth in remote sensing benchmarks (cadastral maps) is often imperfect, due to spurious deformations. We tackle this issue by *learning* how to register images of different modalities (RGB pictures vs. binary cadastral maps). If one tries to predict, given an RGB photography and an associated cadastral map, the deformation that warps one onto the other, by outputting a 2D vector field indicating the predicted displacement of each pixel (which can be as large as ± 32 px), then the problem considered is too hard (32×32 possibilities for each pixel 2D displacement vector). Instead, we simplifly the problem by decomposing it in a cascade of increasing resolutions. The idea is that if one zooms out by a factor 32, while knowing that the maximum possible displacement is of magnitude 32 px, then at this low resolution one has to move pixels by at most 1 pixel. Learning the task at this low resolution is thus easy. When it is done, if we zoom in by a factor 2, thus reaching a resolution lower than the original one by a factor 16, then the maximum displacement is again of 1 pixel (since larger displacements have been dealt with at the previous scale). And so on. In the end, we train a multi-scale chain of neural networks (double U-nets) [34], and later combine it with a segmentation task [27] in order to benefit from multi-task training, known to improve results.

7.5.3. Space Weather Forecasting

Participants: Cyril Furtlehner, Michèle Sebag
PhD: Mandar Chandorkar
Collaboration: Enrico Camporeale (CWI)

Space Weather is broadly defined as the study of the relationships between the variable conditions on the Sun and the space environment surrounding Earth. Aside from its scientific interest from the point of view of fundamental space physics phenomena, Space Weather plays an increasingly important role on our technology-dependent society. In particular, it focuses on events that can affect the performance and reliability of space-borne and ground-based technological systems, such as satellite and electric networks that can be damaged by an enhanced flux of energetic particles interacting with electronic circuits.[6]

Since 2016, in the context of the Inria-CWI partnership, a collaboration between TAU and the Multiscale Dynamics Group of CWI aims to long-term Space Weather forecasting. The project is extremely timely, as the huge amount of (freely available) space missions data has not yet been systematically exploited in the current computational methods for space weather. Specifically, the goal is to take advantage of the data produced everyday by satellites surveying the sun and the magnetosphere, and more particularly to relate solar images and the quantities (e.g., electron flux, proton flux, solar wind speed) measured on the L1 libration point between the Earth and the Sun (about 1,500,000 km and 1 hour time forward of Earth). The project is very ambitious: the accurate prediction of e.g., geomagnetic storms, or solar wind speed from solar images, would represent a giant leap in the field. A challenge is to formulate such goals in terms of supervised learning problem, while the "labels" associated to solar images are recorded at L1 (thus with a varying and unknown time lag). In essence, while typical ML models aim to answer the question *What*, our goal here is to answer both questions *What* and *When*. Concerning the prediction of solar wind impacting earth magnetosphere from solar images, we encountered an interesting sub-problem related to the non deterministic travel time of a solar eruption to earth's magnetosphere. We have formalized it as the joint regression task of predicting the magnitude of signals as well as the time delay with respect to their driving phenomena and provided a solution tested on synthetic data.

7.5.4. Genomic Data and Population Genetics

Participants: Guillaume Charpiat, Flora Jay
PhD: Théophile Sanchez
Collaboration: TIMC-IMAG (Grenoble), Estonian Biocentre (Institute of Genomics, Tartu, Estonia)

Thanks to the constant improvement of DNA sequencing technology, large quantities of genetic data should greatly enhance our knowledge about evolution and in particular the past history of a population. This history can be reconstructed over the past thousands of years, by inference from present-day individuals: by comparing their DNA, identifying shared genetic mutations or motifs, their frequency, and their correlations at different genomic scales. Still, the best way to extract information from large genomic data remains an open problem; currently, it mostly relies on drastic dimensionality reduction, considering a few well-studied population genetics features.

On-going work at TAU, around Théophile Sanchez' PhD, co-supervised by G. Charpiat and Flora Jay, aims at extracting information from genomic data using deep neural networks; the key difficulty is to build flexible problem-dependent architectures, supporting transfer learning and in particular handling data with variable size. In collaboration with the Bioinfo group at LRI, we designed new generic architectures, that take into account DNA specificities for the joint analysis of a group of individuals, including its variable data size aspects [141]. In the short-term these architectures can be used for demographic inference; the longer-term goal is to integrate them in various systems handling genetic data (e.g., epidemiological statistics) or other biological sequence data. In collaboration with the Estonian Biocentre (Tartu, Estonia), applications will consider thousands of sequenced human genomes, and expand our knowledge of the past human history. To this aim Burak Yelmen (PhD student at the Estonian Biocentre) will visit the lab from February to April 2019. Indeed, TAU expertise regarding the methodologies of exploiting missing and noisy data, and the resulting modeling biases, can contribute to enhance these novel population genetics methods, particularly so for methods heavily relying on simulated data (thus potentially suffering from the *reality gap*).

[6] After a recent survey conducted by the insurance company Lloyd's, an extreme Space Weather event could produce up to $2.6 trillion in financial damage.

We also contributed to tess, a method for fast inference of population genetic structure, through a collaboration with TIMC-IMAG. This method analyses SNP data and estimates the admixture coefficients (that is, the probability that an individual belongs to different groups given the genetic data) via matrix factorization. The observed high dimensional genetic data are reduced automatically via the rank-k approximation of the matrix factorization and thereby highlight the latent structure of the data: the matrix factorization scores correspond to the admixture coefficients while the loadings give the genetic characteristics of each cluster. This method is faster than the hierarchical Bayesian models that we had previously developed and hence well suited for large NGS data. We participated in the tess3 R package, that implements this algorithm, facilitates the visualization of population genetic structure and the projection on maps [14]. We are currently adapting closely related algorithms to enable dimension reduction of temporal data with an application to paleogenomics.

7.5.5. Sampling molecular conformations

Participants: Guillaume Charpiat
PhD: Loris Felardos
Collaboration: Jérôme Hénin (IBPC), Bruno Raffin (InriAlpes)

Numerical simulations on massively parallel architectures, routinely used to study the dynamics of biomolecules at the atomic scale, produce large amounts of data representing the time trajectories of molecular configurations. The configuration space is high-dimensional (10,000+), hindering the use of standard data analytics approaches. The use of advanced data analytics to identify intrinsic configuration patterns could be transformative for the field.

The high-dimensional data produced by molecular simulations live on low-dimensional manifolds; the extraction of these manifolds will enable to drive detailed large-scale simulations further in the configuration space. Among the possible options are i) learning a parameterization of the local, low-dimensional manifold and performing a geometric extrapolation of the molecule trajectories; ii) learning a coarse description of the system and its dynamics, supporting a fast prediction of its evolution. In both cases, the states estimated from the time- or configuration-simplified models will be used for steering large scale simulations, thus accelerating the sampling of stable molecular conformations.

This task will be tackled by combining manifold learning (to find a relevant low-dimensional representation space) and reinforcement learning (for the efficient exploration of the space), taking inspiration from Graph Neural Networks [86]. On-going studies use Graph Auto-encoders to extract a meaningful representation of the conformation of molecules and to predict dynamics.

7.5.6. Storm trajectory prediction

Participants: Mo Yang, Guillaume Charpiat
Collaboration: Claire Monteleoni, Sophie Giffard-Roisin (LAL / Boulder University), Balazs Kegl (LAL)

Cyclones, hurricanes or typhoons all designate a rare and complex event characterized by strong winds surrounding a low pressure area. Their trajectory and intensity forecast, crucial for the protection of persons and goods, depends on many factors at different scales and altitudes. Additionally storms have been more numerous since the 1990s, leading to both more representative and more consistent error statistics.

Currently, track and intensity forecasts are provided by numerous guidance models. Dynamical models solve the physical equations governing motions in the atmosphere. While they can provide precise results, they are computationally demanding. Statistical models are based on historical relationships between storm behavior and other parameters [82]. Current national forecasts are typically driven by consensus methods able to combine different dynamical models.

Statistical models perform poorly compared to dynamical models, although they rely on steadily increasing data resources. ML methods have scarcely been considered, despite their successes in related forecasting problems [160]. A main difficulty is to exploit spatio-temporal patterns. Another difficulty is to select and merge data coming from heterogeneous sensors. For instance, temperature and pressure are real values on a 3D spatial grid, while sea surface temperature or land indication rely on a 2D grid, wind is a 2D vector field, while many indicators such as geographical location (ocean, hemisphere...) are just real values (not fields), and displacement history is a 1D vector (time). An underlying question regards the *innate* vs *acquired* issue, and how to best combine physical models with trained models. On-going studies, conducted in collaboration with S. Giffard-Roisin and C. Monteleoni (now Univ. Boulder), outperform the state-of-the-art in many cases [26], [36], [35].

7.5.7. Analyzing Brain Activity

Participants: Guillaume Charpiat
Collaboration: Hugo Richard, Bertrand Thirion (Parietal team, Inria Saclay / CEA)

With the goal of understanding brain functional architecture, the brain activity of ten subjects is recorded by an fMRI scanner, while they are watching movies (sequences of short pieces of real movies). The analysis of the ensuing complex stimulation streams proceeds by extracting relevant features from the stimuli and correlating the occurrence of these features with brain activity recorded simultaneously with the presentation of the stimuli. The analysis of video streams has been carried in [87] or [108] using a deep convolutional network trained for image classification. The question is then to build good descriptors of videos, possibly involving motion.

We consider a deep neural network trained for action recognition on the largest dataset available [115], and use its activations as descriptors of the input video. This provides deep representations of the watched movies, from an architecture that relies either on optical flow, or on image content, or both simultaneously. We then train a linear model to predict brain activity from these features. From the different layers of the deep neural networks, we build video representations that allow us to segregate (1) occipital and lateral areas of the visual cortex (reproducing the results of [108] and (2) foveal and peripheric areas of the visual cortex. We also introduce an effi- cient spatial compression scheme for deep video features that allows us to speed up the training of our predictive algorithm [41]. We show that our compression scheme outperforms PCA by a large margin.

7.6. Challenges

Participants: Cécile Germain, Isabelle Guyon, Michèle Sebag
PhD: Zhengying Liu, Lisheng Sun
Collaboration: D. Rousseau (LAL), Andre Elisseeff (Google Zurich), Jean-Roch Vilmant (CERN)

Following the highly successful ChaLearn **AutoML** Challenges (NIPS 2015 – ICML 2016 [106] – PKDD 2018 [45]), the **AutoDL** challenge [37], to be run in 2019, addresses the problem of tuning the hyperparameters of Deep Neural Networks, including the topology of the network itself. Co-sponsored by Google Zurich, it will require participants to upload their code on the Codalab platform.

In conjunction with AutoDL, we will organize a challenge in computer vision called **AutoCV**, to promote automatic machine learning for video processing, in collaboration with University of Barcelona. This will make use of the TAU GPU cluster.

Part of the HEP activities of the team, **TrackML** [30], [61] first phase was run and co-sponsored by Kaggle, until September 2018. The second phase is presently running on Codalab, and will end in March 2019. The challenge has been presented at WCCI [61] and NIPS [30]. I. Guyon and C. Germain are in the organizing committee, and M. Schoenauer is member of the Advisory Committee. The TAU team, in collaboration with CERN, has taken a leading role in stimulating both the ML and HEP communities to address the combinatorial complexity explosion created by the next generation of particle detectors.

Beyond the LAP (Looking At People) series of challenges (see details and references in Section 3.4), the domain of autonomous analysis of human behavior from multimodal information has recently gained momentum. We have been involved in two Special Issues dedicated to these topics, *The Computational Face*, in PAMI [17], and *Apparent Personality Analysis*, in IEEE Trans. on Affective Computing [16]. Two other challenges were organized at ICPR 2018, one about the information fusion task in the context of multi-modal image retrieval in social media, the other one regarding the inference of personality traits from written essays, including textual and handwritten information [29].

The **HADACA** project (EIT Health) aims to run a series of challenges to promote and encourage innovations in data analysis and personalized medicine. The data challenges will gather transdisciplinary instructors (researchers and professors), students, and health professionals (clinicians). The outcome of the data challenges should provide: i) analytical frameworks to bridge the gap between large dataset and personalized medicine in disease treatments and ii) innovative pedagogical methods to sensitize students to big data analysis in health. As a synergistic activity, TAU is also engaged in a collaboration with the Rensselaer Polytechnic Institute (RPI, New-York, USA) to use challenges in the classroom, as part of their health-informatics curriculum.

The **L2RPN** (Learning to Run a Power Network) project (coll. RTE) [39] addresses the difficult problem of using Reinforcement Learning to assist human operator in their daily tasks of maintaining the French Ultra-High Voltage grid safety while routing power without interruption. We are collaborating with O. Pietquin (Google Brain) to firm up the challenge protocol, largely inspired by AlphaGo and other RL challenges, like the NIPS 2017 “Learning to run” challenge.

It is important to introduce **challenges in ML teaching**. This has been done (and is on-going) in I. Guyon’s Licence and Master courses: some assignments to Master students are to design small challenges, which are then given to Licence students in labs, and both types of students seem to love it. Along similar line, F. Landes proposed a challenge in the context of S. Mallat’s course, at Collège de France.

8. Bilateral Contracts and Grants with Industry

8.1. Bilateral Contracts with Industry

TAU will continue TAO policy about technology transfer, accepting any informal meeting following industrial requests for discussion (and we are happy to be too much solicited), and deciding about the follow-up based upon the originality, feasibility and possible impacts of the foreseen research directions, provided they fit our general canvas. This lead to the following 5 on-going CIFRE PhDs, with the corresponding side-contracts with the industrial supervisor, plus 3 other bilateral contracts. In particular, we now have a first “Affiliate” partner, the SME DMH, and hope to further develop in the future this form of transfer. Note that it can also sometimes lead to collaborative projects, as listed in the following sections.

- **CIFRE RTE** 2015-2018 (72 kEuros), with Réseau Transport d’Electricité, related to Benjamin Donnot’s CIFRE PhD
  Coordinator: Olivier Teytaud (until May 2016), then Isabelle Guyon, and Antoine Marot (RTE)
  Participants: Benjamin Donnot, Marc Schoenauer
- **Myndblue**, 2017-2018 (1 an, 50kEuros) related to consulting activities with DMH (Digital for Mental Health)[7].
  Coordinator: Aurélien Decelle and Simon Moulieras (DMH)
  Participants: Michèle Sebag
- **Contrat LFI** 2017-2018 (30kEuros), with La Fabrique de l’Industrie, related to quality of life at work (Section 7.3.1).
  Coordinator: Michèle Sebag and Thierry Weil (La Fabrique de l’Industrie)

[7] This “Affiliate” contract has been inspired by the affiliate program of Technion

Participants: Olivier Goudet, Diviyan Kalainathan

- **POC Renault** 2017-2018 (125 kEuros), *Clusterisation et optimisation de scenarii pour la validation des véhicules autonomes*
  Coordinator: Marc Schoenauer and Philippe Reynaud (Renault)
  Participants: Guillaume Charpiat, Raphaël Jaiswal (engineer), Marc Schoenauer
- **CIFRE Renault** 2017-2020 (45 kEuros), related to Marc Nabhan's CIFRE PhD *Sûreté de fonctionnement d'un véhicule autonome - évaluation des fausses détections au travers d'un profil de mission réduit*
  Coordinator: Marc Schoenauer and Hiba Hage (Renault)
  Participants: Marc Nabhan (PhD), Yves Tourbier (Renault)
- **OPLa** 2017-2018, Organizing Platform Labor (27k euros), funded by Force Ouvrière.
  Coordinator: A.A. Casilli (Telecom ParisTech)
  Participants: Paola Tubaro
- **DiPLab** 2017-2018, Digital Platform Labor (24k euros), funded by MSH Paris-Saclay.
  Coordinators: Paola Tubaro (avec A.A. Casilli, Telecom ParisTech)
- **CIFRE Thalès** 2018-2021 (45 kEuros), with Thales Teresis, related to Nizam Makdoud's CIFRE PhD
  Coordinator: Marc Schoenauer and Jérôme Kodjabatchian
  Participants: Nizam Makdoud
- **CIFRE RTE** 2018-2021 (72 kEuros), with Réseau Transport d'Electricité, related to Balthazar Donon's CIFRE PhD
  Coordinator: Isabelle Guyon and Antoine Marot (RTE)
  Participants: Balthazar Donon, Marc Schoenauer
- **CIFRE FAIR** 2018-2021 (45 kEuros), with Facebook AI Research, related to Leonard Blier's CIFRE PhD
  Coordinator: Marc Schoenauer and Yann Olliver (Facebook)
  Participatns: Guillaume Charpiat, Michèle Sebag, Léonard Blier
- **Google Zurich** 2018 (50kEuros), related to the **AutoDL** (see Section 3.4)
  Coordinator: Isabelle Guyon and Olivier Bousquet (Google)
  Participants: Zhengying Liu and Lisheng Sun
- **IFPEN** (Institut Français du Pétrole Energies Nouvelles) 2018-2022 (300 kEuros), to hire an Inria Starting Research Position (PhD + 4-6 years) to work in all topics mentioned in Section 3.2 relevant to IFPEN activity (see also Section 4.2).

9. Partnerships and Cooperations

9.1. National Initiatives

9.1.1. ANR

- **ACTEUR** 2014-2018 (236kEuros). Cognitive agent development for urban simulations,
  Coordinator: P. Taillandier (IDEES, Univ Rouen)
  Participant: Philippe Caillou
- **EPITOME** 2017-2020 (225kEuros), *Efficient rePresentatIon TO structure large-scale satellite iMagEs* (Section 7.5.2).
  Coordinator: Yuliya Tarabalka (Titane team, Inria Sophia-Antipolis)
  Participant: Guillaume Charpiat

9.1.2. Others

- **E-LUCID** 2014-2018 (194 kEuros), anomaly detection in network packets.
  Coordinator: Thales Communications & Security S.A.S
  Participants: Marc Schoenauer, Cyril Furtlehner, Luis Marti (until 12/2017)
- **Nutriperso** 2017-2020, 87 kEuros. Personalized recommendations toward healthier eating practices (Section 7.3.2).
  U. Paris-Saclay IRS (*Initiative de Recherche Stratégique*)
  Partners: INRA (coordinator), INSERM, Agro Paristech, Mines Telecom
  Participants: Philippe Caillou, Flora Jay, Michèle Sebag, Paola Tubaro
- **PIA Adamme** 2015-2018 (258 kEuros) Machine Learning on a mass-memory architecture.
  Coordinator: Bruno Farcy (Bull SAS)
  Participants: Marc Schoenauer, Guillaume Charpiat, Cécile Germain-Renaud, Yasmina Bouzbiba, Etienne Brame
- **NEXT** 2017-2021 (675 kEuros). Simulation, calibration, and optimization of regional or urban power grids (Section 4.2).
  ADEME (Agence de l'Environnement et de la Maîtrise de l'Energie)
  Coordinator: ARTELYS
  Participants Isabelle Guyon, Marc Schoenauer, Michèle Sebag, Victor Berger (PhD), Herilalaina Rakotoarison (PhD), Berna Bakir Batu (Post-doc)
- **DATAIA Vadore** 2018-2020 (105 kEuros) VAlorizations of Data to imprOve matching in the laboR markEt, with CREST (ENSAE) and Pôle Emploi (Section 7.3.1).
  Coordinator: Michèle Sebag
  Participants: Philippe Caillou, Isabelle Guyon
- **PIA JobAgile** 2018-2021 (379 kEuros) *Evidence-based Recommandation pour l'Emploi et la Formation* (Section 7.3.1).
  Coordinator: Michèle Sebag and Stéphanie Delestre (Qapa)
  Participants: Philippe Caillou, Isabelle Guyon
- **HADACA** 2018-2019 (50 kEuros), within EIT Health, for the organization of challenges toward personalized medicine (Section 7.6).
  Coordinator: Magali Richard (Inria Grenoble)
  Participants: Isabelle Guyon
- **IPL HPC-BigData** 2018-2022 (100 kEuros) High Performance Computing and Big Data (Section 7.5.5)
  Coordinator: Bruno Raffin (Inria Grenoble)
  Participants: Guillaume Charpiat, Loris Felardos (PhD)

9.2. European Initiatives

9.2.1. Collaborations with Major European Organizations

MLSpaceWeather 2015-2019. Coupling physics-based simulations with Artificial Intelligence (Section 7.5.3).
Coordinator: CWI
Participants: Aurélien Decelle, Cyril Furtlehner, Michèle Sebag

9.3. International Initiatives

9.3.1. Inria International Labs

IIL CWI-Inria
Associate Team involved in the International Lab:

9.3.1.1. MDG-TAO

Title: Data-driven simulations for Space Weather predictions

International Partner (Institution - Laboratory - Researcher):

CWI (Netherlands) - Multiscale Dynamics Group - Enrico Camporeale

Start year: 2017

See also: http://pages.saclay.inria.fr/cyril.furtlehner/html/mdg-tao.html and Section 7.5.3.

We propose an innovative approach to Space Weather modeling: the synergetic use of state-of-the-art simulations with Machine Learning and Data Assimilation techniques, in order to adjust for errors due to non-modeled physical processes, and parameter uncertainties. We envision a truly multidisciplinary collaboration between experts in Computational Science and Data assimilation techniques on one side (CWI), and experts in Machine Learning and Data Mining on the other (Inria). Our research objective is to realistically tackle long-term Space Weather forecasting, which would represent a giant leap in the field. This proposal is extremely timely, since the huge amount of (freely available) space missions data has not yet been systematically exploited in the current computational methods for Space Weather. Thus, we believe that this work will result in cutting-edge results and will open further research topics in space Weather and Computational Plasma Physics.

9.3.2. Inria International Partners

9.3.2.1. Declared Inria International Partners

Isabelle Guyon partner of Google Zurich *Preparation of a competition AutoDL: Automatic Deep Learning*. See Section 7.6.

9.3.2.2. Informal International Partners

Marc Schoenauer partner of the ARC-DP (Australian Research Council Discovery Project) *Bio-inspired computing methods for dynamically changing environments*. Coordinator: University of Adelaide (Frank Neumann), 5 years from Nov. 2015, 400 k$-AUS. Visit to Adelaide: 2 weeks in Feb. 2017, 2 weeks planned in 2019.

Isabelle Guyon Partner of UC Berkeley *Fingerprint verification with deep siamese neural networks using ultratonic sensor data.* Co-advisor of a master student (Baiyu Chen). Partners: Alyosha Efros, Bernhard Boser.

Guillaume Charpiat partner of Boulder University *Hurricane trajectory prediction*. Co-advisor of a master student (Mo Yang). Partners: Sophie Giffard-Roisin, Claire Monteleoni. See Section 7.5.6.

10. Dissemination

10.1. Promoting Scientific Activities

10.1.1. Scientific Events Organisation

10.1.1.1. General Chair, Scientific Chair

Guillaume Charpiat Workshop Statistics/Learning at Paris-Saclay 2018

Isabelle Guyon Competition co-chair, ECML 2019

Michele Sebag Séminaire Annuel Académie des Technologies, 2018.

In 2016, Isabelle Guyon was Program Chair of NIPS (Neural Information Processing Systems) – with an increase of more than 40% in the number of submissions, 96% in terms of reviewers, and over 100% in terms of attendees as compared to the previous year. Lessons learned from the review process are described in a JMLR paper [19].

10.1.1.2. Member of Organizing Committees

Isabelle Guyon Advisory committee BayLearn 2018; Co-organizer WCCI 2018 Special Session on Intelligent Power Systems; Co-organizer WCCI 2018 Special Session on Machine Learning and Deep Learning Methods applied to Vision and Robotics (MLDLMVR); Co-organizer ECCV 2018 workshop Chalearn Looking at People: Inpainting and Denoising in the Deep Learning Age; Co-organizer 2018 Multimedia Information Processing for Personality & Social Networks Analysis Workshop at ICPR; Co-organizer NeurIPS 2018 workshop on Challenges in Machine Learning;

Marc Schoenauer Steering Committee, Parallel Problem Solving from Nature (PPSN); Steering Committee, Learning and Intelligent OptimizatioN (LION); organizer (with Herilalaina Rokotoarison), Workshop COSEAL, Paris, Sept. 17-18, 2018.

Michele Sebag President of Steering Committee, Eur. Conf. on Machine Learning and Principles and Practice of Knowledge Discovery in Databases (ECML-PKDD).

10.1.2. Scientific Events Selection

10.1.2.1. Member of Conference Program Committees

All TAU members are members of the Program Committees of the main conferences in their respective fields of expertise.

10.1.2.2. Reviewer

All TAU member review papers for the most prestigious conferences in their respective fields of expertise.

10.1.3. Journal

10.1.3.1. Member of the Editorial Boards

Isabelle Guyon Action editor, *Journal of Machine Learning Research* (JMLR); series editor, *Springer series Challenges in Machine Learning* (CiML).

Marc Schoenauer Advisory Board, *Evolutionary Computation Journal*, MIT Press, and *Genetic Programming and Evolutionary Machines*, Springer Verlag; Action editor, *Journal of Machine Learning Research*(JMLR).

Michèle Sebag Editorial Board, Machine Learning, Springer Verlag.

Paola Tubaro Associate Editorial Board, *Sociology*, Sage; Member of Editorial Board, *Revue Française de Sociologie*, Presses de Sciences Po.

10.1.3.2. Reviewer - Reviewing Activities

All members of the team reviewed numerous articles for the most prestigious journals in their respective fields of expertise.

10.1.4. Invited Talks

Guillaume Charpiat *Introduction aux réseaux de neurones*, Séminaire Parisien de Mathématiques Appliquées à l'Imagerie, Paris, 3 May. 2018; *Recalage et mise à jour d'images à l'aide de réseaux de neurones*, Journée Extraction d'attributs et apprentissage pour l'analyse des images de télédétection, GDR ISIS, Paris, 18 Oct. 2018.

Flora Jay *Deep Learning Methods for Population Genetics: Inferring Changes Population Size*, Journée Inférences évolutives, GDR GE et AEIM, Paris, 16 Mai 2018; *Inferring past history from genetic data using ABC and Deep Learning approaches*, INRA GenPhySE Seminar, Toulouse, 12 Dec. 2018.

Isabelle Guyon *Codalab: crowdsourcing DataIA* DATAIA Institute Kick-Off (Data Science, Intelligence & Society), 15 Feb. 2018; *Contests of contests*, La Recherche scientifique « hors murs » au 21e siècle, Colloque de l'Académie des sciences, Fondation Del Duca, 29 Nov. 2018; *Evaluating causation coefficients*, NeurIPS 2018 workshop on causal learning, 7 Dec, 2018.

Michèle Sebag *Qualité de la vie et santé économique, étude causale*: Colloque de Cerisy (Sept. 18); séminaire Université Québec à Montréal (Dec. 18); *Causal Modeling*: KAUST Conference on Computational and Statistical Interface to Big Data (Mar. 18); Leiden wshop on Space Weather (2018); *MonteCarlo Tree Search for Algorithm Selection and Calibration*: Dagstuhl Seminar (Sept. 18); NIPS Wshop on AutoML (Dec. 18); *Ingénieures et Scientifiques*, ENPC (Juin 18). Exposés Journées Cabourg, Mar. 18; Rennes, Sep. 18; Toulouse, Oct. 18.

Marc Schoenauer *The Villani mission on Artificial Intelligence*, CISCO Heaadquarters, 9 Apr. 2018; *Le rapport Villani*, journée AFIA, 12 Apr. 2018; *Intelligence Artificielle : le rapport Villani*, Journée de la Recherche de l'Université de Brest, 25 May 2018; *Intelligence Artificielle, mythes et réalités*, Colloque Grands Projets et Systemes Complexes, Arcachon, 18 Jun. 2018; *Intelligence Artificielle, mythes et réalités*, Journée lab. CRISTAL (U. Lille), Gand, 6 Jul. 2018; *Shallow and Deep learning at TAU*, Keynote at the DATAIA-JST International Symposium on Data Science and AI, 10 Jul. 2018; *Une brève introduction à l'Intelligence Artificielle et au rapport Villani*, Académie des Technologies, 10 Oct. 2018; *Une brève introduction à l'Intelligence Artificielle*, Open-Lab PSA, 11 Oct. 2018; *A brief introduction to AI and Deep Learning*, Toulouse Symposium on Deep Learning, 18 oct. 2018; *A brief introduction to AI and Deep Learning*, PSA Stellab Seminar, Paris, 14 nov. 2018; *IA, une stratégie française : le rapport Villani*, Université Franco Italienne, Università Italo Francese, annual seminar, Paris, 21 Nov. 2018; *Some issues with Deep Learning*, Inria / Nokia-Bell Labs seminar, 27 Nov. 2018; *L'Intelligence Artificielle hier, aujourd'hui et demain*, 29e journée CASCIMODOT, Orléans, 12 Dec. 2018.

Paola Tubaro *Un champ de mines? Éthique, droit et politique dans la recherche sur les réseaux sociaux*, conférence MARAMI (Modèles & Analyse des Réseaux : Approches Mathématiques & Informatiques), Avignon, 17 Oct. 2018; *Modèles multi-agents et simulation*, Ecole thématique CNRS "Réseaux et complexité", 28 Sept. 2018; *Microworking in France: an inquiry into the human labour that makes AI possible*, OECD, Paris, 5 Dec. 2018; *Micro-work, artificial intelligence and the automotive industry*, Sant'Anna School of Advnced Studies, Pisa, 31 May 2018; *Online platform labor*, EIT Digital, Rennes, 14 Nov. 2018; *Les promesses et les périls du travail sur plateformes*, France Stratégie, 6 July 2018; *Faut-il interdire la parole problématique en ligne ?*, GEPS medical conference, Montpellier, 12 Jan. 2018

10.1.5. Leadership within the Scientific Community

Isabelle Guyon President and co-founder of ChaLearn, a non-for-profit organization dedicated to the organization of challenge.

Marc Schoenauer Chair of ACM-SIGEVO (Special Interest Group on Evolutionary Computation), 2015-2017, re-elected July 2017 (2-years term); Founding President (since 2015) of SPECIES (Society for the Promotion of Evolutionary Computation In Europe and Surroundings), that organizes the yearly series of conferences *EvoStar*.

Michèle Sebag Elected Chair of Steering Committee, ECML-PKDD; Head of the Research Programme, Institut de Convergence DataIA.

Paola Tubaro Convenor of the Social Network Analysis Group of British Sociological Association; co-founder of European Network on Digital Labor.

10.1.6. Scientific Expertise

Cécile Germain Evaluator for the H2020-2016-CNECT program; member of the DFG review panel within Germany's excellence strategy selection process.

Marc Schoenauer Member, Villani Mission on Artificial Intelligence [50] (see also the AIforHumanity Web Site); Conseil scientifique, MoveInSalcay platform, coordinated by Nokia-Bell Labs; Comité Scientifique IA, SCube (Scientipôle Savoirs & Société), Orsay; Scientific Committee, TrackML (see Section 7.6); Comité de sélection, Chaire ABEONA-ENS "Biais et Equité en IA"; Conseil Scientifique, Fondation de Recherche pour l'Aéronautique et l'Espace (FRAE).

Michèle Sebag Jury de sélection, LRI; ENS-Lyon; LIX-Ecole Polytechnique; LORIA; Univ. Dortmund; Univ. Liège. Evaluation NSERC, Canada.

10.1.7. Research Administration

Cécile Germain University officer for scientific computing; member of the Board of the Lidex *Center for Data Science*; member of the scientific council of faculty of Medicine (UPsud).

Isabelle Guyon Representative of UPSud in the DataIA *Institut de Convergence* Program Committee, University of Paris-Saclay.

Marc Schoenauer Deputy Scientific Director of Inria (in French, Directeur Scientifique Adjoint, DSA), in charge of AI.

Michele Sebag Deputy director of LRI, CNRS UMR 8623; elected member of the Research Council of Univ. Paris-Saclay; member of the STIC department council of Univ. Paris-Saclay; member of the Scientific Council of Labex AMIES, Applications des Mathématiques ds l'Industrie, l'Entreprise et la Société; member of the Scientific Council of IRT System'X; member of the CSFRS (Conseil supérieur de la formation et de la recherche stratégique).

Paola Tubaro Representative of CNRS in the DataIA *Institut de Convergence* Program Committee, University of Paris-Saclay; member of the Board, Maison des Sciences de l'Homme Paris-Saclay.

10.2. Teaching - Supervision - Juries

10.2.1. Teaching

Licence : Philippe Caillou, Computer Science for students in Accounting and Management, 192h, L1, IUT Sceaux, Univ. Paris Sud.

Licence : Aurélien Decelle, Computer Architecture, 26h, L2, Univ. Paris-Sud.

Licence : Aurélien Decelle, Introdution to Machine Learning, 57h, L2, Univ. Paris-Sud.

Licence : Aurélien Decelle, Object-oriented programming , 26h, L2, Univ. Paris-Sud.

Licence : Aurélien Decelle, Computer Architecture, 26h, L3, Univ. Paris-Sud.

Licence : François Landes, Mathematics for Computer Scientists, 51h, L2, Univ. Paris-Sud.

Licence : François Landes, Machine Learning and Artificial Life, 48h, L2, Univ. Paris-Sud.

Licence and Polytech : Cécile Germain, Computer Architecture

Licence : Isabelle Guyon, Project: Resolution of mini-challenges (created by M2 students), L2, Univ. Paris-Sud.

Master : François Landes, Machine Learning, 22h, M1 Polytech, U. Paris-sud.

Master : Guillaume Charpiat and Victor Berger, Advanced Machine Learning, 34h, M2 Recherche, Centrale-Supélec.

Master : Guillaume Charpiat, Introduction to Deep Learning, 6h, M2 Recherche, Telecom.

Master : Aurélien Decelle, Machine Learning, 26h, M1, Univ. Paris-Sud.

Master : Aurélien Decelle, Probability and statistics, 26h, M1, Univ. Paris-Sud.

Master : Cécile Germain, Parallel Programming

Master : Isabelle Guyon, Project: Creation of mini-challenges, M2, Univ. Paris-Sud.

Master : Michèle Sebag, Machine Learning, 12h; Deep Learning, 9h; Reinforcement Learning, 12h; M2 Recherche, U. Paris-sud. Summer School Deep Learning, Genova (Italy), 5h.

Master : François Landes, Machine Learning, 9h, M2 Recherche, U. Paris-sud.

Master : Paola Tubaro, Start -up project for engineering students, 24h, Telecom ParisTech.

Master : Paola Tubaro, Sociology of social networks, 24h, M2, EHESS/ENS.

Master : Flora Jay, Population Genetics, 10h, M2, Univ. Paris-Sud.

Doctorate: Paola Tubaro, Research Methods, 12h, University of Insubria, Italy.

10.2.2. Supervision

PhD François GONARD, *Cold-start recommendation : from Algorithm Portfolios to Job Applicant Matching*, Université Paris-Saclay, May 2018

PhD Thomas SCHMITT, *Collaborative Matching of Job Openings and Job Seekers*, Université Paris-Saclay, June 2018

PhD Hoang M. LUONG, *Squaring the Circle in Modelling Corporate Governance, Market Structure and Innovation: A Tobin's Q Approach to R&D Investment when Network Effects Are Present*, Paola Tubaro, with M. Ugur and S. Gorgoni, University of Greenwich, London, UK, Oct. 2018.

PhD in progress Eléonore BARTENLIAN, *Deep Learning pour le traitement du signal*, 1/10/2018, Michèle Sebag and Frédéric Pascal (Centrale-Supélec)

PhD in progress Victor BERGER, *Variational Anytime Simulator*, 1/10/2017, Michèle Sebag

PhD in progress Leonard BLIER, *Vers une architecture stable pour les systèmes d'apprentissage par renforcement*, 1/09/2018, Yann Ollivier (Facebook AI Research, Paris) and Marc Schoenauer

PhD in progress Tony BONNAIRE, *Reconstruction de la toile cosmique*, from 1/10/2018, Nabila Aghanim (Institut d'Astrophysique Spatiale) and Aurélien Decelle

PhD in progress Benjamin DONNOT, *Optimisation et méthodes d'apprentissage pour une conduite robuste et efficace du réseau électrique par anticipation sur base de parades topologiques.*, 1/09/2015, Isabelle Guyon and Antoine Marot (RTE)

PhD in progress Balthazar DONON, *Apprentissage par renforcement pour une conduite stratégique du système électrique*, 1/10/2018, Isabelle Guyon and Antoine Marot (RTE)

PhD in progress Guillaume DOQUET, *ML Algorithm Selection and Domain Adaptation*, 1/09/2015, Michele Sebag

PhD in progress Victor ESTRADE *Robust domain-adversarial learning, with applications to High Energy Physics,* 01/10/2016, Cécile Germain and Isabelle Guyon.

PhD in progress Loris FELARDOS, *Neural networks for molecular dynamics simulations*, 1/10/2018, Guillaume Charpiat, Jérôme Hénin (IBPC) and Bruno Raffin (InriAlpes)

PhD in progress Giancarlo FISSORE, *Statistical physics analysis of generative models*, 1/10/2017, Aurélien Decelle and Cyril Furtlehner

PhD in progress Julien GIRARD, *Vérification et validation des techniques d'apprentissage automatique*, 1/10/2018, Zakarian Chihani (CEA) and Guillaume Charpiat

PhD in progress Diviyan KALAINATHAN, *Causal models and quality of life at work*, 1/10/2017, Michèle Sebag and Isabelle Guyon

PhD in progress Zhengying LIU, *Automation du design des reseaux de neurones profonds*, 1/10/2017, Isabelle Guyon

PhD in progress Nizam MAKDOUD, *Motivations intrinsèques en apprentissage par renforcement. Application à la recherche de failles de sécurité*, 1/02/2018, Marc Schoenauer and Jérôme Kodjabachian (Thalès ThereSIS, Palaiseau).

PhD in progress Marc NABHAN, *Sûreté de fonctionnement d'un véhicule autonome - évaluation des fausses détections au travers d'un profil de mission réduit*, 1/10/2017, Marc Schoenauer and Hiba Hage (Renault)

PhD in progress Anna PIAZZA, *Inter-Organisational Relationships and Organisational Performance: Network Analysis Applications to a Health Care System*, 01/09/2014, Paola Tubaro, with F. Pallotti and A. Lomi, at the University of Greenwich, London, UK

PhD in progress Adrian POL *Machine Learning Anomaly Detection, with application to CMS Data Quality Monitoring,* 01/10/2016, Cécile Germain.

PhD in progress Herilalaina RAKOTOARISON, *Automatic Algorithm Configuration for Power Grid Optimization*, 1/10/2017, Marc Schoenauer and Michèle Sebag

PhD in progress Théophile SANCHEZ, *Reconstructing the past: deep learning for population genetics*, 1/10/2017, Guillaume Charpiat and Flora Jay

PhD in progress Lisheng SUN, *Apprentissage Automatique: Vers une analyse de données automatisé*, 1/10/2016, Isabelle Guyon and Michèle Sebag

PhD in progress Corentin TALLEC, *Reinforcement Learning and Recurrent Neural Networks: Dynamical approaches*, 1/10/2016, Yann Ollivier

PhD in progress Marion ULLMO, *Detection et classification de la toile et des filaments cosmiques*, from 1/10/2018, Nabila Aghanim (Institut d'Astrophysique Spatiale) and Aurélien Decelle

PhD in progress Pierre WOLINSKI, *Learning the Architecture of Neural Networks*, 1/9/2016, Yann Ollivier (Facebook AI Research, Paris) and Guillaume Charpiat

10.2.3. Juries

- Guillaume Charpiat As a member of the “Commission Scientifique" of Inria Saclay: selection committee for post-docs and PhD students hiring; jury of the Gilles Khan PhD prize (SIF); jury for a “Maître de conférence” position at Université Paris-Sud.
- Cécile Germain PhD jury for Mehdi Cherti 26/01/18, Wenjie ZHENG, 13/06/2018; jury of the Telecom PhD prize 23/03/2018
- Isabelle Guyon PhD jury for Giorgos Borboudakis, 21 Nov. 2018, University of Crete, Heraklion, Greece; Master thesis jury for Marvin Lerousseau, 28 June 2018, INP Grenoble; Master thesis jury for Adrien Pavao, 5 Sep. 2018, U.P-Sud, Orsay.
- Michèle Sebag PhD reviewer: Antonio Vergari (Univ. Bari, Italy); Gaétant Hadjeres, LIX, Ecole Polytechnique; Romain Warlop, Univ. Lille. Pdt Jury: Hafiz Tiomoko, Centrale-Supélec; Stanislas Chambon, Telecom.
- Marc Schoenauer PhD jury for Wen SUN, Université d'Angers, 29/11/2018;
- Paola Tubaro PhD jury for Victorien Barbet, Aix-Marseille Université, 13/12/2018.

10.3. Popularization

10.3.1. Articles and contents

Isabelle Guyon

- Pionnière : Isabelle Guyon, professeur à l'université de Paris-Saclay, 7 Feb. 2018, Usine Nouvelle

- Isabelle Guyon veut démocratiser l'intelligence artificielle, Apr. 2018, Le Monde
- Portrait : Isabelle Guyon, sélectionneuse d'algorithmes, 16 May 2018, Industries et Technologie

Paola Tubaro *Notre vie privée, un concept négociable* [52], Antonio Casilli and Paola Tubaro, in *Le Monde*, Jan. 2018.

10.3.2. Interventions

Guillaume Charpiat Séminaire d'Actualité Critique, *L'intelligence artificielle, entre fantasmes et recherche*, ENS Paris, 5 Apr. 2018.

Isabelle Guyon *Codalab, createur de defis*, UniThe ou Café, Inria Saclay, 5 Apr. 2018

Marc Schoenauer

- Congrès Européen Ethique et Gouvernance 2018, OCDE, Paris, 30 Mar. 2018;
- Audition publique sur l'Intelligence Artificielle et le travail, Comité économique et social européen (CESE), Bruxelles, 30 May 2018;
- Public debate with Jean-Marc David, Convention Systematic, 5 Jun. 2018; Conférence Legrain, ENS Paris, 5 Jul. 2018;
- Prix Design et Science de l'Université Paris-Saclay, 11 Oct. 2018.

Michèle Sebag Usine Nouvelle; Podcast Science et Avenir, discussion avec Cédric Villani.

11. Bibliography

Major publications by the team in recent years

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[3] C. FURTLEHNER, A. DECELLE. *Cycle-based Cluster Variational Method for Direct and Inverse Inference*, in "Journal of Statistical Physics", August 2016, vol. 164, n^o^ 3, pp. 531–574, https://hal.inria.fr/hal-01214155

[4] S. GELLY, M. SCHOENAUER, M. SEBAG, O. TEYTAUD, L. KOCSIS, D. SILVER, C. SZEPESVARI. *The Grand Challenge of Computer Go: Monte Carlo Tree Search and Extensions*, in "Communications- ACM", 2012, vol. 55, n^o^ 3, pp. 106-113, https://hal.inria.fr/hal-00695370

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[6] T. LUCAS, C. TALLEC, J. VERBEEK, Y. OLLIVIER. *Mixed batches and symmetric discriminators for GAN training*, in "ICML - 35th International Conference on Machine Learning", Stockholm, Sweden, July 2018, https://hal.inria.fr/hal-01791126

[7] E. MAGGIORI, Y. TARABALKA, G. CHARPIAT, P. ALLIEZ. *Convolutional Neural Networks for Large-Scale Remote Sensing Image Classification*, in "IEEE Transactions on Geoscience and Remote Sensing", 2017, vol. 55, n° 2, pp. 645-657, https://hal.inria.fr/hal-01369906

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[9] Y. OLLIVIER, L. ARNOLD, A. AUGER, N. HANSEN. *Information-Geometric Optimization Algorithms: A Unifying Picture via Invariance Principles*, in "Journal of Machine Learning Research", 2017, vol. 18, n° 18, pp. 1-65, https://hal.inria.fr/hal-01515898

[10] X. ZHANG, C. FURTLEHNER, C. GERMAIN-RENAUD, M. SEBAG. *Data Stream Clustering with Affinity Propagation*, in "IEEE Transactions on Knowledge and Data Engineering", 2014, vol. 26, n° 7, 1 p. , https://hal.inria.fr/hal-00862941

Publications of the year

Doctoral Dissertations and Habilitation Theses

[11] F. GONARD. *Cold-start recommendation : from Algorithm Portfolios to Job Applicant Matching*, Université Paris-Saclay, May 2018, https://tel.archives-ouvertes.fr/tel-01825220

[12] T. SCHMITT. *Collaborative Matching of Job Openings and Job Seekers*, Université Paris-Saclay, June 2018, https://tel.archives-ouvertes.fr/tel-01886623

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