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 | 2015

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

skills

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

software
gnu-linux
git
ml frameworks
python scientific stack
spss
sas
excel

languages
spanish (native)
english (C2)

experience

RETHINK | ETH Zürich (Switzerland)
Postdoctoral fellow
Nov. 2019 (current)
Explainable AI in drug discovery.

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

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

- investigated 3d volumetric representations for biological systems
- applied 3d-convolutional neural networks for binding site prediction, protein-ligand affinity prediction and generative modeling
- research on ligand selectivity prediction
- development and deployment of production machine learning models

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

- development of statistical models in sociodemographic studies
- statistical support and analysis with a focus on data visualization

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, J., Sabbadin, D., Cuzzolin, A., Martínez-Rosell, G., Gora, J., Manchester, J., Duca, J., & Gianni De Fabritiis (2019). PathwayMap: Molecular Pathway Association with Self-Normalizing Neural Networks. Journal of Chemical Information and Modeling, 59 (3), 1172-1181

posters

- Jiménez, J. , Skalic, M. & De Fabritiis, G. K_{DEEP}: Protein–Ligand Absolute Binding Affinity Prediction via 3D-Convolutional Neural Networks. 1st DCEXS PhD symposium. Barcelona (Spain) Nov. 2017.
- 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.