

Abridged CV

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Academic education

INSTITUTION AND LOCATION	DEGREE	Completion Date	FIELD OF STUDY
University of Lisbon, Lisbon	Licenciatura	3/1993	Forest Eng.
University of Lisbon, Lisbon	MSc	7/1998	Nat. Res Management
University of Lisbon, Lisbon	PhD	10/2001	Forest. Eng
New University of Lisbon, Almada	MSc	7/2004	Comp. Science

Personal Statement

Although coming from Forest Engineering, all my post graduate works were in Computer Science related works. I developed and defined information systems and data quality methods for biometric data in my First MSc and addressed complex spatial optimization problems with metaheuristics [Forest Science 608-621(14)]. I have a very strong quantitative background, including statistics and operations research. I have co-authored several reference works in bioontologies [PLoS Comput Biol 5 (7), e1000443] and automatic protein annotation [PloS one 7 (7), e40519], having supervised one PhD student in the area. Currently my research interests are focused in machine learning methods for in silico virtual screening having developed several models and prototypes. In particular the team I led has hit top scores in the international NIHS-NCATS-UNC DREAM Toxicogenetics competition [Nat Biotechnol. 33, 933–940 (2015)]. My second PhD student has completed her work in this area. I have further experience in the identification differential gene expression profiles [Genomics 106 (5), 268-277]. Due to my quantitative background coupled with a good biological foundation, I am capable of adapting to a large variety of problems as it is visible in my published works.

Positions and Employment

Jan 1999 - Oct 2001	Doctoral Studenta at Instituto Superior de Agronomia
Jan 2002 - Dec 2003	Post-Doctoral Student at Instituto Superior de Agronomia
Jan 2004 –Aug 2007	Invited assistant professor in the Department of Informatics, FCUL, University of Lisbon
Since Sep 2007-	Assistant professor in the Department of Informatics, FCUL, University of Lisbon. Tenured since 2011

Contribution to Science

In my PhD I addressed and solved a complex optimization problem untacked in the published literature until then. I formalized it mathematically and proposed a metaheuristic solution, having implemented it for a variety of real world situations [Falcao and Borges 2002]. In the process I created and implemented a new metaheuristic procedure that compares favorably to most published approaches. I have proposed and implemented an extension of radial basis function neural networks, which provide a more flexible and robust approximation to many types of machine learning

problems [Falcao et al 2006]. I have also been the driving force behind the B3PP model, a Quantitative Structure Activity Relationship model for inferring Blood-Brain barrier penetration [Martins et al 2012]. However, I believe that that my most important scientific contribution is a new method that is able to accurately measure molecular similarity, which I developed during my sabbatical license. This method has proved to be much more robust and accurate than most other published approaches and is able to identify close homologues in very large databases [Teixeira et al 2013]

Relevant authored and co-authored published work (in chronological order)

- Falcão, A O, Borges, J. G., 2002, Combining random and systematic search heuristic procedures for solving spatially constrained forest management scheduling models. *Forest Science* 608-621(14)
- Falcão, A.O., Langlois, T., Wichert, A. 2006 Flexible Kernels for RBF Networks. *Neurocomputing*. Vol 69. pp. 2356-2359
- Pesquita, C., Faria, D., Falcão, A. O, Lord, P., Couto, FM 2009: Semantic Similarity in Biomedical Ontologies. *PLoS Computational Biology* 5(7): e1000443. doi:10.1371/journal.pcbi.1000443
- D Faria, A Schlicker, C Pesquita, H Bastos, AEN Ferreira, M Albrecht, AO Falcao. 2012. Mining GO Annotations for Improving Annotation Consistency *PloS ONE* 7 (7), e40519
- Martins, IF, Teixeira, AL, Pinheiro, L., Falcao, AO. 2012. A Bayesian approach to in silico blood-brain barrier penetration modeling. *Journal of chemical information and modeling* 52 (6), 1686-1697
- Teixeira, AL. Falcao AO. 2013 Noncontiguous atom matching structural similarity function. *Journal of Chemical Information and Modeling*. 2013, 53 (10), pp 2511–2524 DOI: 10.1021/ci400324u.
- Eduati F, Mangravite LM, Wang T#, Tang H, Bare JC, Huang R, Norman T, Kellen M, Menden MP, Yang J, Zhan X, Zhong R, Xiao G, Xia M, Abdo N, Kosyk O, NIEHS-NCATS-UNC DREAM Toxicogenetics Collaboration[including Falcao AO], Friend S, Stolovitzky G, Dearry A, Tice RR, Simeonov A, Rusyn I, Wright FA, Xie Y, Saez-Rodriguez J. 2015. Prediction of human population responses to toxic compounds by a collaborative competition. *Nat Biotechnol*. 33, 933–940. doi:10.1038/nbt.3299. PMID: 26258538
- Clarke LA, Botelho HM, Sousa L, Falcao AO, Amaral MD [2015] Transcriptome meta-analysis reveals common differential and global gene expression profiles in cystic fibrosis and other respiratory disorders and identifies CFTR regulators. *Genomics*. 2015 Jul 29. pii: S0888-7543(15)30020-3. doi: 10.1016/j.ygeno.2015.07.005

Complete List of Published Works:

- <http://www.researcherid.com/rid/A-3545-2010>
- <https://scholar.google.com/citations?user=SU5DRhkAAAAJ>

Lecturing Activity

As a professor of the Department of Informatics I lecture both graduate and undergraduate courses in Information Systems [Introduction to Databases, Bioinformatics, Web Applications, Information Systems Analysis, Data warehousing and data mining]

Research Support

In 2014 the ASSUME [Data mining methods for ASessing Similarity of molecular structUres in MEtric spaces] project [<http://xldb.di.fc.ul.pt/wiki/ASSUME>] was completed, being a partially nationally funded project [SFRH/BD/64487/2009] which has produced most of the relevant research for in silico modeling within my research group. A new project MIMED [Mining the Molecular Metric Space for Drug Design] has been approved in 2015 with a total budget of €127,000 In both of these projects I am the PI