Carlos Xavier Hernández

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NSF Graduate Research Fellow at Stanford University interested in tackling emerging challenges in machine learning. Experience with deep learning, causal inference, statistical modeling, and simulation.

Education

Stanford University — Stanford, CA, USA
Ph.D. in Biophysics — 2013 - PRESENT
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

Skills

Primary languages: Python, Javascript. Familiar with R, C++, MATLAB, Perl, SQL.
Frameworks: PyTorch, Keras.
Proficient in Git, Vim, LaTeX, HTML/CSS, Unix, HPC (e.g. SLURM, MPI)

Software

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 ★ 13 ⑂ 5

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 ★ 10 ⑂ 12

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 ★ 74 ⑂ 55

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 ★ 48 ⑂ 20

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 ★ 169 ⑂ 115

Publications

Kinetic Machine Learning Unravels Ligand-Directed Conformational Change of μ-Opioid Receptor — 2018
EN Feinberg, AB Farimani, CX Hernández, and VS Pande
Science Advances (accepted)

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

Variational Encoding of Complex Dynamics — 2017
CX Hernández*, HK Wayment-Steele*, MM Sultan*, BE Husic, and VS Pande
arXiv (arXiv: 1711.08576)

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

2015

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

2013

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

2011

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"

Research

Stanford University   Stanford, CA, USA
NSF Graduate Research Fellow w/ Vijay S. Pande   2013 - PRESENT
- Developed a method to construct optimized representations of biomolecular motions using deep learning
- Developed a method for inferring causality within biomolecular dynamics
- Investigated folding-upon-binding interactions using Markov state modeling
- Maintained several Python projects related to statistical modeling and visualization of biomolecular dynamics

Center for Computational Biology and Bioinformatics   New York, NY, USA
Undergraduate Research Assistant w/ Raul Rabadan   2010 - 2013
- Studied the role of viruses in the onset of pediatric brain tumors
- Investigated the swine-origin of the 2009 H1N1 influenza pandemic using a Markov chain Monte Carlo approach

University of California, San Diego   La Jolla, CA, USA
HHMI EXROP Undergraduate Research Fellow w/ J. Andrew McCammon   2012
- Developed a network-based algorithm to study the role of evolution in protein dynamics
- Studied the homodimerization of CXCR4 using aforementioned method

Columbia University Medical Center   New York, NY, USA
Genentech Undergraduate Research Fellow w/ Stephen P. Goff   2011
- Studied the co-localization of $TRIM5\alpha$ with HIV capsid within mammalian cells
- Performed viral protein extraction from leucemic long-necked clams

Teaching Experience

Future Advancers of Science and Technology (FAST)   Stanford, CA, USA
Mentor and Founding Member   2015-2017
- Prepared IB students at Andrew P. Hill High School in San Jose, CA to register for Bay Area science fairs
- Guided students towards completion of their own original research projects
- Organized and trained other mentors from Stanford University

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