## RESEARCH CENTRE

Inria Centre at Université Grenoble Alpes

IN PARTNERSHIP WITH: CNRS, Université de Grenoble Alpes

## 2023 ACTIVITY REPORT

# Project-Team STATIFY

## Bayesian and extreme value statistical models for structured and high dimensional data

IN COLLABORATION WITH: Laboratoire Jean Kuntzmann (LJK)

## DOMAIN

Applied Mathematics, Computation and Simulation

## THEME

Optimization, machine learning and statistical methods



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## **Project-Team STATIFY**

Creation of the Project-Team: 2020 April 01

## Keywords

### Computer sciences and digital sciences

- A3.1.1. Modeling, representation
- A3.1.4. Uncertain data
- A3.3.2. Data mining
- A3.3.3. Big data analysis
- A3.4.1. Supervised learning
- A3.4.2. Unsupervised learning
- A3.4.4. Optimization and learning
- A3.4.5. Bayesian methods
- A3.4.7. Kernel methods
- A5.3.3. Pattern recognition
- A5.9.2. Estimation, modeling
- A6.2. Scientific computing, Numerical Analysis & Optimization
- A6.2.3. Probabilistic methods
- A6.2.4. Statistical methods
- A6.3. Computation-data interaction
- A6.3.1. Inverse problems
- A6.3.3. Data processing
- A6.3.5. Uncertainty Quantification
- A9.2. Machine learning
- A9.3. Signal analysis

## Other research topics and application domains

- B1.2.1. Understanding and simulation of the brain and the nervous system
- B2.6.1. Brain imaging
- B3.3. Geosciences
- B3.4.1. Natural risks
- B3.4.2. Industrial risks and waste
- B3.5. Agronomy
- B5.1. Factory of the future
- B9.5.6. Data science
- B9.11.1. Environmental risks

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## 2 Overall objectives

The STATIFY team focuses on statistics. Statistics can be defined as a science of variation where the main question is how to acquire knowledge in the face of variation. In the past, statistics were seen as an opportunity to play in various backyards. Today, the statistician sees his own backyard invaded by data scientists, machine learners and other computer scientists of all kinds. Everyone wants to do data analysis and some (but not all) do it very well. Generally, data analysis algorithms and associated network architectures are empirically validated using domain-specific datasets and data challenges. While winning such challenges is certainly rewarding, statistical validation lies on more fundamentally grounded bases and raises interesting theoretical, algorithmic and practical insights. Statistical questions can be converted to probability questions by the use of probability models. Once certain assumptions about the mechanisms generating the data are made, statistical questions can be answered using probability theory. However, the proper formulation and checking of these probability models is just as important, or even more important, than the subsequent analysis of the problem using these models. The first question is then how to formulate and evaluate probabilistic models for the problem at hand. The second question is how to obtain answers after a certain model has been assumed. This latter task can be more a matter of applied probability theory, and in practice, contains optimization and numerical analysis.

The STATIFY team aims at bringing strengths, at a time when the number of solicitations received by statisticians increases considerably because of the successive waves of *big data, data science* and *deep learning*. The difficulty is to back up our approaches with reliable mathematics while what we have is often only empirical observations that we are not able to explain. Guiding data analysis with statistical justification is a challenge in itself. STATIFY has the ambition to play a role in this task and to provide answers to questions about the appropriate usage of statistics.

Often statistical assumptions do not hold. Under what conditions then can we use statistical methods to obtain reliable knowledge? These conditions are rarely the natural state of complex systems. The central motivation of STATIFY is to establish the conditions under which statistical assumptions and associated inference procedures approximately hold and become reliable.

However, as George Box said "Statisticians and artists both suffer from being too easily in love with their models". To moderate this risk, we choose to develop, in the team, expertise from different statistical domains to offer different solutions to attack a variety of problems. This is possible because these domains share the same mathematical food chain, from probability and measure theory to statistical modeling, inference and data analysis.

Our goal is to exploit methodological resources from statistics and machine learning to develop models that handle variability and that scale to high dimensional data while maintaining our ability to assess their correctness, typically the uncertainty associated with the provided solutions. To reach this goal, the team offers a unique range of expertise in statistics, combining probabilistic graphical models and mixture models to analyze structured data, Bayesian analysis to model knowledge and regularize ill-posed problems, non-parametric statistics, risk modeling and extreme value theory to face the lack, or impossibility, of precise modeling information and data. In the team, this expertise is organized to target five key challenges:

- 1. Models for high dimensional, multimodal, heterogeneous data;
- 2. Spatial (structured) data science;
- 3. Scalable Bayesian models and procedures;
- 4. Understanding mathematical properties of statistical and machine learning methods;
- 5. The big problem of small data.

The first two challenges address sources of complexity coming from data, namely, the fact that observations can be: 1) high dimensional, collected from multiple sensors in varying conditions *i.e.* multimodal and heterogeneous and 2) inter-dependent with a known structure between variables or with unknown interactions to be discovered. The other three challenges focus on providing reliable and interpretable models: 3) making the Bayesian approach scalable to handle large and complex data; 4) quantifying the information processing properties of machine learning methods and 5) allowing to draw reliable conclusions from datasets that are too small or not large enough to be used for training machine/deep learning methods.

These challenges rely on our four research axes:

- 1. Models for graphs and networks;
- 2. Dimension reduction and latent variable modeling;
- 3. Bayesian modeling;
- 4. Modeling and quantifying extreme risk.

In terms of applied work, we will target high-impact applications in neuroimaging, environmental and earth sciences.

## **3** Research program

#### 3.1 Models for graphs and networks

**Participants:** Jean-Baptiste Durand, Florence Forbes, Julyan Arbel, Sophie Achard, Olivier Francois, Mariia Vladimirova, Lucrezia Carboni, Hana Lbath, Minh-tri Le, Yuchen Bai.

**Keywords:** graphical models, Markov properties, hidden Markov models, clustering, missing data, mixture of distributions, EM algorithm, image analysis, Bayesian inference.

Graphs arise naturally as versatile structures for capturing the intrinsic organization of complex datasets. The literature on graphical modeling is growing rapidly and covers a wide range of applications, from bioinformatics to document modeling, image analysis, social network analysis, *etc.* When faced with multivariate, possibly high dimensional, data acquired at different sites (or nodes) and structured according to an underlying network (or graph), the objective is generally to understand the dependencies or associations present in the data so as to provide a more accurate statistical analysis and a better understanding of the phenomenon under consideration.

Structure learning. This refers to the inference of the existing dependences between variables from observed samples. The limits of obtaining graph edges using sample correlation between nodes is well known. We have investigated alternative approaches, both Bayesian and frequentist, the former were rather used to account for constraints on the structure while for the latter we focused on robust modeling and estimation in presence of outliers. We proposed a fast Bayesian structure learning based on pre-screening of categorical variables, in the PhD thesis of T. Rahier with Schneider Electric. In the continuous variable case, we studied the design of tractable estimators and algorithms that can provide robust estimation of covariance structures. Many covariance estimation methods rely on the Gaussian graphical model but a viable model for data contaminated by outliers requires the use of more robust and complex procedures and is therefore more challenging to build. Then, the problem of robust structure learning is especially acute in the high-dimensional setting, in which the number of variables p is of the same order or is much larger than the number of available observations n. We have investigated different ways to handle both the above mentioned issues, in order to provide models for application such as modeling brain connectivity from functional magnetic resonance imaging (fMRI) data. Each brain region is associated with a time series, and the goal is to study the connectivity among these regions. Interactions between the regions can be described by covariance or precision matrices that quantify the links between time series and can then be represented as graphs. We have first proposed an approach, initiated with the PhD of K. Ashurbekova, to generalize the Gaussian approach to multivariate heavy-tailed distributions with dimensionality relatively larger than the number of observations. This encompasses methods related to shrinkage and M-estimators for which we aimed at designing algorithms with proved convergence results and optimal values for shrinkage coefficients. Second, still motivated by the brain connectivity

application, we have investigated in the PhD of H. Lbath (QFunC project), the possibility to compute more subtle correlations between brain regions using a new notion of correlation of local averages. At last, to go beyond the Gaussian assumption, we also investigated copulas approaches or characterized graphical dependencies for multivariate counts, with potential applications to branching processes.

Structure modelling. Once the structure is identified, the following questions are about comparing the discovered graph structures together, or with regards to a reference graph. If the structure is not itself the object of consideration, the goal is usually to account for it in a subsequent analysis. Except for simple graphs (chains or trees), this is problematic because mainstream statistical models and algorithms are based on the independence assumption and become intractable for even moderate graph sizes. The analysis of graphs as the objects of interest with the design of tools to model and compare them has been studied in the PhD of L. Carboni. We proposed new mathematical tools based on equivalence relation between graph statistics in order to be able to take into account the location in space of the nodes. To account for dependences in a tractable way we often rely on Markov modelling and variational inference. When dependence in time is considered, Gaussian processes are an interesting tractable tool. With the PhD of A. Constantin, we have investigated those in the context of a collaboration with INRAE and CNES in Toulouse, for the classification and reconstruction of irregularly sampled satellite image times series. The proposed approach is able to deal with irregular temporal sampling and missing data directly in the classification process. It is based on Gaussian processes and allows to perform jointly the classification of the pixel labels as well as the reconstruction of the pixel time series. The method complexity scales linearly with the number of pixels, making it amenable in large scale scenario. In a different context, we have developed hidden semi-Markov models for the analysis of eye movements, in particular with the PhD of B. Olivier in collaboration with A. Guérin-Dugué (GIPSA-lab) and B. Lemaire (Laboratoire de Psychologie et Neurocognition). New coupling methods for hidden semi-Markov models driven by several underlying state processes have been proposed.

**Structured anomaly detection.** The vast majority of deep learning architectures for medical image analysis are based on supervised models requiring the collection of large datasets of annotated examples. Building such annotated datasets, which requires skilled medical experts, is time consuming and hardly achievable, especially for some specific tasks, including the detection of small and subtle lesions that are sometimes impossible to visually detect and thus manually outline. This critical aspect significantly impairs performances of supervised models and hampers their deployment in clinical neuroimaging applications, especially for brain pathologies that require the detection of small size lesions (*e.g.* multiple sclerosis, microbleeds) or subtle structural or morphological changes (*e.g.* Parkinson's disease). We have developed unsupervised anomaly detection methods based on generalized Student mixture models and deep statistical unsupervised learning model for the detection of early forms of Parkinson's disease. We have also compared parametric mixture approaches to non parametric machine learning techniques for change detection in the context of time series analysis of glycemic curves for diabetes.

## 3.2 Dimension reduction and latent variable modeling

**Participants:** Jean-Baptiste Durand, Florence Forbes, Stephane Girard, Julyan Arbel, Olivier Francois, Daria Bystrova, Giovanni Poggiato, Geoffroy Oudoumanessah, Louise Alamichel.

**Keywords:** mixture of distributions, EM algorithm, missing data, conditional independence, statistical pattern recognition, clustering, unsupervised and partially supervised learning.

Extracting information from raw data is a complex task, all the more so as this information is measured in a high dimensional space. Fortunately, this information usually lives in a subspace of smaller size. Identifying this subspace is crucial but difficult. One approach is to perform appropriate changes of representation that facilitate the identification and characterization of the desired subspace. Latent random variables are a key concept to encode in a structured way representations that are easier to handle and capture the essential features of the data. **Regression in high dimensions.** Methods adapted to high dimensions include inverse regression methods, *i.e.* SIR, partial least squares (PLS), approaches based on mixtures of regressions with different variants, *e.g.* Gaussian locally linear mapping (GLLiM) and extensions, Mixtures of Experts, cluster weighted models, *etc.* SIR-like methods are flexible in that they reduce the dimension in a way optimal for the subsequent regression task that can itself be carried out by any desired regression tool. In that sense these methods are said to be non parametric or semi-parametric and they have a potential to provide robust procedures. We have also proposed a new approach, called Extreme-PLS, for dimension reduction in conditional extreme values settings where the goal is to best explain the extreme values of the response variable.

**Simulation-based inference (SBI) for high dimensional inverse problems.** To account for uncertainty in a principled manner, we also considered Bayesian inversion techniques. We investigated the use of learning approaches to handle Bayesian inverse problems in a computationally efficient way when the observations to be inverted present a moderately high number of dimensions and are in large number. We proposed tractable inverse regression approaches, based on GLLiM and normalizing flows. They have the advantage to produce full probability distributions as approximations of the target posterior distributions. These distributions have several interesting features. They provide confidence indices on the predictions and can be combined with importance sampling or approximate Bayesian computation (ABC) schemes for a better exploration when multiple equivalent solutions exist. They generalise easily to variants that can handle non Gaussian data, dependent or missing observations. The relevance of the proposed approach has been illustrated on synthetic examples and on two real data applications, in the context of planetary remote sensing and neuroimaging. In addition, we addressed the issue of model selection for some of the GLLiM models, *i.e.* Mixture of experts (MoE) models and contributed to a number of theoretical results.

**Online and incremental inference.** Most SBI methods scale poorly when the number of observations is too large, which makes them unsuitable for modern data, which are often acquired in real time, in an incremental nature, and are often available in large volume. Computation of inferential quantities in an incremental manner may be forcibly imposed by the nature of data acquisition (*e.g.* streaming and sequential data) but may also be seen as a solution to handle larger data volumes in a more resource friendly way, with respect to memory, energy, and time consumption. To produce feasible and practical online algorithms for streaming data and complex models, we have investigated the family of stochastic approximation (SA) algorithms for a certain class of models, *e.g.*, exponential family distributions and their mixtures.

## 3.3 Bayesian modelling

Bayesian methods have become the center of attraction to model the underlying uncertainty of statistical models. Bayesian models and methods are already used in all of our other axes, whenever the Bayesian choice provides interesting features, *e.g.* for model selection, dependence modeling (copulas), inverse problems, *etc.* This axis emphasizes more specifically our theoretical and methodological research in Bayesian learning. In particular, we will focus on techniques referred to as Bayesian nonparametrics (BNP).

Participants:Julyan Arbel, Daria Bystrova, Giovanni Poggiato, Florence Forbes, Jean-<br/>Baptiste Durand, Pedro Coelho Rodrigues, Pierre Wolinski, Konstanti-<br/>nos Pitas, Louise Alamichel, Trung Tin Nguyen, Theo Moins.

**Keywords:** Bayesian statistics, Bayesian nonparametrics, Markov Chain Monte Carlo, Experimental design, Bayesian neural networks, Approximate Bayesian Computation.

**Markov priors for Bayesian nonparametric models.** We have proposed Bayesian nonparametric priors for hidden Markov random fields, first for continuous, Gaussian observations with an illustration in image segmentation. Second, for discrete observed data typically issued from counts, *e.g.* Poisson distributed observations with an illustration on risk mapping model. The inference was done by Variational Bayesian Expectation Maximization (VBEM).

Asymptotic properties of BNP models. A common way to assess a Bayesian procedure is to study the asymptotic behavior of posterior distributions, that is their ability to estimate a true distribution when the number of observations grows. Mixture models have attracted a lot of attention in the last decade due to some negative results regarding the number of clusters. More specifically, it was shown that Bayesian nonparametric mixture models are inconsistent for some choices of priors. We proposed ways to compute the prior distribution of the number of clusters. This is a notoriously difficult task, and we proposed approximations in order to enable such computations for real-world applications. We studied and justified BNP models based on their asymptotic properties. We showed that mixture models based on many different BNP processes are inconsistent in the number of clusters and discuss possible solutions. Notably, we showed that a post-processing algorithm introduced for the simplest process (Dirichlet process) extends to more general models and provides a consistent method to estimate the number of components.

**Amortized Approximate Bayesian computation.** Approximate Bayesian computation (ABC) has become an essential part of the Bayesian toolbox for addressing problems in which the likelihood is prohibitively expensive or entirely unknown. A key ingredient in ABC is the choice of a discrepancy that describes how different the simulated and observed data are, often based on a set of summary statistics when the data cannot be compared directly. The choice of the appropriate discrepancies is an active research topic, which has mainly considered data discrepancies requiring samples of observations or distances between summary statistics. We have first investigated sample-based discrepancies and established new asymptotic results using so-called energy-based distances. We have then considered a summary-based approach and proposed a new ABC procedure that can be seen as an extension of the semi-automatic ABC framework to a functional summary statistics setting and can also be used as an alternative to sample-based approaches. The resulting ABC approach also exhibits amortization properties via the use of the GLLiM inverse regression model.

**Bayesian neural networks.** The connection between Bayesian neural networks and Gaussian processes gained a lot of attention in the last few years, with the flagship result that hidden units converge to a Gaussian process limit when the layers width tends to infinity. Underpinning this result is the fact that hidden units become independent in the infinite-width limit. Our aim is to shed some light on hidden units dependence properties in practical finite-width Bayesian neural networks. In addition to theoretical results, we assessed empirically the depth and width impacts on hidden units dependence properties. Hidden units are proven to follow a Gaussian process limit when the layer width tends to infinity. Recent work has suggested that finite Bayesian neural networks may outperform their infinite counterparts because they adapt their internal representations flexibly. To establish solid ground for future research on finite-width neural networks, our goal is to study the prior induced on hidden units. Our main result is an accurate description of hidden units tails which shows that unit priors become heavier-tailed going deeper, thanks to the introduced notion of generalized Weibull-tail. This finding sheds light on the behavior of hidden units of finite Bayesian neural networks.

## 3.4 Modelling and quantifying extreme risk

Participants:Julyan Arbel, Daria Bystrova, Giovanni Poggiato, Stephane Girard,<br/>Florence Forbes, Pedro Coelho Rodrigues, Pascal Dkengne Sielenou,<br/>Meryem Bousebata, Theo Moins, Pierre Wolinski, Sophie Achard

Keywords: dimension reduction, extreme value analysis, functional estimation.

Extreme events have a major impact on a wide variety of domains from environmental sciences (heat waves, flooding), reliability, to finance and insurance (financial crashes, reinsurance). While usual statistical approaches focus on the modeling of the bulk of the distribution, extreme-value analysis aims at building models adapted to distribution tails, where by nature, observations are rare. Extreme value analysis is a relatively recent domain in statistics focusing on distribution tails.

**Extreme quantile estimation.** One of the most popular risk measures is the Value-at-Risk (VaR) introduced in the 1990's. In statistical terms, the VaR at level  $\alpha \in (0, 1)$  corresponds to the upper  $\alpha$ -quantile of the loss distribution. We have proposed estimators and studied their theoretical properties for extreme quantiles, that is when  $\alpha \rightarrow 0$ . We have also investigated Weissman extrapolation device for estimating extreme quantiles from heavy-tailed distributions. This is based on two estimators: an order statistic to estimate an intermediate quantile and an estimator of the tail-index. The common practice is to select the same intermediate sequence for both estimators. We showed how an adapted choice of two different intermediate sequences leads to a reduction of the asymptotic bias associated with the resulting refined Weissman estimator. This new bias reduction method is fully automatic and does not involve the selection of extra parameters.

**New measures of extreme risk.** A simple way to assess the (environmental, industrial or financial) risk is to compute a measure linked to the value of the phenomena of interest (rainfall height, wind speed, river flow). Candidate measures include quantiles (which correspond to traditional Value at Risk or return levels), expectiles, tail conditional moments, spectral risk measures, distorsion risk measures, *etc.* We have mainly focused on the first two measures, quantiles and expectiles, and investigated estimation procedures for extensions of these measures. The main drawback of quantiles is that they do not provide a coherent risk measure. Two distributions may have the same extreme quantile but very different tail behaviors. Moreover, standard estimators do not use the most extreme values of the sample and consequently induce a loss of information. Our strategy was to adapt the definition of quantiles to take into account the whole distribution tail.

We have introduced new measures of extreme risk based on  $L_p$ - quantiles encompassing both expectiles and quantiles. We believe this generalization of the concept of extreme quantile to extreme  $L_p$ - quantile opens promising new research directions. We have first explored to what extent univariate extreme-value estimators can be improved on the basis of these novel  $L_p$ - quantiles. We built tractable estimators of these quantities with guaranteed theoretical properties.

**Extremes with covariates.** A second challenge was to extend this concept to the regression framework where the variable of interest depends on a set of covariates. When the number of covariates is large, two research directions have been explored to overcome the curse of dimensionality: 1) we designed a dimension reduction method for the extreme-value context, 2) we also considered semi-parametric models to reduce the complexity of the fitted model.

Another challenge with expectiles is that their sample versions do not benefit from a simple explicit form, making their analysis significantly harder than that of quantiles and order statistics. This difficulty is compounded when one wishes to integrate auxiliary information about the phenomenon of interest through a finite-dimensional covariate, in which case the problem becomes the estimation of conditional expectiles. We exploited the fact that the expectiles of a distribution are in fact the quantiles of another distribution explicitly linked to the former one, in order to construct nonparametric kernel estimators of extreme conditional expectiles. We analyze the asymptotic properties of our estimators in the context of conditional heavy tailed distributions. The extension to functional covariates was investigated. Since quantiles and expectiles belong to the wider family of  $L_p$ -quantiles, we also proposed to construct kernel estimators of extreme conditional  $L_p$ -quantiles. We studied their asymptotic properties in the context of conditional heavy-tailed distributions and we showed through a simulation study that taking  $p \in (1,2)$ may allow to recover extreme conditional quantiles and expectiles accurately.

We built a general theory for the estimation of extreme conditional expectiles in heteroscedastic regression models with heavy-tailed noise. Our approach is supported by general results of independent interest on residual-based extreme value estimators in heavy-tailed regression models, and is intended

to cope with covariates having a large but fixed dimension. We demonstrated how our results could be applied to a wide class of important examples, among which linear models, single-index models as well as ARMA and GARCH time series models.

**Extremes and machine learning.** This is the topic of a more recent collaboration with E. Gobet from CMAP. Feedforward neural networks based on Rectified linear units (ReLU) cannot efficiently approximate quantile functions which are not bounded, especially in the case of heavy-tailed distributions. We have thus proposed a new parametrization for the generator of a Generative adversarial network (GAN) adapted to this framework, basing on extreme-value theory. We provided an analysis of the uniform error between the extreme quantile and its GAN approximation. It appears that the rate of convergence of the error is mainly driven by the second-order parameter of the data distribution. A similar investigation has been conducted to simulate fractional Brownian motion with ReLU neural networks.

## 4 Application domains

#### 4.1 Image Analysis

**Participants:** Florence Forbes, Jean-Baptiste Durand, Stephane Girard, Pedro Coelho Rodrigues, Geoffroy Oudoumanessah, Sophie Achard.

As regards applications, several areas of image analysis can be covered using the tools developed in the team. More specifically, in collaboration with team PERCEPTION, we address various issues in computer vision involving Bayesian modelling and probabilistic clustering techniques. Other applications in medical imaging are natural. We work more specifically on MRI and functional MRI data, in collaboration with the Grenoble Institute of Neuroscience (GIN). We also consider other statistical 2D fields coming from other domains such as remote sensing, in collaboration with the Institut de Planétologie et d'Astrophysique de Grenoble (IPAG) and the Centre National d'Etudes Spatiales (CNES). In this context, we worked on hyperspectral and/or multitemporal images. In the context of the "pole de competivité" project I-VP, we worked of images of PC Boards.

#### 4.2 Biology, Environment and Medicine

Participants: Florence Forbes, Stephane Girard, Jean-Baptiste Durand, Julyan Arbel, Sophie Achard, Pedro Coelho Rodrigues, Olivier Francois, Yuchen Bai, Theo Moins, Lucrezia Carboni, Hana Lbath.

A third domain of applications concerns biology and medicine. We considered the use of mixture models to identify biomakers. We also investigated statistical tools for the analysis of fluorescence signals in molecular biology. Applications in neurosciences are also considered. In the environmental domain, we considered the modelling of high-impact weather events and the use of hyperspectral data as a new tool for quantitative ecology.

## 5 Social and environmental responsibility

#### 5.1 Footprint of research activities

The footprint of our research activities has not been assessed yet. Most of the team members have validated the "charte d'éco-responsabilité" written by a working group from Laboratoire Jean Kuntzmann, which should have practical implications in the near future.

## 5.2 Impact of research results

A lot of our developments are motivated by and target applications in medicine and environmental sciences. As such they have a social impact with a better handling and treatment of patients, in particular with brain diseases or disorders. On the environmental side, our work has an impact on geoscience-related decision making with e.g. extreme events risk analysis, planetary science studies and tools to assess biodiversity markers. However, how to truly measure and report this impact in practice is another question we have not really addressed yet.

## 6 Highlights of the year

## 6.1 Awards

Sophie Achard received the silver medal from CNRS in 2023.

## 7 New software, platforms, open data

#### 7.1 New software

7.1.1 Planet-GLLiM

Name: Planet-GLLiM

Keyword: Inverse problem

**Functional Description:** The application implements the GLLiM statistical learning technique in its different variants for the inversion of a physical model of reflectance on spectro-(gonio)-photometric data. The latter are of two types: 1. laboratory measurements of reflectance spectra acquired according to different illumination and viewing geometries, 2. and 4D spectro-photometric remote sensing products from multi-angular CRISM or Pléiades acquisitions.

URL: https://gitlab.inria.fr/kernelo-mistis/planet-gllim-front-end/-/wikis/Home

Publications: insu-03705153, hal-02908364

Contact: Sylvain Douté

Participants: Florence Forbes, Benoit Kugler, Sami Djouadi, Samuel Heidmann, Stanislaw Borkowski

Partner: Institut de Planétologie et d'Astrophysique de Grenoble

#### 7.1.2 Kernelo

Name: Kernelo-GLLiM

Keywords: Inverse problem, Clustering, Regression, Gaussian mixture, Python, C++

- **Scientific Description:** Building a regression model for the purpose of prediction is widely used in all disciplines. A large number of applications consists of learning the association between responses and predictors and focusing on predicting responses for the newly observed samples. In this work, we go beyond simple linear models and focus on predicting low-dimensional responses using high-dimensional covariates when the associations between responses and covariates are non-linear.
- **Functional Description:** Kernelo-GLLiM is a Gaussian Locally-Linear Mapping (GLLiM) solver. Kernelo-GLLiM provides a C++ library and a python module for non linear mapping (non linear regression) using a mixture of regression model and an inverse regression strategy. The methods include the GLLiM model (Deleforge et al (2015) ) based on Gaussian mixtures.

#### URL: https://gitlab.inria.fr/kernelo-mistis/kernelo-gllim-is/-/wikis/home

Publications: hal-00863468, hal-02908364

**Contact:** Florence Forbes

Participants: Florence Forbes, Benoit Kugler, Sami Djouadi, Samuel Heidmann, Stanislaw Borkowski

Partner: Institut de Planétologie et d'Astrophysique de Grenoble

## 8 New results

#### 8.1 Models for graphs and networks

8.1.1 TriadNet: Sampling-free predictive intervals for lesional volume in 3D brain MRI.

Participants: Florence Forbes, Benjamin Lambert, Michel Dojat.

#### Joint work with: Senan Doyle from Pixyl.

The volume of a brain lesion (e.g. infarct or tumor) is a powerful indicator of patient prognosis and can be used to guide the therapeutic strategy. Lesional volume estimation is usually performed by segmentation with deep convolutional neural networks (CNN), currently the state-of-the-art approach. However, to date, few work has been done to equip volume segmentation tools with adequate quantitative predictive intervals, which can hinder their usefulness and acceptation in clinical practice. In this work, we propose TriadNet, a segmentation approach relying on a multi-head CNN architecture, which provides both the lesion volumes and the associated predictive intervals simultaneously, in less than a second. We demonstrate its superiority over other solutions on BraTS 2021, a large-scale MRI glioblastoma image database.

#### 8.1.2 Multi-layer Aggregation as a Key to Feature-Based OOD Detection.

Participants: Florence Forbes, Benjamin Lambert, Michel Dojat.

#### Joint work with: Senan Doyle from Pixyl.

Deep Learning models are easily disturbed by variations in the input images that were not observed during the training stage, resulting in unpredictable predictions. Detecting such Out-of-Distribution (OOD) images is particularly crucial in the context of medical image analysis, where the range of possible abnormalities is extremely wide. Recently, a new category of methods has emerged, based on the analysis of the intermediate features of a trained model. These methods can be divided into 2 groups: single-layer methods that consider the feature map obtained at a fixed, carefully chosen layer, and multi-layer methods that consider the ensemble of the feature maps generated by the model. While promising, a proper comparison of these algorithms is still lacking. In this work, we compared various feature-based OOD detection methods on a large spectra of OOD (20 types), representing approximately 7800 3D MRIs. Our experiments shed the light on two phenomenons. First, multi-layer methods consistently outperform single-layer approaches, which tend to have inconsistent behaviour depending on the type of anomaly. Second, the OOD detection performance highly depends on the architecture of the underlying neural network.

#### 8.1.3 Anisotropic Hybrid Networks for liver tumor segmentation with uncertainty quantification.

Participants: Florence Forbes, Benjamin Lambert, Michel Dojat.

#### Joint work with: Senan Doyle, Pauline Roca from Pixyl.

The burden of liver tumors is important, ranking as the fourth leading cause of cancer mortality. In case of hepatocellular carcinoma (HCC), the delineation of liver and tumor on contrast-enhanced magnetic resonance imaging (CE-MRI) is performed to guide the treatment strategy. As this task is time-consuming, needs high expertise and could be subject to inter-observer variability there is a strong need for automatic tools. However, challenges arise from the lack of available training data, as well as the high variability in terms of image resolution and MRI sequence. In this work we propose to compare two different pipelines based on anisotropic models to obtain the segmentation of the liver and tumors. The first pipeline corresponds to a baseline multi-class model that performs the simultaneous segmentation of the liver and tumor classes. In the second approach, we train two distinct binary models, one segmenting the liver only and the other the tumors. Our results show that both pipelines exhibit different strengths and weaknesses. Moreover we propose an uncertainty quantification strategy allowing the identification of potential false positive tumor lesions. Both solutions were submitted to the MICCAI 2023 Atlas challenge regarding liver and tumor segmentation.

## 8.1.4 Uncertainty-based Quality Control for Subcortical Structures Segmentation in T1-weighted Brain MRI.

**Participants:** Florence Forbes, Benjamin Lambert, Michel Dojat.

Joint work with: Senan Doyle, Alan Tucholka from Pixyl.

Deep Learning (DL) models are presently the gold standard for medical image segmentation. However, their performance may drastically drop in the presence of characteristics in test images not present in the training set. The automatic detection of these Out-Of-Distribution (OOD) inputs is the key to prevent the silent failure of DL models, especially when the visual inspection of the input is not systematically carried out. For MRI segmentation, a wide range of covariables can perturbate a DL model : noise, artifacts or MR sequence parameters. Deterministic Uncertainty Methods (DUM) are novel and promising techniques for OOD detection. They propose to analyze the intermediate activations of a trained segmentation DL model to detect OOD inputs. In a previous study, we demonstrated that DUM achieved high OOD detection performance on a task of Multiple Sclerosis lesions segmentation in T2-weighted FLAIR MRI. To evaluate the generalization capability of this technique, we propose to evaluate DUM in the context of automatic subcortical structures segmentation. We focus our results on the hippocampus and thalamus structures segmentation from T1-weighted MR brain scans of healthy subjects.

## 8.1.5 Brain subtle anomaly detection based on Auto-Encoders latent space analysis: Application to *de novo* Parkinson patients

Participants: Florence Forbes, Geoffroy Oudoumanessah.

**Joint work with**: Michel Dojat from Grenoble Institute of Neurosciences, Carole Lartizien, Nicolas Pinon, Robin Trombetta from Creatis.

Neural network-based anomaly detection remains challenging in clinical applications with little or no supervised information and subtle anomalies such as hardly visible brain lesions. Among unsupervised

methods, patch-based auto-encoders with their efficient representation power provided by their latent space, have shown good results for visible lesion detection. However, the commonly used reconstruction error criterion may limit their performance when facing less obvious lesions. In this work, we design two alternative detection criteria. They are derived from multivariate analysis and can more directly capture information from latent space representations. Their performance compares favorably with two additional supervised learning methods, on a difficult *de novo* Parkinson Disease (PD) classification task.

#### 8.1.6 Estimation of leaf area densities in tropical forests

Participants: Jean-Baptiste Durand, Florence Forbes, Yuchen Bai.

Joint work with: Grégoire Vincent, IRD, AMAP, Montpellier, France.

Covering just 7% of the Earth's land surface, tropical forests play a disproportionate role in the biosphere: they store about 25% of the terrestrial carbon and contribute to over a third of the global terrestrial productivity. They also recycle about a third of the precipitations through evapotranspiration and thus contribute to generate and maintain a humid climate regionally, with positive effects also extending well beyond the tropics. However, the seasonal variability in fluxes between tropical rainforests and atmosphere is still poorly understood. Better understanding the processes underlying flux seasonality in tropical forests is thus critical to improve our predictive ability on global biogeochemical cycles. Leaf area, one key variable controlling water efflux and carbon influx, is poorly characterized. To monitor evolutions of biomass, leaf area density (LAD) or gas exchange, aerial and terrestrial laser scanner (LiDAR) measurements have been frequently used.

The principle is, for different LiDAR shoots assumed as independent, to measure the portions of beam lengths between successive hits. Possible censoring comes from beams not being intercepted within a given voxel. Current approaches aim at connecting LAD to the distribution of beam lengths through some statistical model. Such a simplified model does not currently take into account several effects that may bias LAD estimators or lessen their accuracies: heterogeneity and dependencies in the vegetation properties in different voxels, nature of hit material (wood vs. leaves), unknown leaf angles, underdetection of vegetal elements due to gradual loss of laser power (inducing censoring in data sets).

This collaboration, supported by Y. Bai's PhD work, aims at developping machine learning methods to address these issues. Semantic segmentation of hits on wood vs. leaves was addressed by neural networks, some extensions to PointNet++ were developped [38] to cope with local data sparsity and severe class imbalance. Current work is now focusing on assessing the robustness of estimators to deviations from different assumptions using simulated data sets.

#### 8.1.7 Efficient Neural Networks for Tiny Machine Learning

Participants: Julyan Arbel, Pierre Wolinski, Minh Tri Lê.

The field of Tiny Machine Learning (TinyML) has gained significant attention due to its potential to enable intelligent applications on resource-constrained devices. The review [73] provides an in-depth analysis of the advancements in efficient neural networks and the deployment of deep learning models on ultra-low power microcontrollers (MCUs) for TinyML applications. It begins by introducing neural networks and discussing their architectures and resource requirements. It then explores MEMS-based applications on ultra-low power MCUs, highlighting their potential for enabling TinyML on resource-constrained devices. The core of the review centres on efficient neural networks for TinyML. It covers techniques such as model compression, quantization, and lowrank factorization, which optimize neural network architectures for minimal resource utilization on MCUs. The paper then delves into the deployment of deep learning models on ultra-low power MCUs, addressing challenges such as limited computational capabilities and memory resources. Techniques like model pruning, hardware acceleration, and algorithm-architecture co-design are discussed as strategies to enable efficient deployment.

Lastly, the review provides an overview of current limitations in the field, including the trade-off between model complexity and resource constraints. Overall, this review paper presents a comprehensive analysis of efficient neural networks and deployment strategies for TinyML on ultra-low-power MCUs. It identifies future research directions for unlocking the full potential of TinyML applications on resource-constrained devices.

#### 8.1.8 Graph comparisons

Participants: Sophie Achard, Lucrezia Carboni.

Joint work with: Michel Dojat from GIN, Univ. Grenoble Alpes

In recent accepted publication [18], we worked on the notion of graph comparisons. Node role explainability in complex networks is very difficult, yet is crucial in different application domains such as social science, neurosciences or computer science. Many efforts have been made on the quantification of hubs revealing particular nodes in a network using a given structural property. Yet, in several applications, when multiple instances of networks are available and several structural properties appear to be relevant, the identification of node roles remains largely unexplored. Inspired by the node automorphically equivalence relation, we define an equivalence relation on graph's nodes associated with any collection of nodal statistics (i.e. any functions on the node set). This allows us to define new graph global measures, the power coefficient and the orthogonality score to evaluate the collection parsimony and heterogeneity of a given nodal statistics collection. In addition, we introduce a new method based on structural patterns to compare graphs that have the same vertices set. This methods assigns a value to a node to determine its role distinctiveness in a graph family. Extensive numerical results of our method are conducted on both generative graph models and real data concerning human brain functional connectivity. The differences in nodal statistics are shown to be dependent on the underlying graph structure. Comparisons between generative models and real networks combining two different nodal statistics reveal the complexity of human brain functional connectivity with differences at both global and nodal levels. Using a group of 200 healthy controls connectivity networks, our method is able to compute high correspondence scores among the whole population, to detect homotopy, and finally to quantify differences between comatose patients and healthy controls.

Participants: Sophie Achard, Hana Lbath.

**Joint work with**: Jonas Richiardi from CHUV, Lausanne, Pierre Lafaye de Micheaux from Université Montpellier, Jean-Francois Coeurjolly from LJK Univ. Grenoble Alpes.

Functional magnetic resonance imaging (fMRI) functional connectivity between brain regions is often computed using parcellations defined by functional or structural atlases. Typically, some kind of voxel averaging is performed to obtain a single temporal correlation estimate per region pair. However, several estimators can be defined for this task, with various assumptions and degrees of robustness to local noise, global noise, and region size. In this paper [11], we systematically present and study the properties of 9 different functional connectivity estimators taking into account the spatial structure of fMRI data, based on a simple fMRI data spatial model. These include 3 existing estimators and 6 novel estimators. We demonstrate the empirical properties of the estimators using synthetic, animal, and human data, in terms of graph structure, repeatability and reproducibility, discriminability, dependence on region size, as well as local and global noise robustness.

#### 8.1.9 Spatio-temporal data

Participants: Sophie Achard, Hana Lbath.

Joint work with: Alex Petersen, Brigham Young University, US and Wendy Meiring, University Santa Barbara California, US

A novel non-parametric estimator of the correlation between regions, or groups of arbitrarily dependent variables, is proposed in the presence of noise. The challenge resides in the fact that both noise and low intra-regional correlation lead to inconsistent inter-regional correlation estimation using classical approaches. While some existing methods handle one of these issues or the other, none tackle both at the same time. To address this problem, we propose a trade-off between two approaches: correlating regional averages, which is not robust to low average intra-regional correlation, and averaging pairwise inter-regional correlations, which is not robust to high noise. To that end, we project the data onto a space where the Euclidean distance can be used as a proxy for the sample correlation. We then leverage hierarchical clustering to gather together highly correlated variables within each region prior to averaging. We prove our estimator is consistent for an appropriate cut-off height of the dendogram. We also empirically show our approach surpasses popular estimators in terms of quality and provide illustrations on real-world datasets that further demonstrate its usefulness. [22]

Participants: Sophie Achard.

Joint work with: Irène Gannaz, Univ. Grenoble Alpes

In the general setting of long-memory multivariate time series, the long-memory characteristics are defined by two components. The long-memory parameters describe the autocorrelation of each time series. And the long-run covariance measures the coupling between time series, with general phase parameters. It is of interest to estimate the long-memory, long-run covariance and general phase parameters of time series generated by this wide class of models although they are not necessarily Gaussian nor stationary. This estimation is thus not directly possible using real wavelets decomposition or Fourier analysis. Our purpose in the paper [12] is to define an inference approach based on a representation using quasi-analytic wavelets. We first show that the covariance of the wavelet coefficients provides an adequate estimator of the covariance structure including the phase term. Consistent estimators based on a local Whittle approximation are then proposed. Simulations highlight a satisfactory behavior of the estimation on finite samples on linear time series and on multivariate fractional Brownian motions. An application on a real neuroscience dataset is presented, where long-memory and brain connectivity are inferred.

#### 8.1.10 Uniform in time modulus of continuity of Brownian motion

Participants: Julien Chevallier.

The main objective of [68] is to find a control of the modulus of continuity of the standard Brownian motion in the spirit of what appears in (Kurtz, 1978). By letting the modulus depend on the time horizon we are able to get a control uniform in time in the sense that is is valid for the whole trajectory from 0 to infinity. Moreover, a stability inequality for diffusion processes is then derived and applied to two simple frameworks.

#### 8.1.11 Neuroimaging datasets and consensus protocol

Participants: Sophie Achard.

**Joint work with**: Guillaume Becq from GIPSA-lab, Univ. Grenoble Alpes, Emmanuel Barbier from GIN, University Grenoble Alpes, Joanes Grandjean and collaborators from Department of Cognitive Neuroscience, Donders Institute for Brain, Cognition, and Behaviour, Radboud University Medical Centre, 6525 AJ, Nijmegen, the Netherlands.

Task-free functional connectivity in animal models provides an experimental framework to examine connectivity phenomena under controlled conditions and allows for comparisons with data modalities collected under invasive or terminal procedures. Currently, animal acquisitions are performed with varying protocols and analyses that hamper result comparison and integration. Here we introduce StandardRat, a consensus rat functional magnetic resonance imaging acquisition protocol tested across 20 centers. To develop this protocol with optimized acquisition and processing parameters, we initially aggregated 65 functional imaging datasets acquired from rats across 46 centers. We developed a reproducible pipeline for analyzing rat data acquired with diverse protocols and determined experimental and processing parameters associated with the robust detection of functional connectivity patterns relative to previous acquisitions. The protocol and processing pipeline described here is openly shared with the neuroimaging community to promote interoperability and cooperation toward tackling the most important challenges in neuroscience [20].

#### 8.2 Latent variable modelling

#### 8.2.1 Stochastic Majorization-Minimization with sample-average approximation

Participants: Florence Forbes.

Joint work with: Hien Nguyen, University of Queensland, Brisbane Australia, Gersende Fort, IMT Toulouse.

To extend the applicability of Majorization-Minimization algorithms (MM) in a stochastic optimization context, we propose to combine MM with Sample Average Approximation (SAA). So doing, we avoid the setting of step sizes that goes with stochastic approximation approaches while augmenting SAA with the possibility to consider smaller samples of increasing sizes. In addition SAA does not require to assume uniqueness of the solution or quasi-convexity of the majorizers.

#### 8.2.2 Bayesian Synthetic Likelihoods with Mixture of Experts

Participants: Florence Forbes, Trung Tin Nguyen.

#### Joint work with: Hien Nguyen, University of Queensland, Brisbane Australia.

We extend Bayesian Synthetic Likelihood (BSL) methods to non-Gaussian approximations of the likelihood function. In this setting, we introduce Mixture of Experts (MoEs), a class of neural network models, as surrogate likelihoods that exhibit desirable approximation theoretic properties. Moreover, MoEs can be estimated using Expectation–Maximization algorithm-based approaches, such as the Gaussian Locally Linear Mapping model estimators that we implement. Further, we provide theoretical evidence towards the ability of our procedure to estimate and approximate a wide range of likelihood functions. Through simulations, we demonstrate the superiority of our approach over existing BSL variants in terms of both posterior approximation accuracy and computational efficiency.

#### 8.2.3 Towards frugal unsupervised detection of subtle abnormalities in medical imaging

Participants: Florence Forbes, Geoffroy Oudoumanessah, Michel Dojat.

Joint work with: Carole Lartizien, Creatis Lyon.

Anomaly detection in medical imaging is a challenging task in contexts where abnormalities are not annotated. This problem can be addressed through unsupervised anomaly detection (UAD) methods, which identify features that do not match with a reference model of normal profiles. Artificial neural networks have been extensively used for UAD but they do not generally achieve an optimal trade-off between accuracy and computational demand. As an alternative, we investigate mixtures of probability distributions whose versatility has been widely recognized for a variety of data and tasks, while not requiring excessive design effort or tuning. Their expressivity makes them good candidates to account for complex multivariate reference models. Their much smaller number of parameters makes them more amenable to interpretation and efficient learning. However, standard estimation procedures, such as the Expectation-Maximization algorithm, do not scale well to large data volumes as they require high memory usage. To address this issue, we propose to incrementally compute inferential quantities. This online approach is illustrated on the challenging detection of subtle abnormalities in MR brain scans for the follow-up of newly diagnosed Parkinsonian patients. The identified structural abnormalities are consistent with the disease progression, as accounted by the Hoehn and Yahr scale.

#### 8.2.4 Latent factor models: a tool for dimension reduction in joint species distribution models

Participant: Julyan Arbel, Daria Bystrova, Giovanni Poggiato.

Joint work with: Wilfried Thuiller, LECA - Laboratoire d'Ecologie Alpine.

We investigate modelling species distributions over space and time which is one of the major research topics in both ecology and conservation biology. Joint Species Distribution models (JSDMs) have recently been introduced as a tool to better model community data, by inferring a residual covariance matrix between species, after accounting for species' response to the environment. However, these models are computationally demanding, even when latent factors, a common tool for dimension reduction, are used. To address this issue, previous research proposed to use a Dirichlet process, a Bayesian nonparametric prior, to further reduce model dimension by clustering species in the residual covariance matrix. Here, we built on this approach to include a prior knowledge on the potential number of clusters, and instead used a Pitman-Yor process to address some critical limitations of the Dirichlet process. We therefore propose a framework that includes prior knowledge in the residual covariance matrix, providing a tool to analyze clusters of species that share the same residual associations with respect to other species. We applied our methodology to a case study of plant communities in a protected area of the French Alps (the Bauges Regional Park), and demonstrated that our extensions improve dimension reduction and reveal additional information from the residual covariance matrix, notably showing how the estimated clusters are compatible with plant traits, endorsing their importance in shaping communities. A book chapter describing latent factor models as a tool for dimension reduction in joint species distribution models is aslo available.

#### 8.3 Bayesian modelling

#### 8.3.1 Concentration results for approximate Bayesian computation without identifiability

Participants: Florence Forbes, Julyan Arbel, Trung Tin Nguyen.

Joint work with: Hien Nguyen, University of Queensland, Brisbane Australia.

We study the large sample behaviors of approximate Bayesian computation (ABC) posterior measures in situations when the data generating process is dependent on non-identifiable parameters. In particular, we establish the concentration of posterior measures on sets of arbitrarily small size that contain the equivalence set of the data generative parameter, when the sample size tends to infinity. Our theory also makes weak assumptions regarding the measurement of discrepancy between the data set and simulations, and in particular, does not require the use of summary statistics and is applicable to a broad class of kernelized ABC algorithms. We provide useful illustrations and demonstrations of our theory in practice, and offer a comprehensive assessment of the nature in which our findings complement other results in the literature.

#### 8.3.2 Bayesian mixture models (in)consistency for the number of clusters

Participants: Julyan Arbel, Louise Alamichel, Daria Bystrova.

#### Joint work with: Guillaume Kon Kam King (INRAE).

Bayesian nonparametric mixture models are common for modeling complex data. While these models are well-suited for density estimation, their application for clustering has some limitations. Recent results proved posterior inconsistency of the number of clusters when the true number of clusters is finite for the Dirichlet process and Pitman–Yor process mixture models. In [62], we extend these results to additional Bayesian nonparametric priors such as Gibbs-type processes and finite-dimensional representations thereof. The latter include the Dirichlet multinomial process, the recently proposed Pitman–Yor, and normalized generalized gamma multinomial processes. We show that mixture models based on these processes are also inconsistent in the number of clusters and discuss possible solutions. Notably, we show that a post-processing algorithm introduced for the Dirichlet process can be extended to more general models and provides a consistent method to estimate the number of components.

#### 8.3.3 Diagnosing convergence of Markov chain Monte Carlo

Participants: Julyan Arbel, Theo Moins, Stephane Girard.

#### Joint work with: A. Dutfoy (EDF R&D).

Diagnosing convergence of Markov chain Monte Carlo (MCMC) is crucial in Bayesian analysis. Among the most popular methods, the potential scale reduction factor (commonly named  $\hat{R}$ ) is an indicator that monitors the convergence of output chains to a stationary distribution, based on a comparison of the between- and within-variance of the chains. Several improvements have been suggested since its introduction in the 90'ss. We analyse some properties of the theoretical value *R* associated to  $\hat{R}$  in the case of a localized version that focuses on quantiles of the distribution. This leads to proposing a new indicator [24], which is shown to allow both for localizing the MCMC convergence in different quantiles of the distribution, and at the same time for handling some convergence issues not detected by other  $\hat{R}$ versions.

#### 8.3.4 Bayesian neural networks

Participants: Julyan Arbel, Pierre Wolinski, Konstantinos Pitas.

Joint work with: Hong-Phuong Dang, Clement Elvira, Cédric Herzet, Zacharie Naulet, Mariia Vladimirova.

The study of feature propagation at initialization in neural networks lies at the root of numerous initialization designs. An assumption very commonly made in the field states that the pre-activations are

Gaussian. Although this convenient *Gaussian hypothesis* can be justified when the number of neurons per layer tends to infinity, it is challenged by both theoretical and experimental works for finite-width neural networks. Our major contribution of this work is to construct a family of pairs of activation functions and initialization distributions that ensure that the pre-activations remain Gaussian throughout the network's depth, even in narrow neural networks. In the process, we discover a set of constraints that a neural network should fulfill to ensure Gaussian pre-activations. Additionally, we provide a critical review of the claims of the Edge of Chaos line of works and build an exact Edge of Chaos analysis. We also propose a unified view on pre-activations propagation, encompassing the framework of several well-known initialization procedures. Finally, our work provides a principled framework for answering the much-debated question: is it desirable to initialize the training of a neural network whose pre-activations are ensured to be Gaussian?

We also investigate the cold posterior effect through the lens of PAC-Bayes generalization bounds. We argue that in the non-asymptotic setting, when the number of training samples is (relatively) small, discussions of the cold posterior effect should take into account that approximate Bayesian inference does not readily provide guarantees of performance on out-of-sample data. Instead, out-of-sample error is better described through a generalization bound. In this context, we explore the connections of the ELBO objective from variational inference and the PAC-Bayes objectives. We note that, while the ELBO and PAC-Bayes objectives are similar, the latter objectives naturally contain a temperature parameter  $\lambda$  which is not restricted to be  $\lambda = 1$ . For classification tasks, in the case of Laplace approximations to the posterior, we show how this PAC-Bayesian interpretation of the temperature parameter captures important aspects of the cold posterior effect.

[15] summarizes some recent works and associated challenges in the field of Bayesian statistics that were presented during the Journées MAS 2020. The goal of the session was to give an overview of the many aspects of Bayesian statistics investigated by young researchers of the community.

#### 8.3.5 Particle and Gradient-based approach for sequential Bayesian optimal design.

Participants: Florence Forbes, Jacopo Iollo.

Joint work with: Pierre Alliez, Inria Titane and Christophe Heinkele, Cerema Strasbourg.

We propose a new procedure, for Bayesian experimental design, that performs sequential design optimization by simultaneously providing accurate estimates of successive posterior distributions for parameter inference. The sequential design process is carried out via a contrastive estimation principle, using stochastic optimization and Sequential Monte Carlo (SMC) samplers to maximise the Expected Information Gain (EIG). As larger information gains are obtained for larger distances between successive posterior distributions, this EIG objective may worsen classical SMC performance. To handle this issue, tempering is proposed to have both a large information gain and an accurate SMC sampling, that we show is crucial for performance. This novel combination of stochastic optimization and tempered SMC allows to jointly handle design optimization and parameter inference. We provide a proof that the obtained optimal design estimators benefit from some consistency property. Numerical experiments confirm the potential of the approach, which outperforms other recent existing procedures.

#### 8.3.6 Bayesian nonparametric mixture of experts for high-dimensional inverse problems.

Participants: Julyan Arbel, Florence Forbes, Trung Tin Nguyen.

Joint work with: Hien Duy Nguyen, University of Queensland, Brisbane, Australia.

A wide class of problems can be formulated as inverse problems where the goal is to find parameter values that best explain some observed measures. Typical constraints in practice are that relationships

between parameters and observations are highly nonlinear, with high-dimensional observations and multi-dimensional correlated parameters. To handle these constraints, we consider probabilistic mixtures of locally linear models, which can be seen as particular instances of mixtures of experts (MoE). We have shown in previous studies that such models had a good approximation ability provided the number of experts was large enough. This contribution is to propose a general scheme to design a tractable Bayesian nonparametric (BNP) MoE model to avoid any commitment to an arbitrary number of experts. A tractable estimation algorithm is designed using a variational approximation and theoretical properties are derived on the predictive distribution and the number of components. Illustrations on simulated and real data show good results in terms of selection and computing time compared to more traditional model selection procedures.

#### 8.3.7 Hierarchical Bayesian models for simulation-based inference

Participants: Pedro Rodrigues, Julia Linhart.

**Joint work with**: Thomas Moreau and Alexandre Gramfort from Inria Saclay and Gilles Louppe from Université de Liège.

Inferring the parameters of a stochastic model based on experimental observations is central to the scientific method. A particularly challenging setting is when the model is strongly indeterminate, i.e. when distinct sets of parameters yield identical observations. This arises in many practical situations, such as when inferring the distance and power of a radio source (is the source close and weak or far and strong?) or when estimating the amplifier gain and underlying brain activity of an electrophysiological experiment. In a recent work, we have proposed the hierarchical neural posterior estimation (HNPE), a novel method for cracking such indeterminacy by exploiting additional information conveyed by an auxiliary set of observations sharing global parameters. This method extends recent developments in simulation-based inference (SBI) based on normalizing flows to Bayesian hierarchical models. We validated HNPE quantitatively on a motivating example amenable to analytical solutions and then applied it to invert a well known non-linear model from computational neuroscience, using both simulated and real EEG data.

#### 8.3.8 Bayesian inference on a large-scale brain simulator

Participants: Pedro Rodrigues.

Joint work with: Nicholas Tolley and Stephanie Jones from Brown University, Alexandre Gramfort from Inria Saclay

The Human Neocortical Neurosolver (HNN) is a framework whose foundation is a cortical column model with cell and circuit level detail designed to connect macroscale signals to meso/microcircuit level phenomena. We apply this model to study the cellular and circuit mechanisms of beta generation using local field potential (LFP) recordings from the non-human primate (NHP) motor cortex. To characterize beta producing mechanisms, we employ simulation based inference (SBI) in the HNN modeling tool. This framework leverages machine learning techniques and neural density estimators to characterize the relationship between a large space of model parameters and simulation output. In this setting, Bayesian inference can be applied to models with intractable likelihood functions (Gonçalves 2020, Papamakarios 2021). The main goal of this project is to provide a set of guidelines for scientists that wish to apply simulation-based inference to their neuroscience studies with a large-scale simulator such as HNN. This involves developing new methods for extracting summary features, checking the quality of the posterior approximation, etc. This work is mostly carried out by the Ph.D. student Nicholas Tolley from Brown University.

#### 8.4 Modelling and quantifying extreme risk

#### 8.4.1 Extreme events and neural networks

Participants: Stephane Girard.

Joint work with: M. Allouche and E. Gobet (CMAP, Ecole Poytechnique).

In [14], we propose new parametrizations for neural networks in order to estimate extreme quantiles in both non-conditional and conditional heavy-tailed settings. All proposed neural network estimators feature a bias correction based on an extension of the usual second-order condition to an arbitrary order. The convergence rate of the uniform error between extreme log-quantiles and their neural network approximation is established. The finite sample performances of the non-conditional neural network estimator are compared to other bias-reduced extreme-value competitors on simulated data. It is shown that our method outperforms them in difficult heavy-tailed situations where other estimators almost all fail. Finally, the conditional neural network estimators are implemented to investigate the behaviour of extreme rainfalls as functions of their geographical location in the southern part of France.

#### 8.4.2 Estimation of univariate extreme risk measures

Participants: Jonathan El Methni, Stephane Girard.

Joint work with: M. Allouche (CMAP, Ecole Polytechnique).

One of the most popular risk measures is the Value-at-Risk (VaR) introduced in the 1990's. In statistical terms, the VaR at level  $\alpha \in (0, 1)$  corresponds to the upper  $\alpha$ -quantile of the loss distribution. Weissman extrapolation device for estimating extreme quantiles (when  $\alpha \rightarrow 0$ ) from heavy-tailed distributions is based on two estimators: an order statistic to estimate an intermediate quantile and an estimator of the tail-index. The common practice is to select the same intermediate sequence for both estimators. In [13], we show how an adapted choice of two different intermediate sequences leads to a reduction of the asymptotic bias associated with the resulting refined Weissman estimator. This new bias reduction method is fully automatic and does not involve the selection of extra parameters. Our approach is compared to other bias reduced estimators of extreme quantiles both on simulated and real data. This work is extended to more general risk measures in [63] and to Weibull-tail distributions in [70], the results are submitted for publication.

#### 8.4.3 Estimation of multivariate risk measures

Participants: Julyan Arbel, Stephane Girard.

Joint work with: H. Nguyen (University of Queensland, Brisbane, Australia), T. Opitz (INRAe Avignon) and A. Usseglio-Carleve (Univ. Avignon).

Expectiles form a family of risk measures that have recently gained interest over the more common value-at-risk or return levels, primarily due to their capability to be determined by the probabilities of tail values and magnitudes of realisations at once. However, a prevalent and ongoing challenge of expectile inference is the problem of uncertainty quantification, which is especially critical in sensitive applications, such as in medical, environmental or engineering tasks. In [16], we address this issue by developing a novel distribution, termed the multivariate expectilebased distribution (MED), that possesses an expectile as a closed-form parameter. Desirable properties of the distribution, such as

log-concavity, make it an excellent fitting distribution in multivariate applications. Maximum likelihood estimation and Bayesian inference algorithms are described. Simulated examples and applications to expectile and mode estimation illustrate the usefulness of the MED for uncertainty quantification.

Analysis of variance (ANOVA) is commonly employed to assess differences in the means of independent samples. However, it is unsuitable for evaluating differences in tail behaviour, especially when means do not exist or empirical estimation of moments is inconsistent due to heavy-tailed distributions. Here, we propose an ANOVA-like decomposition to analyse tail variability, allowing for flexible representation of heavy tails through a set of user-defined extreme quantiles, possibly located outside the range of observations. Building on the assumption of regular variation, we introduce a test for significant tail differences among multiple independent samples and derive its asymptotic distribution. We investigate the theoretical behaviour of the test statistics for the case of two samples, each following a Pareto distribution, and explore strategies for setting hyperparameters in the test procedure. To demonstrate the finite-sample performance, we conduct simulations that highlight generally reliable test behaviour for a wide range of situations. The test is applied to identify clusters of financial stock indices with similar extreme log-returns and to detect temporal changes in daily precipitation extremes at rain gauges in Germany. The results are submitted for publication [72].

#### 8.4.4 Dimension reduction for extremes

Participants: Julyan Arbel, Meryem Bousebata, Stephane Girard.

#### Joint work with: G. Enjolras (CERAG).

In the context of the PhD thesis of Meryem Bousebata, we proposed a new approach, called Extreme-PLS (EPLS), for dimension reduction in regression and adapted to distribution tails. The objective is to find linear combinations of predictors that best explain the extreme values of the response variable in a non-linear inverse regression model. The asymptotic normality of the EPLS estimator is established in the single-index framework and under mild assumptions. The performance of the method is assessed on simulated data. A statistical analysis of French farm income data, considering extreme cereal yields, is provided as an illustration [17].

Further, a novel interpretation of EPLS directions as maximum likelihood estimators is introduced in [66], utilizing the von Mises-Fisher distribution applied to hyperballs. The dimension reduction process is enhanced through the Bayesian paradigm, enabling the incorporation of prior information into the projection direction estimation. The maximum a posteriori estimator is derived in two specific cases, elucidating it as a regularization or shrinkage of the EPLS estimator. We also establish its asymptotic behavior as the sample size approaches infinity. A simulation data study is conducted in order to assess the practical utility of our proposed method. This clearly demonstrates its effectiveness even in moderate data problems within high-dimensional settings. Furthermore, we provide an illustrative example of the method's applicability using French farm income data, highlighting its efficacy in real-world scenarios. The results are submitted for publication.

#### 8.4.5 Bayesian inference for extreme values

Participants: Julyan Arbel, Theo Moins, Stephane Girard.

#### Joint work with: A. Dutfoy (EDF R&D).

Combining extreme value theory with Bayesian methods offers several advantages, such as a quantification of uncertainty on parameter estimation or the ability to study irregular models that cannot be handled by frequentist statistics. However, it comes with many options that are left to the user concerning model building, computational algorithms, and even inference itself. Among them, the parameterization of the model induces a geometry that can alter the efficiency of computational algorithms, in addition to making calculations involved. In [25], we focus on the Poisson process characterization of extremes and outline two key benefits of an orthogonal parameterization addressing both issues. First, several diagnostics show that Markov chain Monte Carlo convergence is improved compared with the original parameterization. Second, orthogonalization also helps deriving Jeffreys and penalized complexity priors, and establishing posterior propriety. The analysis is supported by simulations, and our framework is then applied to extreme level estimation on river flow data.

## 9 Bilateral contracts and grants with industry

## 9.1 Bilateral contracts with industry

Participants: Florence Forbes, Pedro Luiz Coelho Rodrigues, Stephane Girard, Julyan Arbel.

- **Plan de Relance project with GE Healthcare (2022-24).** The topic of the collaboration is related to early anomaly detection of failures in medical transducer manufacturing. The financial support for STATIFY is of 155K euros.
- **Contract with EDF (2020-2023).** Julyan Arbel and Stephane Girard are the advisors of the PhD thesis of Theo Moins founded by EDF. The goal is to investigate sensitivity analysis and extrapolation limits in extreme-value theory Bayesian methods. The financial support for STATIFY is of 150K euros.
- **Contract with TDK-Invensense (2020-2023).** Julyan Arbel is the advisor of the PhD thesis of Minh Tri Lê founded by TDK-Invensense. The goal is to apply deep learning methods on small size systems, thus investigating compression methods in deep learning. The financial support for STATIFY is of 150K euros.
- **Contract with Valeo (2022-2023).** Stephane Girard is supervising the work of Pascal Dkengne Sielenou (engineer at STATIFY) funded by a contract between STATIFY and Valeo. The goal is to design statistical method for autonomous vehicle data analysis [69]. The total financial support for STATIFY is of 50K euros.

## 10 Partnerships and cooperations

## 10.1 International initiatives

- **Participants:** Jean-Baptiste Durand, Florence Forbes, Julyan Arbel, Sophie Achard, Pedro Luiz Coelho Rodrigues.
- Sophie Achard is coPI of the ANR project (PRCI) QFunC (2020-23) in partnership with University of Santa Barbara (USA) and Université de Lausanne (Switzerland). The aim of the project is to build spatio-temporal models for brain connectivity. The financial support for STATIFY is 260K euros.
- Julyan Arbel is coPI of the Bayes-Duality project launched with a funding of \$2.76 millions by Japan JST -French ANR for a total of 5 years starting in October 2021. The goal is to develop a new learning paradigm for Artificial Intelligence that learns like humans in an adaptive, robust, and continuous fashion. The financial support for the French side is 464K euros.
- Australian Research Council Discovery project (2023-25): Florence Forbes is coPI of 3 year project with Hien Duy Nguyen from University of Queensland, Brisbane, Australia. The financial support is about 233K euros.

#### 10.1.1 Inria associate team not involved in an IIL or an international program

#### WOMBAT

Title: Variance-reduced Optimization Methods and Bayesian Approximation Techniques for scalable inference

**Duration:** 2023 ->

Coordinator: Hien Duy Nguyen (h.nguyen7@uq.edu.au)

#### **Partners:**

• University of Queensland Brisbane (Australie)

Inria contact: Florence Forbes

Summary: Many inferential tools, such as machine learning algorithms and statistical models, require the estimation of model parameters, structures, quantities, and properties, from data. In practice, it is common that model characterizations are available through high-fidelity simulations of the data generating processes, but only through "black-boxes" that are poorly suited for optimization under uncertainty or conventional statistical inference procedures. The main statistical challenge is that model likelihoods are typically intractable or unavailable in closed form. Approaches suited for these scenarios are typically referred to as likelihood-free or simulation-based inference (SBI) methods, and have received a great deal of attention in recent years, with momentum coming from mixing of ideas from the interface between statistics and machine learning. However, most SBI methods scale poorly when the number of observations is too large, which makes them unsuitable for modern data, which are often acquired in real time, in an incremental nature, and are often available in large volume. Computation of inferential quantities in an incremental manner may be forcibly imposed by the nature of data acquisition (e.g. streaming and sequential data) but may also be seen as a solution to handle larger data volumes in a more resource friendly way, with respect to memory, energy, and time consumption. To produce feasible and practical online algorithms for streaming data and complex models, we propose to study the family of stochastic approximation (SA) algorithms. The overall goal of the project is to combine recent ideas from the SBI and SA literature, to propose efficient methods for handling complex inferential problems. We shall demonstrate our approaches via applications to problems in challenging domains, such as Magnetic Resonance Imaging (MRI) or road network management as initial targets. So doing, we hope to achieve both breakthroughs in applied methodology and the development of new SBI and SA techniques that wide-spread applicability.

#### 10.2 International research visitors

**10.2.1** Visits of international scientists

Other international visits to the team

Filippo Ascolani

Status PhD

Institution of origin: Bocconi Milano

Country: Italy

Dates: February 2023

Context of the visit: Collaboration

## 10.3 National initiatives

**Participants:** Jonathan El Methni, Jean-Baptiste Durand, Florence Forbes, Julyan Arbel, Sophie Achard, Stephane Girard, Pedro Luiz Coelho Rodrigues.

#### ANR

- STATIFY is involved in the ANR project GAMBAS (2019-2023) hosted by CIRAD, Montpellier. The project Generating Advances in Modeling Biodiversity And ecosystem Services (GAMBAS) develops statistical improvements and ecological relevance of joint species distribution models. The project supports the PhD thesis of Giovanni Poggiato.
- An ANR project RADIO-AIDE (2022-26) for *Radiation induced neurotoxicity assessed by Spatiotemporal modeling and AI after brain radiotherapy* coordinated by S.Ancelet from IRSN has been granted for 4 years starting from April 2022. It involves STATIFY, Grenoble Insitute of Neurosciences, Pixyl, ICANS, APHP, ICM and ENS P.Saclay. The available funding for STATIFY is 94K euros.
- ANR project PEG2 (2022-26) on Predictive Ecological Genomics: STATIFY is involved in this 4-year project recently accepted in July 2022. The PI is prof. Olivier Francois who spent 2 years (2021-22) in the team on a *Delegation* position.
- Julyan Arbel is coPI of the Bayes-Duality project launched with a funding of \$2.76 millions by Japan JST French ANR for a total of 5 years starting in October 2021. The goal is to develop a new learning paradigm for Artificial Intelligence that learns like humans in an adaptive, robust, and continuous fashion. On the Japan side the project is led by Mohammad Emtiyaz Khan as the research director, and Kenichi Bannai and Rio Yokota as Co-PIs.
- STATIFY is involved in the 5-year ANR project ExtremReg (2019-2023) hosted by Toulouse University. This research project aims to provide new adapted tools for nonparametric and semiparametric modeling from the perspective of extreme values. Our research program concentrates around three central themes. First, we contribute to the expanding literature on non-regular boundary regression where smoothness and shape constraints are imposed on the regression function and the regression errors are not assumed to be centred, but one-sided. Our second aim is to further investigate the study of the modern extreme value theory built on the use of asymmetric least squares instead of traditional quantiles and order statistics. Finally, we explore the less-discussed problem of estimating high-dimensional, conditional and joint extremes The financial support for STATIFY is about 15K euros.

#### **PEPR Digital Health**

• Florence Forbes and Sophie Achard are involved in the REWIND project (2023-2028), pRecision mEdicine WIth loNgitudinal Data. The goal is to develop models for longitudinal for understanding the progression of chronic diseases.

## France Life Imaging (FLI)

 Funding from "comité" de pilotage national du Réseau d'Expertise « Traitement et Analyse en Imagerie Multimodale » (RE4) de l'Infrastructure France Life Imaging (FLI) for a project entitled « Détection d'Anomalies en Imagerie Médicale par apprentissage faiblement Supervisé ». Joint project with Carole Lartizien and Michel Dojat.

#### **INRAe projects**

- Stephane Girard was awarded 80K euros for the project "Analysis of variability in extremes AN-OVEX" via the AMI INRAe-Inria "*Risques naturels et environnementaux*", 2023–2024.
- Jonathan El Methni and Stephane Girard were awarded 3.5K euros for the project "Warm Winter Risk WWR" via the AMI INRAe *"projets exploratoires pour le métaprogramme XRISQUES"*, 2023–2024.

#### 10.3.1 Networks

**MSTGA and AIGM INRAE (French National Institute for Agricultural Research) networks:** F. Forbes and J.B Durand are members of the INRAE network called AIGM (ex MSTGA) network since 2006, website, on Algorithmic issues for Inference in Graphical Models. It is funded by INRAE MIA and RNSC/ISC Paris. This network gathers researchers from different disciplines. STATIFY co-organized and hosted 2 of the network meetings in 2008 and 2015 in Grenoble.

## 10.4 Regional initiatives

Participants:Jonathan El Methni, Jean-Baptiste Durand, Florence Forbes,<br/>Sophie Achard, Stephane Girard, Pedro Luiz Coelho Rodrigues.

#### **Grenoble Idex projects**

- MIAI, Multidisciplinary Institute in Artificial Intelligence: In the context of the MIAI institute, Sophie Achard is co-PI of a chair (2020-23) on *Toward Robust and Understandable Neuromorphic Systems* funding one PhD student and several post-doc fellows. Sophie Achard is PI of an international chair with partners from USA and Switzerland (400 keuros).
- MIAI: Stephane Girard was awarded 3.5K euros for his project *"How AI models can deal with extreme values? Application to risk assessment"* via the open call to sustain the development and promotion of AI, 2022–2023.
- MIAI: Pedro Rodrigues was awarded 13K euros for his project on *Machine Learning for Experimental Data* via the IRGA 2022 call for projects.
- MIAI: Florence Forbes, Jean-Baptiste Durand and Yuchen Bai were awarded 4.5K euros for their project on *Developing IA for estimating leaf area density area in tropical forests from LiDAR data*, Nov. 2022.

## **11** Dissemination

#### **11.1** Promoting scientific activities

#### 11.1.1 Scientific events: organisation

#### Member of the organizing committees

- Pedro Rodrigues was member of the organizing commitee of the GRETSI 2023: Colloque Francophone de Traitement du Signal et des Images. The event gathered around 500 researchers in Grenoble and lasted for 5 days. Pedro Rodrigues was responsible for all visual aspects of the communication of the conference, such as editing the conference booklet, preparing the signs to indicate where participants should go, etc.
- Julyan Arbel was member of the organizing commitee of the Bayes at CIRM Autumn School, organized in CIRM in Marseille in Oct-Nov 2023. The event gathered 100 participants and lasted for 5 days. Julyan Arbel was the treasurer of the event with a budget of 35K euros.

- Florence Forbes was member of the organizing commitee of the IABM workshop on Biomedical Imaging, 2 days in Paris.
- Florence Forbes was member of the organizing commitee of the Monte Carlo Methods (MCM 2023) conference, one week in June, Paris.

#### 11.1.2 Scientific events: selection

#### Member of the conference program committees

- Stephane Girard, Member of the Scientific Program Committee of the 16th International Conference of the ERCIM WG on computational and methodological statistics, Berlin, 2023. He organized an invited session entitled "Extreme and machine learning" and he was chair of a contributed session entitled "Extreme values".
- Julyan Arbel, Member of the Scientific Program Committee of the Journées de Statistique of SFDS, organized in Université libre de Bruxelles (ULB) in July 2023. The event gathered 400+ participants.
- Julyan Arbel, Member of the Scientific Program Committee of the Statistical Methods for Post Genomic Data analysis (SMPGD) meeting, in January 2023.

#### Reviewer

- Pedro Rodrigues, Reviewer, NeurIPS 2023.
- Pedro Rodrigues, Reviewer, ICML 2023.
- Pedro Rodrigues, Reviewer, AISTATS 2023.
- Pedro Rodrigues, Reviewer, NeurIPS 2023 workshop on Machine Learning for Physical Sciences.
- Julyan Arbel, Reviewer, NeurIPS 2023.
- Julyan Arbel, Reviewer, Advances in Approximate Bayesian Inference AABI 2023.
- Julyan Arbel, Reviewer, AISTATS 2023.
- Julyan Arbel, Reviewer, Journées de Statistique of SFDS 2023.

#### 11.1.3 Journal

#### Member of the editorial boards

- Stephane Girard, Associate Editor, Revstat Statistical Journal since 2019.
- Stephane Girard, Member of the Advisory Board, Dependence Modeling since 2015.
- Julyan Arbel, Associate Editor, Bayesian Analysis since 2019.
- Julyan Arbel and Florence Forbes, Associate Editor, Australian and New Zealand Journal of Statistics since 2019.
- Julyan Arbel, Associate Editor, Statistics & Probability Letters since 2019.
- Julyan Arbel, Associate Editor, Computational Statistics & Data Analysis since 2020.
- Julyan Arbel, Associate Editor, Statistical Methods & Applications since 2023.

#### **Reviewer - reviewing activities**

- Stephane Girard, Reviewer, Journal of Machine Learning Research.
- Stephane Girard, Reviewer, Computational Statistics and Data Analysis.
- Stephane Girard, Reviewer, Advances in Data Analysis and Classification.
- Stephane Girard, Reviewer, Communications in Statistics Theory and Methods.
- Stephane Girard, Reviewer, Croatian Operational Research Review.
- Julien Chevallier, Reviewer, ALEA Latin American Journal of Probability and Mathematical Statistics.
- Julien Chevallier, Reviewer, Annals of Applied Probability.
- Julien Chevallier, Reviewer, Kinetic and Related Models.
- Julyan Arbel, Reviewer, Journal of Computation and Graphical Statistics.
- Julyan Arbel, Reviewer, Journal of Machine Learning Research.
- Julyan Arbel, Reviewer, Statistics and Computing.
- Julyan Arbel, Reviewer, Statistical Science.
- Julyan Arbel, Reviewer, Stochastic Processes and their Applications.
- Julyan Arbel, Reviewer, Methodology and Computing in Applied Probability.
- Julyan Arbel, Reviewer, Computo.

#### 11.1.4 Invited talks

- Stephane Girard was invited to give a talk at the EVTA seminar (joint extreme value seminar of Delft, Tilburg and Amsterdam universities).
- Julyan Arbel was invited to give a talk at the Approximation Methods in Bayesian Analysis workshop, CIRM, Marseille, in June 2023.
- Julyan Arbel was invited to give a talk at the Université de Montréal statistics seminar, Montréal, in July 2023.
- Julyan Arbel was invited to give a talk at the CMStatistics conference in Berlin, in December 2023.
- Julyan Arbel was invited to give a talk at the University of Edinburgh statistics seminar, Edinburgh, in October 2023.
- Florence Forbes was invited to the ICMSE workshop, Edimburgh, January 2023.
- Florence Forbes was invited to the Bayes for Health workshop, University of Oxford, March 2023.
- Florence Forbes was invited to the GeoSto days, Dijon, June 2023.

#### 11.1.5 Leadership within the scientific community

Florence Forbes is in charge of representing the Grenoble Inria Center for activities and events related to digital health.

#### 11.1.6 Research administration

- Julyan Arbel, Member of the Scientific Committee of the Data Science axis of Persyval Labex.
- Julyan Arbel, Member of the Board of Directors member of ISBA, the International Society for Bayesian Analysis, 2022-2025.
- Julyan Arbel, Member of the Comité des Emplois Scientifiques at Inria Grenoble since 2019.
- Florence Forbes is a member of the scientific committe COS of Inria Grenoble.

#### 11.2 Teaching - Supervision - Juries

#### 11.2.1 Teaching

- Master: Stephane Girard, *Statistique Inférentielle Avancée*, 18 ETD, M1 level, Ensimag. Grenoble-INP, France.
- Master: Stephane Girard, *Introduction to Extreme-Value Analysis*, 15 ETD, M2 level, Univ-Grenoble Alpes (UGA), France.
- Master: Julyan Arbel, Bayesian nonparametrics and Bayesian deep learning, Master Mathématiques Apprentissage et Sciences Humaines (M\*A\*S\*H), Université PSL (Paris Sciences & Lettres), 25 ETD.
- Master: Julyan Arbel, *Bayesian deep learning*, Master Intelligence Artificielle, Systèmes, Données (IASD), Université PSL (Paris Sciences & Lettres), 12 ETD.
- Master: Julyan Arbel, *Bayesian machine learning*, Master Mathématiques Vision et Apprentissage (MVA), École normale supérieure Paris-Saclay, 36 ETD.
- Master: Julien Chevallier, *Temporal point processes*, 9 ETD, M2 level, Univ-Grenoble Alpes (UGA), France.
- Julien Chevallier is a faculty member at Université Grenoble Alpes (UFR IM2AG).
- Master M1AM and ENSIMAG, Pedro Rodrigues, Statistical Analysis and Document Mining, 35 ETD
- Master M2 DataScience (Institut Polytechnique de Paris), Pedro Rodrigues, DataCamp, 40 ETD

#### 11.2.2 Supervision

- Julyan Arbel was co-supervisor with Wilfried Thuiller of the PhD thesis of Daria Bystrova, "Bayesian learning of species associations", UGA, defended in July 2023.
- Julyan Arbel was supervisor of the PhD thesis of Minh Tri Lê, "Constrained deep neural networks for MEMS sensor-based applications", UGA, defended in July 2023.
- Julyan Arbel was co-supervisor with Wilfried Thuiller of the PhD thesis of Giovanni Poggiatto, "Integrating ecological dependence into biodiversity modelling", UGA, defended in May 2023.
- PhD in progress: Louise Alamichel. "Bayesian Nonparametric methods for complex genomic data" Inria, started in October 2021, advised by Julyan Arbel and Guillaume Kon Kam King (INRAE).
- PhD in progress: Julien Zhou. "Learning combinatorial bandit models under privacy constraints" Inria-Criteo, started in November 2022, advised by Julyan Arbel, Pierre Gaillard and Thibaud Rahier.
- PhD in progress: Mohamed-Bahi Yahiaoui. "Computation time reduction and efficient uncertainty propagation for fission gas simulation" CEA Cadarache-Inria, started in October 2021, advised by Julyan Arbel, Loic Giraldi, Geoffrey Daniel.
- Julyan Arbel and Stephane Girard were co-supervisors of the PhD thesis of Theo Moins, "Bayesian computational methods for estimating extreme quantiles from environmental data", UGA, defended on September 2023.

- PhD in progress: Jean Pachebat "How AI models can deal with extreme values? Application to risk assessment", started on February 2023, Stephane Girard (with Emmanuel Gobet, Ecole Polytechnique), Institut Polytechnique de Paris.
- Pedro Rodrigues co-supervises the Ph.D. thesis of Julia Linhart (2021-2024) with Alexandre Gramfort (META, ex-Inria Saclay)
- Pedro Rodrigues co-supervises the Ph.D. thesis of Pierre-Louis Ruhlmann (2023-2026) with Michael Arbel (THOTH) and Florence Forbes (STATIFY).
- PhD in progress: Yuchen Bai, "Hierarchical Bayesian Modelling of leaf area density from UAV-lidar", started in October 2021, supervised by Jean-Baptiste Durand, Florence Forbes and Gregoire Vincent (IRD, Montpellier).
- PhD in progress: Jacopo Iollo, started in January 2022, supervised by Florence Forbes, P. Alliez (DR Inria Sophia) and C. Heinkele (Cerema, Strasbourg).
- PhD in progress: Geoffroy Oudoumanessah, started in October 2022, supervised by Florence Forbes, C. Lartizien (Creatis, Lyon) and Michel Dojat (GIN).
- PhD in progress: Theo Sylvestre, started in October 2022, supervised by Florence Forbes and S. Ancelet (IRSN).
- PhD in progress: Benjamin Lambert, started in January 2022, supervised by Florence Forbes and M. Dojat (GIN).
- PhD in progress: Brice Marc, started in January 2023, supervised by Florence Forbes, Philippe Foucher and Pierre Charbonier, Cerema Strasbourg.

#### 11.2.3 Juries

- Stephane Girard, Reviewer of the PhD thesis of Michel Kamel, "Modèles probabilistes et apprentissage statistique/automatique avancé pour la détection des anomalies : Application dans l'industrie de télécommunication", Ecole des Mines de Saint-Etienne, July 2023.
- Stephane Girard, Member of the HDR committee of Sylvain Lespinats, "L'exploration de données mise en pratique pour l'extraction d'information en conditions réelles", UGA, December 2023.
- Julyan Arbel, Reviewer of the PhD thesis of Miguel Palencia Olivar, ERIC/LIRIS & Lizeo Group, Lyon, France. "A topical approach to capturing customer insight in social media".
- Julyan Arbel, Reviewer of the PhD thesis of Mica Teo, Edinburgh University, UK, "Bayesian scalaron-image regression via random image partition models".
- Julyan Arbel, Reviewer of the PhD thesis of Otmane Sakhi, ENSAE, Institut Polytechnique de Paris, France, "Offline Contextual Bandit : Theory and Large Scale Applications.
- Florence Forbes, Reviewer of the PhD thesis of Caroline Lawless, University of Oxford.
- Florence Forbes, Reviewer of the PhD thesis of Mohamed Fakhfakh, University of Toulouse.
- Florence Forbes, Member of the PhD committee of Hugo Schmutz, Universite Cote d'Azur, Nice.
- Florence Forbes, Member of the PhD committee of Pierre Palud, University of Lille.
- Florence Forbes, Member of the PhD committee of Martial Amovin, University of Lyon.
- Florence Forbes, Member of the PhD committee of Paul Youssef, University of Grenoble.
- Florence Forbes, Member of the HDR committee of Tabea Rebafka, Sorbonne University, Paris.

## 11.3 Popularization

#### 11.3.1 Articles and contents

• Stephane Girard published a popularization paper entitled "Les statistiques de l'extrême" coauthored with R. Barbero, T. Opitz (INRAe Avignon) and A. Usseglio-Carleve (Avignon university) in the "Pour la Science" journal, issue 546.

## 12 Scientific production

## 12.1 Major publications

- [1] C. Bouveyron, S. Girard and C. Schmid. 'High dimensional data clustering'. In: *Computational Statistics and Data Analysis* 52 (2007), pp. 502–519.
- [2] F. Boux, F. Forbes, J. Arbel, B. Lemasson and E. L. Barbier. 'Bayesian inverse regression for vascular magnetic resonance fingerprinting'. In: *IEEE Transactions on Medical Imaging* 40.7 (July 2021), pp. 1827–1837. DOI: 10.1109/TMI.2021.3066781. URL: https://hal.archives-ouvertes.fr /hal-02314026.
- [3] A. Daouia, S. Girard and G. Stupfler. 'Estimation of Tail Risk based on Extreme Expectiles'. In: *Journal of the Royal Statistical Society series B* 80 (2018), pp. 263–292.
- [4] A. Deleforge, F. Forbes and R. Horaud. 'High-Dimensional Regression with Gaussian Mixtures and Partially-Latent Response Variables'. In: *Statistics and Computing* (Feb. 2014). DOI: 10.1007/s112 22-014-9461-5. URL: https://hal.inria.fr/hal-00863468.
- [5] F. Forbes and G. Fort. 'Combining Monte Carlo and Mean field like methods for inference in hidden Markov Random Fields'. In: *IEEE trans. Image Processing* 16.3 (2007), pp. 824–837.
- [6] F. Forbes, H. D. Nguyen, T. T. Nguyen and J. Arbel. 'Summary statistics and discrepancy measures for ABC via surrogate posteriors'. In: *Statistics and Computing* 32.85 (2022). DOI: 10.1007/s11222 -022-10155-6. URL: https://hal.archives-ouvertes.fr/hal-03139256.
- [7] F. Forbes and D. Wraith. 'A new family of multivariate heavy-tailed distributions with variable marginal amounts of tailweights: Application to robust clustering'. In: *Statistics and Computing* 24.6 (Nov. 2014), pp. 971–984. DOI: 10.1007/s11222-013-9414-4. URL: https://hal.inria.f r/hal-00823451.
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