

Distributed Automated Research Platform

ROBHOOT

Current Team:

Carlos J. Melián¹ Switzerland C1

Victor Eguíluz² Spain C2

Tentative Team:

Swiss Science Data Center³ Switzerland C1

Eawag IT (Harald)⁴ Switzerland C1

iDiv IT ()⁵ Germany C3

Inca (Nterminal, Yupana)⁶

Benoit Baudry (DIVERSIFY-project)⁷ France C4

1 Eawag Center for Ecology, Evolution and Biogeochemistry, Switzerland

2 Inst. de Física Interdisciplinar y Sistemas Complejos, IFISC
(CSIC-UIB), Palma de Mallorca, Spain.

3 Tentative team

Contents

1	Funding scheme A	3
2	Funding scheme B	4
3	Summary	5
4	State of the art	6
5	Milestones	7
5.1	Milestone 1: <i>ROBHOOT</i> testnet	7
5.1.1	Milestone 1.1: Data Integration (<i>DAADI</i>)	8
5.1.2	Milestone 1.2: Complexity Reduction (<i>GOCORE</i>)	8
5.1.3	Milestone 1.3: Pattern-Process Inference (<i>PROPENCE</i>)	8
5.1.4	Milestone 1.4: Validation (<i>VATION</i>)	8
5.1.5	Milestone 1.5: Visualization (<i>VITION</i>)	8
5.2	Milestone 2: <i>ROBHOOT</i> mainnet	8
5.2.1	Milestone 2.1: Data Integration	8
5.2.2	Milestone 2.2: Complexity Reduction	8
5.2.3	Milestone 2.3: Pattern-Process Inference	8
5.2.4	Milestone 2.4: Validation	8
5.2.5	Milestone 2.5: Visualization	8
6	Tables	10
7	Figures	12

1 Funding scheme A

Call ID: FET Proactive: emerging paradigms and communities H2020-FETPROACT-2019-2020

Specific Challenge:

To explore and consolidate a new technological direction in order to put it firmly on the map as a viable paradigm for future technology. To foster the interdisciplinary communities that are able to drive this forward, extending from the participating consortia to a wider European pool of expertise. To stimulate the emergence of a European innovation eco-system around a new technological paradigm, well beyond the world of research alone.

Scope:

Proposals are sought for cutting-edge high-risk / high-reward research and innovation projects that aim to demonstrate a new technological paradigm within the scope of one of the following sub-topics:

Human-Centric AI. Artificial intelligence (AI) is gaining more and more footholds in various aspects of our life. However, machine learning algorithms are difficult to understand, opaque and may have implicit biases in their decision making. Explicability has become an essential element if users are to trust, accept and adopt the next generation of intelligent machines on a wider scale. This initiative seeks to advance to the next AI frontier with verifiable, evidence-based features of trustworthiness (i.e., reliable and unbiased alignment of values, goals and beliefs) and transparency (explainable performance), exploring radically new approaches (e.g., inspired from neuro-science, cognition or social science). For instance, explanation could be more tightly intertwined with the decision making process itself so that decisions can be challenged, interpreted, refined and adjusted through mutual exchange, introspection (e.g., self-awareness of biases, reflecting on the internal functioning of the learning system, or on what caused a wrong or unacceptable decision) and active learning of both system and user, for example through dialogue or other forms of multi-modal interaction aimed at establishing mutual trust. New data collection and ownership/governance models that go beyond the dominant off-line and centralised data processing should be investigated, and new avenues, such as for incremental, unsupervised, active, one-shot and ‘small data’ machine learning, should be explored. The projects are expected to contribute to the wider debate on the sociotechnical, organisational and AI-ethical dimensions of such technologies and systems, and link to the ‘Commission’s broader AI strategy

Deadline: September 3, 2019 12:30:00 AM The submission session is now available for: FETPROACT-EIC-05-2019(RIA), FETPROACT-EIC-06-2019(RIA)

2 Funding scheme B

Call ID: FET-Open Challenging Current Thinking H2020-FETOPEN-01-2018-2019-2020

Specific Challenge:

To lay the foundations for radically new future technologies of any kind from visionary interdisciplinary collaborations that dissolve the traditional boundaries between sciences and disciplines, including the social sciences and humanities. This topic also encourages the driving role of new actors in research and innovation, including excellent young researchers, ambitious high-tech SMEs and first-time participants to FET under Horizon 2020 from across Europe.

Scope:

Proposals are sought for cutting-edge high-risk / high-impact interdisciplinary research with all of the following essential characteristics ("FET gatekeepers"):

Radical vision: the project must address a clear and radical vision, enabled by a new technology concept that challenges current paradigms. In particular, research to advance on the roadmap of a well-established technological paradigm, even if high-risk, will not be funded.

Breakthrough technological target: the project must target a novel and ambitious science-to-technology breakthrough as a first proof of concept for its vision. In particular, blue-sky exploratory research without a clear technological objective will not be funded.

Ambitious interdisciplinary research for achieving the technological breakthrough and that opens up new areas of investigation. In particular, projects with only low-risk incremental research, even if interdisciplinary, will not be funded.

The inherently high risks of the research proposed shall be mitigated by a flexible methodology to deal with the considerable science-and-technology uncertainties and for choosing alternative directions and options.

The Commission considers that proposals requesting a contribution from the EU of up to EUR 3 million would allow this specific challenge to be addressed appropriately. Nonetheless, this does not preclude submission and selection of proposals requesting other amounts.

Expected Impact:

Scientific and technological contributions to the foundation of a new future technology
Potential for future social or economic impact or market creation. Building leading research and innovation capacity across Europe by involvement of key actors that can make a difference in the future, for example excellent young researchers, ambitious high-tech SMEs or first-time participants to FET under Horizon 2020.

Deadline: ID: September 18, 2019 17:00:00 Brussels time FETOPEN-01-2018-2019-2020

3 Summary

Public funded data is the norm in science and engineering landscapes. Yet, distributed and open-source automated knowledge-inspired technology accounting for the interdisciplinary research cycle remains challenging in science and engineering. We propose a decentralized automated research platform to facilitate reproducibility in a knowledge-inspired society, technology and science. The platform will be implemented in two stages. First, a testnet biodiversity research prototype accounting for data integration and inference to visualization and reporting generation. Second, a mainnet platform integrating literature discovery, data integration, inference, validation, visualization and reporting generation. Decentralized and open automated research platforms can strongly contribute to a knowledge-inspired governance to help take informed decisions in solving complex social problems merging interdisciplinary science and technology.

Keywords: Knowledge-inspired society, Data integration, Multilayer networks, Deep explicability-based learning, Transparent governance, Bayesian inference. Probabilistic Bayesian networks.

4 State of the art

Radical vision:

- Decentralized, open and scalable automated research platform accounting for the research cycle, from literature and data integration to visualization and report generation.

Breakthrough technological target:

- Transparent automated data-rule-knowledge-inspired technology fully accounting for the interdisciplinary research cycle.

Ambitious interdisciplinary research:

- Mixing researchers, engineers and society to build an open and transparent data-rule- and knowledge-inspired science, technology and society.

—————How to solve it?—————

1. The problem:

Why? Centralized, Non-transparent and non-reproducible vs decentralized, transparent and reproducible

Is it ~~radical~~ radical?

Is it viable? Efficient?

Which are the Knowns?

Unknowns?

2. Our own plan

How much time?

Existing gaps? Why?

Data available? Methods? Main gaps

Our own method? Why?

3. Carry on the plan

Quantitative assessment

The maths

4. Solutions (Milestones)

5. Go backwards (Reproducibility)

Is it correct? Reproducible? Scalable? Decentralized? Safe?

Apply to other problems? Datasets?

—————

Automation is rapidly occurring in many fronts, from robotics and investments to gaming and ecommerce. Many technologies are in a era of massive data accumulation, integration and pattern detection. Yet, obtaining insights from such an integration accounting for open science, full reproducibility, inference and prediction power is at a very incipient stage (Ioannidis, 2005; Reichstein, M. et al., 2019). There are many challenges when aiming to integrate data, inference and prediction. ~~For example,~~ sampling design and experiments (Voelkl et al., 2018), randomizations to achieve solid statistics , and process- or pattern-based model selection and inference just to name a few. All these steps require many intermediate decisions that make the scientific process challenging to decentralize, repeat, replicate, and reproduce. Currently, there are many protocols and platforms automatizing ~~partial steps of the~~ (Table 1 summarize a non-exhaustive list of automated platforms).

Reproducibility, robustness and minimizing bias across the different stages of a research platform are two of the desire properties of automated research platforms. Reproducibility guarantees the future improvement of the results and many programming languages currently offer tools to facilitate reproducibility (i.e., Jupyter notebooks). Automated research platforms will facilitate tracking the explored paths (i.e., the within and between layer interactions, Figure 1) and can produce statistics on how close each path is to the empirical patterns.

The following are six features of open automated research platforms that might play a leading role in moving towards a information-inspired science, society and technology: 1) Building the science of science to provide quantitative statistics of interdisciplinary science (Figure 1 for the architecture of an automated research platform); 2) Identifying systematically and accounting for bias and uncertainty in inference; 3) Exploring prediction and explanatory gradients to gain synergy between AI predictive approaches and explanatory power to complex problems (Figure 2); 4) Identifying gaps in patterns not explored consequence of lack of syntesis in interdisciplinary research, 5) Allowing for reusability, repeatability, replicability and reproducibility along the many paths in the scientific enterprise, and 6) Building on rapidly evolving open-source computing programming languages to facilitate the decentralization, scalability and integration of the scientific process (Table 2 and Figure 3).

5 Milestones

5.1 Milestone 1: *ROBHOOT* testnet

Building a functional testnet case for an automated research platform. We will use a Biodiversity research case for this testnet as a showcase of how to gain insights about knowledge-inspired technology (See Robhoot testnet box).

ROBHOOT testnet

Develop automated packages for each layer (See Figure 3 and Table 2 for a prototype in the computing language Julia. The platform will have access to data from both centralized and decentralized platforms in Biodiversity research ^a .

5.1.1 Milestone 1.1: Data Integration (*DAADI*)

5.1.2 Milestone 1.2: Complexity Reduction (*GOCORE*)

5.1.3 Milestone 1.3: Pattern-Process Inference (*PROPENCE*)

5.1.4 Milestone 1.4: Validation (*VATION*)

5.1.5 Milestone 1.5: Visualization (*VITION*)

^a<https://github.com/melian009/Robhoot/blob/master/resources/databases.md>

5.2 Milestone 2: *ROBHOOT* mainnet

Develop a platform fully integrated in decentralized network platforms ¹

ROBHOOT mainnet

5.2.1 Milestone 2.1: Data Integration

5.2.2 Milestone 2.2: Complexity Reduction

5.2.3 Milestone 2.3: Pattern-Process Inference

5.2.4 Milestone 2.4: Validation

5.2.5 Milestone 2.5: Visualization

¹<https://golem.network/>

References

- Ioannidis, J. P. A., 2005. Why most published research findings are false. *PLoS medicine* 2:e124. URL <http://www.ncbi.nlm.nih.gov/pubmed/16060722>.
- Reichstein, M., Camps-Valls, G., Stevens, B., Jung, M., Denzler, J., Carvalhais, N., and Prabhat, 2019. Deep learning and process understanding for data-driven earth system science. *Nature* 566:195–2024.
- Voelkl, B., L. Vogt, E. S. Sena, and H. Würbel, 2018. Reproducibility of preclinical animal research improves with heterogeneity of study samples. *PLoS Biology* 16.

6 Tables

Table 1	
Automated platforms	Webpage
Nakamoto Terminal	https://www.nterminal.com
BigQuery	https://cloud.google.com/bigquery/
Automated statistician	https://www.automaticstatistician.com/index/
Modulos	http://www.modulos.ai/
Google AI	https://ai.google/
Iris	https://iris.ai

Table 2: Prototyping a script workflow in *ROBHOOT*

```

SUMMARY=====
This is a prototype for a script workflow to automate interactions among data search,
parsing, integration, database, cleaning, data complexity reduction, pattern and process
inference, validation and visualization. The script is based in two types of packages:
backbone and specialized packages. Backbone packages (B) connect intra- and inter-layer
algorithms to automatically run the workflow. Specialized (S) packages feedback
with backbone packages to run specific tasks: parsing, likelihoods, inference, plotting,
visualizing, etc.

=====
Layers=====
DATA INTEGRATION: D
COMPLEXITY REDUCTION: C
PATTERN-PROCESS INFERENCE: P
VALIDATION: VA
VISUALIZATION: VI
=====
EXAMPLE with julia =====
Julia packages:
https://github.com/melian009/Robhoot/blob/master/packages.md

WORKFLOW NETWORK-----

data.search D S - - - - - > Retriever.jl M1
parsing.data D S - - - - - > Query.jl M1
data.to.table D S - - - - - > MySQL.jl SQLite.jl Clickhouse.jl M1
data.julia D S - - - - - > DataFrames.jl M1
table.comp.reduction C B - - - - - > TensorFlow.jl lm4.jl Clustering.jl OnlineAI.jl
LightGBM.jl
pattern.detection P S - - - - - > TensorFlow.jl DataVoyage.jl DataFitting.jl Mocha.jl
DeepQLearning.jl Flux.jl AnomalyDetection.jl
process.simulation P S - - - - - > Simjulia.jl Agents.jl JuliaDynamics.jl Zygote.jl
pat.proc.infer P S - - - - - > mads.jl temporal.jl GlobalSearchRegression.jl BlackBox-
Optim.jl JuMP.jl GeneticAlgorithms.jl NaiveBayes.jl Mamba.jl ABC.jl ApproxBayes.jl
DynamicHMC.jl
validation.pat.proc VA S - - - - - > mads.jl LearningStrategies.jl Mamba.jl ABC.jl
Measurements.jl
visualiztion.pattern.process - - - - - > Makie.jl VegaLite.jl

```

7 Figures

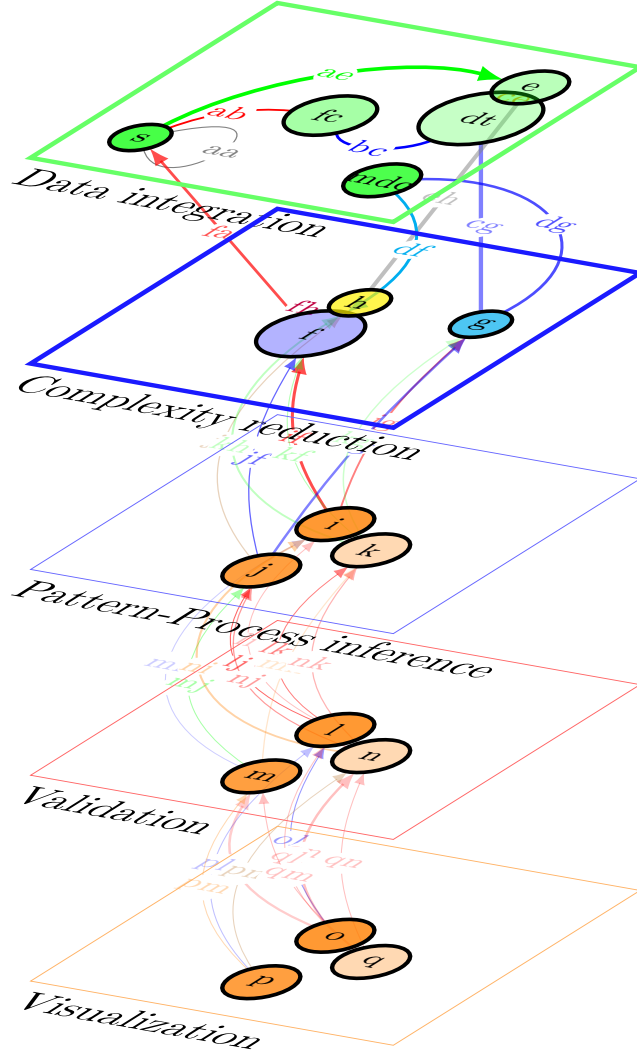


Figure 1: A cartoon of a five layer automated research platform: Data Integration, Complexity reduction, Pattern-process inference, Validation, and Visualization. Nodes and links represent algorithms and interactions between two algorithms, respectively. For example, the figure shows five algorithms in the layer Data integration (**a**, **b**, **c**, **d**, and **e**). Algorithm **a** interacts with algorithm **b** and **e** in the same layer (intra-layer connections) and with algorithm **f** from the second layer (inter-layer connection), Complexity reduction. The cartoon represents many intra- and inter-layer connections to solve a problem. The paths can be quantified by many metrics each producing a distribution of automated solutions. This distribution can be analyzed with the ones used for a specific domain in science, the science of science of a domain, to quantify properties as robustness, reproducibility and bias of a domain.

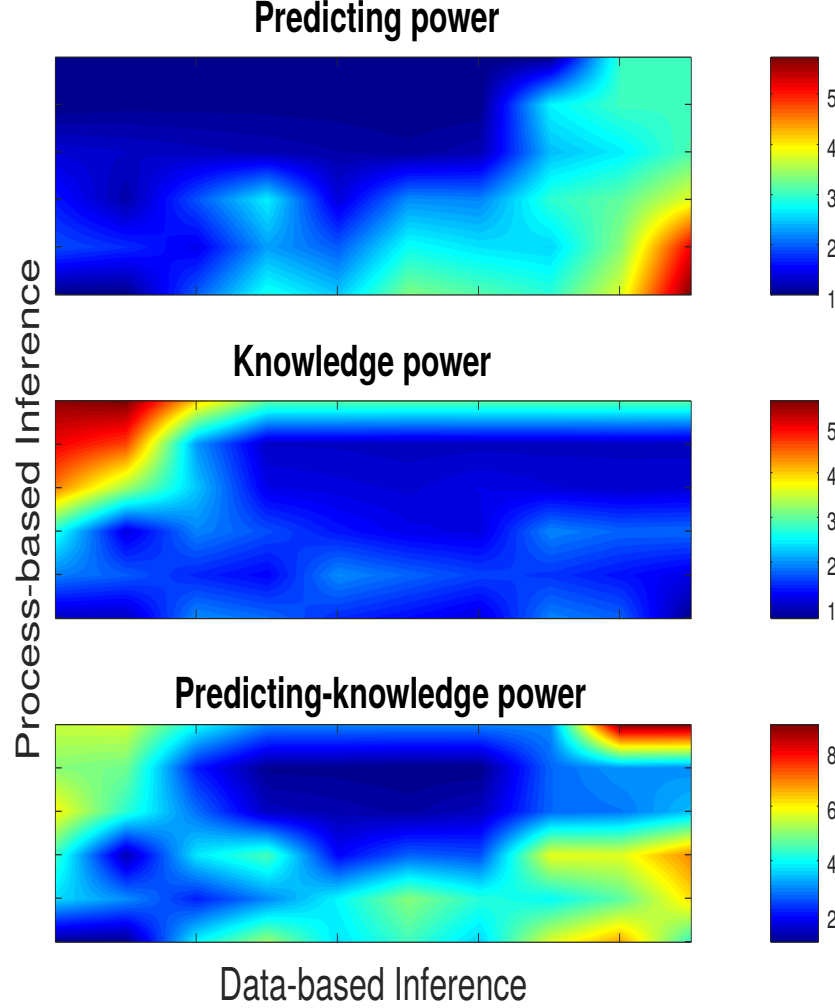


Figure 2: Predicting and knowledge power can be joined to drive open knowledge-inspired societies, technology and science. This figure shows a cartoon of the predicting power (top), the knowledge power (middle), and the predicting-knowledge power (bottom). x- and y-axis represent data-based inference (i.e., gradient of AI methods from low (left) to high (right) predictive power) and process-based inference (i.e., gradient of process-based methods from low (bottom left) to high (top left) knowledge power). The gradient of predicting power (top) shows a hot spot red area in the bottom right highlighting the region where AI methods best predict any given empirical data. The gradient of knowledge power (middle) shows a hot spot red area in the top left highlighting the region where the best mechanistic understanding of a problem occur. The predicting-knowledge power (bottom) integrates the sum of the two previous maps highlighting a red hot spot where interdisciplinary research joining predicting and knowledge power of the empirical data occur.

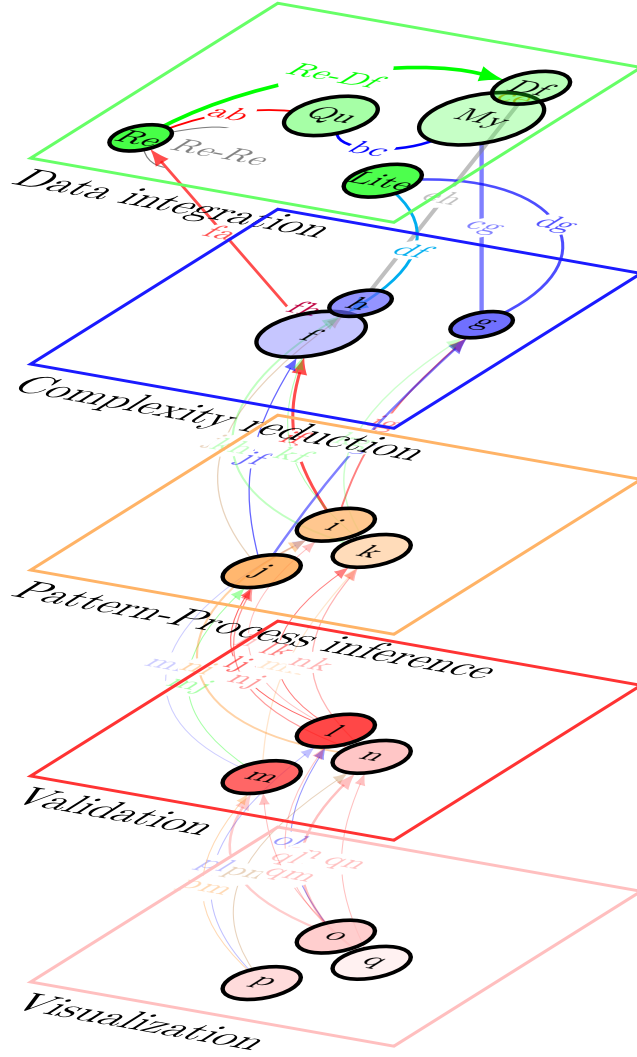


Figure 3: A julia prototype of an automated research platform. Nodes and links in each layer represent julia packages and interactions between two packages, respectively. The figure shows julia packages within each layer. For example, the layer Data integration contains the packages "Retriever.jl" (**Re**), "Query.jl" (**Qu**), "MySQL.jl" (**My**), "SQLite.jl" (**lite**), and "DataFrames.jl" (**df**).

Index

Open automated research platforms, 7

research cycle, 7

robust experiments, 7

robust algorithms, 7

robust inference, 7