

## Machine and Human Intelligence research group (<u>website</u>) Department of Computer Science, University of Helsinki Finnish Center for Artificial Intelligence FCAI

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The Machine and Human Intelligence research group focuses on **probabilistic machine learning** applied to statistical model fitting of complex models in the computational sciences. We are interested in smart probabilistic algorithms that are robust and sample-efficient. Our research is regularly published in top-tier machine learning conferences, such as *NeurIPS* and *ICML*, and in renowned computational journals, such as *PLoS Computational Biology* (see <u>Publications</u>). The group is part of the <u>Department of Computer Science</u> of the University of Helsinki and of the <u>Finnish Center for Artificial Intelligence FCAI</u>.

- **Skills required:** Linear algebra, (Bayesian) statistics and probability, coding (Python or MATLAB).
- Supervisor: Luigi Acerbi (website); Contact: luigi.acerbi@helsinki.fi

## Research projects in sample-efficient probabilistic machine learning:

We develop probabilistic machine learning methods to perform *optimization* and *approximate Bayesian inference* with complex scientific models, with applications largely in (but not limited to) computational and cognitive neuroscience. To work with real models and data, our algorithms are *robust* to noise (e.g., due to Monte Carlo approximations or simulations) and *sample-efficient* in that they require a relatively small number of function evaluations with respect to traditional methods. Our algorithms are released as well-documented toolboxes (see our <u>Resources</u> page and the <u>lab GitHub</u>).

Potential research projects are related to extensions and applications of our algorithms:

- Variational Bayesian Monte Carlo (VBMC). <u>VBMC</u> is a new approach to Bayesian inference that obtains good approximations of the posterior and model evidence with a small number of likelihood evaluations (<u>Acerbi, 2018; NeurIPS</u>). The framework is currently being expanded in various directions, notably with the addition of support for noisy log-likelihood evaluations, such as those estimated via simulation (<u>Acerbi, 2020;</u> <u>NeurIPS</u>). We have also worked on applying surrogate modelling and active learning to the "embarrassingly parallel" setting (<u>de Souza, Mesquita, Kaski & Acerbi, 2022;</u> <u>AISTATS</u>). A Python version (PyVBMC) is about to be released (<u>docs</u>).
- Fast hybrid Bayesian optimization for model fitting via Bayesian Adaptive Direct Search (BADS). BADS is a fast optimization algorithm that combines a model-free approach (mesh-adaptive direct search) with a strong model-based algorithm (Bayesian optimization), achieving the best of both worlds, that is sample-efficiency and robustness to noise (<u>Acerbi & Ma, 2017; NeurIPS</u>). <u>BADS</u> is currently used by dozens of labs across the world. A Python version (PyBADS) is about to be released.
- Estimation of log-likelihoods for simulator-based models via inverse binomial sampling (IBS). IBS is an efficient statistical technique to estimate the log-likelihood when the log-likelihood is unavailable, but we can generate simulated data from the model. Unlike other "likelihood-free" methods, IBS does not use summary statistics, but computes the log-likelihood of the full data set (van Opheusden\*, Acerbi\* & Ma, PLoS Computational Biology, 2020). Moreover, IBS combines very well with BADS and VBMC.