Postdoc position on Graph Kernel for Chemoinformatics in Rouen, France

June 7, 2018

Keywords Kernel methods, machine learning, chemoinformatics, graph kernels, graph representations

Brief Description of the position

Graph kernels [2, 7] can be understood as graph similarity measures corresponding to scalar products between graph's projections in an implicit (and possibly unknown) Hilbert space. On one hand, graph kernels can be used in any kernel method [1, 4–6], thanks to the underlying implicit embedding. On the other hand, relaxing the constraints associated to explicit vectorial representations of graphs limits the loss of structural information. Therefore, graph kernels allows to encode more structural information than classic graph embedding methods while being able to connect to powerful machine learning methods.

Graph kernels have been defined on molecular graphs and applied to chemoinformatics to build prediction models using the structural information encoded within molecular compounds [2, 3, 7]. However, intrinsic properties of atoms and theirs interactions induce some electronic properties which are not explicitly encoded within classic molecular graphs representations. The main purpose of this post doctoral position is to include this information into a new augmented kernel and apply it on some chemoinformatics datasets. The two main steps will be i) to define a new molecular representation encoding local electronic information and ii) to define a new similarity measure as a kernel to compare two molecules encoded in the new proposed representation.

This project will be supervised in close collaboration by LITIS (Rouen, France) and GREYC (Caen, France) laboratories which have a strong expertise on graph kernels for chemoinformatics. The chemical part will be supervised by COBRA laboratory (Rouen, France) which has proposed various atomic descriptors encoding some electronical information. Their expertise will be essential to be able to encode additional information into a new representation for chemical compounds.

Position Details:

Location The research will be conducted at LITIS Laboratory (Rouen, France) in Normandy. The LITIS (EA 4108) is affiliated to Normandie University, University of Rouen and INSA Rouen Normandie.

Start date September 2018

Duration 15 months

Salary about 2200 euros/month (net salary).

Application:

Required skills

- PhD in Applied Mathematics or computer science,
- Experience in C++, Python or Matlab programming,
- Knowledge in kernel methods or graph based approaches constitutes an advantage.

Contact `postdoc-graphkernel@litislab.fr`

Required documents

- up to date CV,
- Any recommendation letter
- A short document on research experience and interests

References

[1] Corinna Cortes and Vladimir Vapnik. Support vector machine. *Machine learning*, 20(3):273–297, 1995.

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[4] Alain Rakotomamonjy, Francis R Bach, Stéphane Canu, and Yves Grandvalet. Simplemkl. *Journal of Machine Learning Research*, 9(Nov):2491–2521, 2008.

[5] Bernhard Schölkopf, Koji Tsuda, and Jean-Philippe Vert. *Kernel methods in computational biology*. MIT press, 2004.

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