

# 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

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, 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  $\mu$ -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

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- 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

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- 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

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- 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

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- 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

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