Xunmo Yang

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Education

University of Houston - Houston, TX, US
Ph.D, Chemistry (GPA: 3.6) May 2016
- Dissertation: *Ab initio* Calculations of Intramolecular Charge and Energy Transfer with Reduced Modes in Donor-bridge-acceptor Species
- Advisor: Dr. Eric R. Bittner

Xiamen University - Xiamen, Fujian, China
Bachelor of Science, Chemistry; Mathematics Minor July 2009
- Thesis: Study of Weak Interaction and Aromatic Carbon Atom in DREIDING Force Field

Udacity - Machine Learning Engineer Nanodegree February 2016
Udacity - Data Analyst Nanodegree September 2015

Skills

Working Knowledge
Python, Mathematica, R, HTML/CSS, D3.js, Octave/MATLAB, SQL, TensorFlow, SAS, Vim, Linux, LaTeX, Q-Chem, Gaussian, various chemistry instruments

Basic Knowledge
JavaScript, OpenCV, MongoDB, Hadoop, HBase, Pig, Hive, Spark, Splunk, FORTRAN, C, Haskell

Languages
Fluent in English, Chinese. Proficient in Taiwanese.

Project Experience

Pseudo-hologram Video Maker May 2016
- Deployed an OpenCV-based program online for pseudo-hologram video conversion using Flask

English Letter Recognition February 2016
- Trained a 6 layer convolutional neural network with 95% accuracy on notMNIST dataset using TensorFlow

Clustering of Vervet Monkey's Alarms February 2016
- Verified the classical discovery of three types of alarms in vervet monkey by hierarchical, k-means and partitioning around medoids (PAM) clustering, achieved at least 75% classification accuracy
- Built an AdaBoost model with 99% prediction accuracy

Creating Customer Segments January 2016
- Applied PCA and independent component analysis (ICA) to a customer dataset of a wholesale distributor to preprocess and understand purchasing behavior better
- Used Gaussian mixture model to find customer segments for better A/B test on policy change

Train a Smartcab to Drive January 2016
- Taught toy smartcab traffic laws and best routing strategy with Q-learning. The driving agent was able to consistently reach the destination within allotted time with 95% success rate

Forum Data Analysis October 2015
- Analyzed the posts on Udacity's forum using Hadoop MapReduce codes

PISA Data Visualization September 2015
- Explored the relations between family possessions and student scores in the Programme for International Student Assessment (PISA) data using R and Python

- Visualized the analysis with interactions using D3.js and dimple.js

Red Wine Study — September 2015

- Modeled the influence of various chemicals to red wine quality on a wine dataset by linear regression with Lasso in RStudio

Increased-by-one Single Tape Turing Machine — June 2015

- Implemented an increased-by-one single tape Turing machine program with only HTML/CSS, inspired by a discussion of the Turing completeness of HTML/CSS

Identifying Fraud from Enron Email — May 2015

- Investigated the Enron email corpus data with decision tree, Gaussian naive Bayesian, and k-means clustering machine learning techniques

Houston Map Data Wrangling — May 2015

- Cleaned the map data on openstreetmap of the great Houston area (file size > 500M)
- Analyzed the cleaned data with MongoDB queries

<The Essential Hayek> Translation — March 2016

- Translated <The Essential Hayek> voluntarily to Chinese

Certificates

SAS Certified Base Programmer for SAS 9 Credential

11 computer science courses on edX, Coursera and Udacity (certificates available on my LinkedIn)

Research & Teaching Experience

University of Houston, Houston, TX

Research & *Teaching Assistant* — August 2010 - present

- Developed and coded in Mathematica a new theoretical molecular dynamics analysis scheme based on Lanczos algorithm and time-convolutionless master equation
- Benchmarked the scheme with a classical series of molecules and researched the dynamics
- Optimized the geometry of tripodal amine-Cu(I) complexes using density functional theory (DFT), to assist further research of their reactivity and stability
- Taught general and physical chemistry labs independently. Instruments used include UV/VIS, FT-IR, ESR, NMR, STM and XRD

Xiamen University, Xiamen, Fujian, China

Research Assistant — August 2009 - June 2010

- Implemented FORTRAN programs for the point group and atom type recognition in AMBER and DREIDING force fields, as part of efficient QM/MM method development

Publications

Intramolecular Charge and Energy Transfer Rates with Reduced Modes: Comparison to Marcus Theory for Donor-Bridge-Acceptor Systems

Yang, Xunmo and Bittner, Eric. *The Journal of Physical Chemistry A*, **2014**, *118*(28), pp 5196-5203

Computing Intramolecular Charge and Energy Transfer Rates using Optimal Modes

Yang, Xunmo and Bittner, Eric. *The Journal of Chemical Physics,* 142*, 244114 (2015)*

Tripodal Amine Ligands for Accelerating Cu-Catalyzed Azide-Alkyne Cycloaddition: Efficiency and Stability against Oxidation and Dissociation

Zhiling Zhu, Siheng Li, Haoqing Chen, Yongkai Huang, Xunmo Yang, Eric Bittner, and Chengzhi Cai. (Submitted to *Organic* & *Biomolecular Chemistry*)

Patent

Coriolis force experiment plate — No.: CN 2665845 Y — Issued: 12/22/2004