Youlin Liu

Purdue University, West Lafayette, IN 765-409-6703 yliu0593@gmail.com Website

Overview

- Research experience in spectroscopic image analysis, chemometrics, physics modeling with relevant statistical methods
- Interdisciplinary problem solving driven combining broad chemistry knowledge and coding skills
- Documentation system management with scripting languages on an aesthetics level
- Comfortable communicating complex data to lay and technical audiences in written, verbal, and visual formats

Education

Purdue University — **West Lafayette, Indiana**
PhD in Chemistry (expected Aug. 2021) — 2016–present

University of Science and Technology of China (USTC) — **Hefei, China**
Bachelor of Science, Chemistry — 2012–2016

Research Experience

Simpson Lab of Nonlinear Optics — **Purdue University**
Graduate Researcher — 11/2016–present

Generative Adversarial Linear Discriminant Analysis

- Designed the structure of the main algorithm
- Optimized coding efficiency by substituting a genetic algorithm with an analytical model
- Evaluated the GALDA model with PCA, PLS-DA, PCA-LDA and Regularized LDA with rigorous cross-validation
- Published a public git repository for the GALDA model

Hyperspectral Infrared Imaging Microscope Design and Digital Image Analysis

- Aligned optical components for a microscope to achieve co-propagation of a visible beam with an IR beam
- Managed and trouble-shoot electronics for synchronized digitization across signal acquisition
- Tested various image segmentation methods for various samples (chemical and tissue)
- Used Machine Learning packages from MATLAB and scikit for classification tasks

High-Throughput Fluorescence Recovery After Photobleaching Diffusion Analysis of Protein/Excipient Interactions

- Modeled an untraditional artificial neural network as a regression model with complex layer design for incorporated physics level parameters with experimental measurables
- Tested and validated DLVO model with simulated FRAP (Fluorescence recovery after photobleaching) data
- Assessed model accuracy with multivariate analysis and error propagation

Synchrotron X-Ray Damage Analysis With Non-Negative Matrix Factorization

- Performed X-ray diffraction experiments at Argonne National Laboratory
- Converted Synchrotron raw data to MATLAB accessible images for in-house analysis
- Indexed peaks with XDS, HKL2000

DNA-Enabled-Nano-Group, USTC — **Hefei, China**
Undergraduate Researcher — 05/2015–06/2016

SERS (Surface-enhanced Raman spectroscopy) with gold nanoparticles

- Optimized inorganic synthesis via reaction control
- Characterized gold dimers for plasmonic properties

Mesoscale Chemical Systems, University of Twente — **Enschede, The Netherlands**
Research Intern — 06/2015–08/2015

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Sonochemical effects analysis with microfluidic sonochemical reactor

- Designed and conducted experiments to analyze sonochemical effects with chemiluminescence
- Analyzed large amount of data for statistical significance
- Validated a microfluidic sonochemical reactor's capability for producing localized radicals

Skills

Hands-on: Standard inorganic&organic synthesis, optics alignment, synchronize digitization, FT-IR, crystallization, X-ray diffraction, HPLC

Proficient coding languages: MATLAB, python, C++

Typesetting and documentation management: LaTeX, Markdown, html, pandoc, git, bash

Other standalone suites: LabView, XDS, HKL2000, CCP4, Vina, ImageJ

Outreach & Teaching

Teaching Assistant: General chemistry teaching assistant, Purdue University 2017-2018
Head TA: General chemistry II course coordinator for interactive teaching 2018
Graduate TA Mentor: Guidance and feedback to new graduate teaching assistants 2018-2019

Conferences

Pittcon Conference Generative Adversarial Linear Discriminant Analysis Atlanta, GA(virtual) 2021
ACS Generative Adversarial Linear Discriminant Analysis San Diego, CA (virtual) 2020
Pittcon Conference Hyperspectral image classification Chicago, IL 2020
Turkey Run Analytical Chemistry Conference Adversarial Spectroscopy Marshall, IN 2019
Pittcon Conference Hyperspectral IR imaging Philadelphia, PA 2019

Publications

Li, M., Razumtcev, A., Yang, C.; Liu, Y., Rong, J.,Razumtcev & Simpson, G. J. "Fluorescence-Detected Mid-Infrared Photothermal Microscopy" (submitted)

Liu, Y., Smith, C., Cao, Z.; Sherman, A., & Simpson, G. J. "Generative Adversarial Linear Discriminant Analysis" (submitted)

"High-Throughput Fluorescence Recovery After Photobleaching Diffusion Analysis of Protein/Excipient Interactions" (manuscript in preparation)

Sarkar, S, Florian, H., Liu, Y., Geiger, A. & Simpson, G. J. "Non-negative Matrix Factorization for Isolating Damage-Free Reflections in Macromolecular Synchrotron Data Collection" (manuscript in preparation)

Smith, C., Liu, Y., & Simpson, G. J. "Defense Against Adversarial Spectroscopic Attacks" (Conference Presentation). In Big Data: Learning, Analytics, and Applications (Vol. 10989, p. 109890F). International Society for Optics and Photonics.

Geiger, A. C., Ulcickas, J. R., Liu, Y., Witinski, M. F., Blanchard, R., & Simpson, G. J. "Sparse-sampling methods for hyperspectral infrared microscopy". In Image Sensing Technologies: Materials, Devices, Systems, and Applications VI (Vol. 10980, p. 1098016). International Society for Optics and Photonics.

Bram, V., Liu, Y., Pérez, A., Castro-Hernandez, E., & Rivas, D. F. "Scaled–up sonochemical microreactor with increased efficiency and reproducibility." ChemistrySelect 1, no. 2 (2016): 136-139.