Carlos Xavier Hernández

Research Scientist

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I am a Research Scientist at Facebook Research. Previously, I worked on neural interfaces at CTRL-labs. Prior to that, I did my thesis at Stanford with Vijay Pande on statistical modeling and representation learning of complex biomolecular dynamics.

Experience

Facebook Research — New York, NY, USA
Research Scientist — 2019 - PRESENT

CTRL-labs — New York, NY, USA
Research Scientist — 2018 - 2019

Stanford University — Stanford, CA, USA
NSF Graduate Research Fellow w/ Vijay S. Pande — 2013 - 2018

Education

Stanford University — Stanford, CA, USA
Ph.D. in Biophysics — 2013 - 2018
Thesis: "Towards a Deeper Understanding of Molecular Mechanics"

Columbia University in the City of New York — New York, NY, USA
B.S. in Applied Mathematics — 2009 - 2013

Publications

Kinetic Machine Learning Unravels Ligand-Directed Conformational Change of μ-Opioid Receptor — 2018
EN Feinberg, AB Farimani, **CX Hernández**, and VS Pande
bioRxiv (doi: 10.1101/170886)

Variational Encoding of Complex Dynamics — 2018
CX Hernández*, HK Wayment-Steele*, MM Sultan*, BE Husic, and VS Pande
Phys. Rev. E (doi: 10.1103/PhysRevE.97.062412)

Using Deep Learning for Segmentation, and Counting within Microscopy Data — 2018
CX Hernández, MM Sultan, and VS Pande
arXiv (arXiv: 1802.10548)

Markov State Models Provide Insights into Dynamic Modulation of Protein Function — 2015
D Shukla, **CX Hernández**, JK Weber, and VS Pande
Accounts of Chemical Research (doi: 10.1021/ar5002999)

Structure-based Network Analysis of An Evolved G-Protein Coupled Receptor Homodimer Interface — 2013
SE Nichols*, **CX Hernández***, Y Wang, and JA McCammon
Protein Science (doi: 10.1002/pro.2258)

Understanding the Origins of a Pandemic Virus — 2011
CX Hernández, J Chan, H Khiabanian, and R Rabadan
arXiv (arXiv: 1104.4568)

Software

MolEncoder: Molecular Autoencoder in PyTorch 2017
CX Hernández
GitHub (url: https://github.com/cxhernandez/molencoder)
● Python ★ 56 ⑂ 10

MDEntropy: Information-Theoretic Analyses for Molecular Dynamics 2017
CX Hernández and VS Pande
The Journal of Open Source Software (doi: 10.21105/joss.00427)
● Python ★ 19 ⑂ 8

MSMExplorer: Data Visualizations for Biomolecular Dynamics 2017
CX Hernández, MP Harrigan, MM Sultan, and VS Pande
The Journal of Open Source Software (doi: 10.21105/joss.00188)
● Python ★ 12 ⑂ 13

MSMBuilder: Statistical Models for Biomolecular Dynamics 2017
MP Harrigan, MM Sultan, CX Hernández, BE Husic, P Eastman, CR Schwantes, KA Beauchamp, RT McGibbon, and VS Pande
Biophysical Journal (doi: 10.1016/j.bpj.2016.10.042)
● Python ★ 95 ⑂ 69

Osprey: Hyperparameter Optimization for Machine Learning 2016
RT McGibbon, CX Hernández, MP Harrigan, S Kearnes, MM Sultan, S Jastrzebski, BE Husic, and VS Pande
The Journal of Open Source Software (doi: 10.21105/joss.00034)
● Python ★ 71 ⑂ 22

MDTraj: A Modern, Open Library for the Analysis of Molecular Dynamics Trajectories 2015
RT McGibbon, KA Beauchamp, MP Harrigan, C Klein, JM Swails, CX Hernández, CR Schwantes, LP Wang, TJ Lane, and VS Pande
Biophysical Journal (doi: 10.1016/j.bpj.2015.08.015)
● Python ★ 253 ⑂ 163

Posters & Presentations

Convolutional Neural Networks for Visual Recognition (CS231N) Stanford, CA, USA
Invited Presentation 2017
"Using Deep Learning for Segmentation and Counting within Microscopy Data"

Biophysical Society Meeting Los Angeles, CA, USA
Poster 2016
"Intrinsic Disorder in the P53 C-Terminal Regulatory Domain Yields Multiple Pathways for Folding-Upon-Binding"

Workshop on Molecular and Chemical Kinetics Berlin, DEU
Poster 2015
"Inferring Causality Along Transition State Pathways"

Honors & Awards

2013 **ADVANCE Summer Research Fellowship,** Stanford University
2013 **Graduate Research Fellowship,** National Science Foundation
2012 **EXROP Undergraduate Research Fellowship,** Howard Hughes Medical Institute
2011 **Genentech Summer Undergraduate Research Fellowship,** Columbia University - Genentech

Press

2012 **Pandemic Flu Risk Raised by Lax Hog-Farm Surveillance,** Wired Magazine
2011 **The Origin and Evolution of a Pandemic Virus,** MAGNet Newsletter