

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 data visualization.

Education

Stanford University

Ph.D. in Biophysics

Thesis: "Towards a Deeper Understanding of Molecular Mechanics"

Stanford, CA, USA

2013 - PRESENT

Columbia University in the City of New York

B.S. in Applied Mathematics

New York, NY, USA

2009 - 2013

Skills

Primary languages: Python, Javascript. Familiar with R, C++, MATLAB, Perl, SQL.

Frameworks: PyTorch, Keras.

Proficient in Git, Vim, LaTeX, D3, 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** 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 Khiabani, and R Rabadan
[arXiv](#) (arXiv: 1104.4568)

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 α 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