josé jiménez

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education

MSc | Statistics and Optimization
Universitat Politècnica de Catalunya | 2015-2017

- Research: bayesian optimization, machine learning
- Advisor: Josep Ginebra
- avg. grade: 9.3/10 (top 1%)

BSc | Statistics
Universidad de Sevilla | 2011-2015

- focus on Markov Chain Monte Carlo methods
- avg. grade: 9.41/10
- awards: best average grade.

skills

programming
python
R
golang
bash
C
matlab
wolfram mathematica
LaTeX
pl/sql
html, css, js, jquery, php

software
gnu-linux (sysadmin)
git
ml frameworks
python scientific stack
cheminformatics software stack
spss
sas
excel

languages
spanish (native)
english (C2)

teaching
computer-aided drug design seminar lecturer (2 lectures)
PhD & MSc-level student supervision

experience

ETH Zürich (Zürich, Switzerland)
Postdoctoral fellow
Nov. 2019 (current)
Advisors: Gisbert Schneider & Nils Weskamp
Research: Explainable AI in drug discovery. Position funded by Boehringer Ingelheim Pharma. GmbH & Co.

Institute for Pure & Applied Mathematics | UCLA (CA, USA)
Research fellow
Sept. 2019 - Nov. 2019
Program: Machine Learning for Physics and the Physics of Learning

Comp. Science Lab. | Universitat Pompeu Fabra (Barcelona, Spain)
PhD studies
Jan. 2016 - Oct. 2019
Advisor: Gianni De Fabritiis
Research: Machine learning in structural biology and computational chemistry

- investigated 3d volumetric representations for atomistic systems and applied neural-network models for binding site prediction, lead optimization, generative modeling and ligand selectivity prediction.
- extensive collaborations with pharmaceutical companies such as Novartis, Pfizer, Biogen and Janssen

Communications and Marketing Institute (Sevilla, Spain)
Internship
Jan. 2015 - Jun. 2015

- development of classical statistical models in sociodemographic studies

selected proceedings

journal papers

- Jiménez, J., Skalic, M., Martínez-Rosell, G., & De Fabritiis, G. (2018). K_{DEEP}: Protein–Ligand Absolute Binding Affinity Prediction via 3D-Convolutional Neural Networks. Journal of chemical information and modeling, 58(2), 287-296.
- Jiménez, J., Doerr, S., Martínez-Rosell, G., Rose, A. S., & De Fabritiis, G. (2017). DeepSite: protein-binding site predictor using 3D-convolutional neural networks. Bioinformatics, 33(19), 3036-3042.
- Jiménez-Luna, J., Pérez-Benito, L., Martínez-Rosell, G., Sciabola, S., Torella, R., Tresadern, G., & De Fabritiis, G. (2019). DeltaDelta neural networks for lead optimization of small molecule potency. Chemical Science, 10(47), 10911-10918.
- Jiménez-Luna, J., Grisoni, F., and Schneider G. (2020). Drug discovery with explainable artificial intelligence. Nature Machine Intelligence 2 (10), 573-584.

posters

- Jiménez, J. & De Fabritiis. Relative Protein-ligand Binding Affinity Prediction with 3d-convolutional Neural Networks. 2018 Workshop on Free Energy Methods, Kinetics and Markov State Models in Drug Design. Boston (MA), May. 2018.
- Jiménez, J. & De Fabritiis. Lead Optimization of Congeneric Series via Convolutional Neural Networks. 1st RSC AI in Chemistry Symposium. London (UK), Jun. 2018.

talks

- Predicting Protein-ligand Affinities with PyTorch. Bioinformatics Open Days 2019. Braga (PT), Feb. 2019.