3iA Côte d'Azur
Interdisciplinary Institute for Artificial Intelligence

Ph.D. research topic

- Title of the proposed topic: **Attention mechanisms for graphical models, with applications to protein structure analysis.**
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- Research axis of the 3IA: AI -for-computional-biology-and-bio-inspired-AI
- **Supervisor (name, affiliation, email): Frederic Cazals, Inria. Email: frederic.cazals@inria.fr**
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- **Keywords:** deep learning, attention mechanisms, transformers, message passing, belief propagation, enumeration, approximation algorithms, free energy, protein structure analysis.
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- **Context.** Emerging from the field of natural language processing, (self-)attention mechanisms have proven essential to understand the coupling between tokens in a sentence [2, 3]. In a different context, graphical models make it possible to express the conditional dependence of random variables encoded in graph nodes via the edges of the graph. On such models, message passing algorithms provide effective ways to compute various quantities of interest, in particular partition functions and free energies [4, 5]. Recently, attention mechanisms have also proven key to encode the coupling between spatial patterns observed between amino acids in a protein structure [6]. The corresponding tool, AlphaFold by Deepmind, is considered a major achievement to predict a plausible structure of a protein from its amino-acid sequence. In related work, message passing algorithms have been used to compute average properties of proteins [1].
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- **Goals.** AlphaFold is a key achievement but outputs a single structure. In fact, statistical physics teaches us that observable properties of molecules depend on ensemble of conformations (weighted by Boltzmann's factor). (See also AI, molecular design and the Covid19.) The goal of this PhD thesis will be to extend attention mechanisms in the context of graphical models, to study ensembles of conformations rather than isolated observations. The work envisioned encompasses the design and analysis of algorithms, their coding (C++ and python), as well their experimental evaluation.

References

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