

Partner search for FET-Open research project : Bayesian Models for Drug Discovery

RDFR20200504001 (under validation)

French SME specialized in the development of dedicated hardware for probabilistic Artificial Intelligence (AI) is looking for a partner in silico drug discovery to join a consortium of already 4 partners to apply to a European project (FET Open)

To complete their consortium, they are looking for a company or an academic partner expert in modelling molecules (expertise in 3D structures of molecules) to define the Bayesian models which will be used for the in silico drug screening.

Description

The aim of the project is to promote the development of new pharmaceutical treatments by combining data and prior knowledge on new or existing molecules.

The framework chosen is that of Bayesian inference. The probabilistic reasoning proposed by Reverend Bayes and by Laplace and then formalised by the physicist Jaynes is well adapted when it is a question of combining scientific knowledge with experimental data. Unfortunately, for complex problems and very large databases such as the one envisaged here, the computational time required to solve inferences remains totally prohibitive even on architectures using specialized processors such as GPUs.

The objectives of the consortium are:

1. Design probabilistic models to combine information from biological databases with scientific knowledge about the molecules and proteins of interest
2. Develop hardware architectures and the associated software to actually implement these models to predict the effects of molecules not yet tested on certain biological targets
3. Verify the validity of these predictions through in vitro experiments

Advantages and Innovations

Traditional machine learning methods are not well suited for in-silico drug discovery. On the opposite, Bayesian models allow to incorporate expert knowledge.

The project will aim to design Bayesian models for this application and develop dedicated hardware to accelerate the search of new molecules for undiscovered drugs.

Technical Specification or Expertise Sought

Expertise in modelling molecules

Stage of Development Proposal under development

Comments Regarding Stage of Development

At this stage, the consortium's competences partially cover those necessary to achieve the targeted objectives:

- A German partner (to be confirmed) (SME) can handle experimental verification and some aspects of modelling,
- A French partner (SME) can bring its knowledge in probabilistic models and its know-how in software design and development.
- A French partner (SME) can design the hardware architecture to achieve the performances.
- A Portuguese partner (Academic) can perform hardware implementations of these architectures and provide the hardware to make the predictions.

Call: FET-Open Challenging Current Thinking"

Dead line of the call: 3/06/2020

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