Jeremy R. Ash

Bioinformatics Ph.D. · Statistics M.S.

Address: 1717 S Dorsey Lane Apt. 1132, Phoenix, AZ 85281. Citations: 224. h-index: 6. i10-index: 6.

jeremyryanash@gmail.com | jrash.github.io/ | jrash | jeremyryanash | @jeremyr_ash | Google Scholar | ORCID iD | Publons

Education

North Carolina State University — *Raleigh, NC, USA*

Bioinformatics, Ph.D. | Statistics, M.S. — *Aug. 2014 - Dec. 2019*

- GPA:3.76

The University of Texas at Austin — *Austin, TX, USA*

Biology, B.S. — *Aug. 2010 - Aug. 2013*

Skills

Research Areas	Improving QSAR models with molecular dynamics, Uncertainty quantification in virtual screening, Cheminformatics methods development, Bioinformatics, Chemometrics, Data visualization
Programming	R, Python (tensorflow, scikit-learn, etc.), C++, Linux, LaTeX, Schrodinger, Knime, High performance computing, Software development (Continuous integration, Version control, Unit testing, Documentation)
Statistics	Machine learning, Statistical modeling (Frequentist, Bayesian, Multivariate, Non-Parametric), Simulation, Methods development, Probability theory, Numerical methods

Experience

Research Statistician — *Cary, NC*

SAS Institute, JMP Division, Stats R&D — *Jan. 2020 - PRESENT*

- Transitioning to Research Statistician Developer with half of my time spent on feature development in C++.
- Research and prototype methodologies in consideration for JMP, using R, Python, SAS and JSl (JMP scripting language).
- Evaluate methodologies using customer and simulation data. Present findings to development as they plan new features.
- Support test driven development by writing and managing suites of unit tests and confirming accuracy in daily software builds.
- Engage with customers through conference presentations, published research and beta feedback.
- Recent projects include: wavelet based functional analysis for chemical spectra, a novel method for avoiding extrapolation in JMP's prediction profilers for machine learning models, a multivariate control chart platform for detecting outliers in high dimensional data.

Graduate Industrial Intern — *Cary, NC*

SAS Institute, JMP Division, Stats R&D — *Aug. 2018 - Dec. 2019*

Graduate Research Assistant — *NCSU*

Advisors: Jacqueline Hughes-Oliver and Denis Fourches — *Aug. 2015 - Dec. 2019*

- Statistical methods development for QSAR models – models predicting the bioactivity of small molecules given their chemical structure.
- Uncertainty quantification in virtual screening: confidence band and hypothesis tests methods for hit enrichment curves at extremely small testing fractions.
- Using information from molecular dynamics simulations to improve machine learning methods for drug activity prediction.
- Developing **chemmodlab**, an R package for building cheminformatics machine learning models.

Graduate Research Assistant — *NCSU*

Advisor: Jeff Thorne — *Aug. 2014 – July 2015*

- Group project with the labs of Scott Schmidler (Duke), and Jotun Hein (Oxford) hosted by The Statistical and Applied Mathematical Sciences Institute.
- Improved the biological realism of insertion and deletion in a Bayesian model for the joint estimation of phylogeny and protein structure alignment. Implemented in the software, **StatAlign**.

Research Associate

LSU

Advisor: Jeremy Brown

Feb. 2014 – Aug. 2014

- Collaborated with the lab of Kyle Gallivan (Florida State University) developing **TreeScaper**, software for analysis of phylogenetic networks.
- Wrote extensive **documentation** as the non-linear dimensionality reduction and network analysis methodologies were unfamiliar in the phylogenetics community.

Research Assistant

UT Austin

Advisors: Harold Zakon and David Hillis

Dec. 2012 – Dec. 2013

- Used phylogenetic methods to predict functional divergences of sodium channels during their evolutionary history.

Research Assistant

UT Austin

Advisor: Daniel Johnston

Oct. 2012 – Oct. 2013

- Studied the involvement of the prefrontal cortex in trace eyelid conditioning in mice using behavioral training, genetic engineering, and histology.

Graduate Courses

Statistics Ph. D.

- Statistical Theory I & II
- Linear Models and Variance Components
- Computing for Statistical Research
- Experimental Statistics For Biological Sciences
- Real Analysis

Statistics Masters

- Introduction to Statistical Learning
- Applied Bayesian Analysis
- Linear Models and Regression

Bioinformatics Ph. D.

- Bioinformatics I & II
- Computational Methods for Molecular Biology
- Bioinformatics Consulting
- Molecular Genetics
- Functional Genomics

Teaching

JMP Blog

Virtual

Blogger

May 2021 - PRESENT

- Writing a series on chemical spectral analysis in JMP, see **here** and **here**.

CH795 Special Topics in Chemistry: Computational Chemistry

Raleigh, NC

Guest Lecturer

Spring 2018

- Taught an introduction to the R programming language. Materials can be found **here**.

Society of Systematics Biologists Conference

Baton Rouge, LA.

Workshop Instructor

Jan. 2017

- Lead a 3 hour workshop on TreeScaper, software I helped develop. Materials can be found **here**.

Awards

Oct 2019	International Conference on Statistical Distributions and Applications Travel Grant
Aug 2018	ACS Division of Chemical Information Scholarship of Excellence
Fall 2017	Triangle Center of Evolutionary Medicine Fellowship
Aug 2017	ACS Division of Chemical Information Scholarship of Excellence
Fall 2014	NCSU Graduate School Fellowship

Publications

Under Review or In Preparation:

14) **Ash, J. R.**; Mishne, G, Chi, E. *Co-manifold Learning: Improved Clustering and Activity Cliff Visualization with Distinct Sets of Descriptors.* (in prep. for J. Cheminform.).

13) **Ash, J. R.**; Hughes-Oliver, J. M. *chemmodlab 2.0: Confidence Bands and Hypothesis Tests for Hit Enrichment Curves.* (in prep. for J. Cheminform.).

12) **Ash, J. R.**; Hughes-Oliver, J. M. *Confidence Bands and Hypothesis Test Methods for Recall Curves at Extremely Small Fractions with Applications to Drug Discovery.* (in prep. for J. Amer. Statist. Assoc.). arXiv paper **here**.

Published (Entries link to papers):

11) Akhtari, F. S.; Havener, T. M.; Hertz, D. J.; **Ash, J. R.**; Larson, A.; McLeod, H. L.; Motsinger-Reif, A. A. *Race and Smoking Status Associated with Paclitaxel Drug Response in Patient-Derived Lymphoblastoid Cell Lines.* Pharmacogenet. Genomics. 2021, 31 (2), 48-52..

10) Odenkirk, M. T.; Zin, P. P. K.; **Ash, J. R.**; Reif, D. M.; Fourches, D.; Baker, E. S. *Structural-based connectivity and omic phenotype evaluations (SCOPE): a cheminformatics toolbox for investigating lipidomic changes in complex systems.* Analyst. 2020, 145 (22), 7197-7209. (Cover Article)

9) **Ash, JR** *Methods Development for Quantitative Structure-Activity Relationships.* North Carolina State University, PhD Dissertation. 2019.

8) Odenkirk, M. T.; Stratton, K. G.; Gritsenko, M. A.; Bramer, L. M.; Webb-Robertson, B. M.; Bloodsworth, K. J.; Weitz, K. K.; Lipton, A. K.; Monroe, M. E.; **Ash, J. R.**; Fourches, D.; Taylor, B. D.; Burnum-Johnson, K. E.; Baker, E. S. *Unveiling molecular signatures of preeclampsia and gestational diabetes mellitus with multi-omics and innovative cheminformatics visualization tools.* Mol. Omics. 2020, 16 (6), 521-532. (Cover Article)

7) Fourches, D.; **Ash, J.** *4D-Quantitative Structure–Activity Relationship Modeling: Making a Comeback.* Expert Opin. Drug Discov. 2019, 14 (12), 1227–1235.

6) **Ash, J. R.**; Kuenemann, M. A.; Rotroff, D.; Motsinger-Reif, A.; Fourches, D. *Cheminformatics Approach to Exploring and Modeling Trait-Associated Metabolite Profiles.* J. Cheminform. 2019, 11 (1), 43.

5) Burnum-Johnson, K. E.; Zheng, X.; Dodds, J. N.; **Ash, J.**; Fourches, D.; Nicora, C. D.; Wendler, J. P.; Metz, T. O.; Waters, K. M.; Jansson, J. K.; Smith, R. D.; Baker, E. S. *Ion Mobility Spectrometry and the Omics: Distinguishing Isomers, Molecular Classes and Contaminant Ions in Complex Samples.* TrAC Trends Anal. Chem. 2019, 116, 292–299.

4) Menden M. P.; Wang D.; Guan Y.; Mason M.; BenceSzalai, Bulusu K. C.; Yu T.; Kang J.; Jeon M.; Wolfinger R.; Nguyen T.; Zaslavskiy M.; **AstraZeneca-Sanger Drug Combination DREAM Consorti**; Jang I. S.; Ghazoui Z.; Ahsen M. E.; Vogel R.; Neto E. C.; Norman T.; Tang E. K. Y.; Garnett M. J.; Di Veroli G.; Fawell S.; Stolovitzky G.; Guinney J.; Dry J. R.; Saez-Rodriguez J. *Community Assessment of Cancer Drug Combination Screens Identifies Strategies for Synergy Prediction.* Nat. Commun. 2019, 10 (1), 2674.

3) **Ash, J. R.**; Hughes-Oliver, J. M. Chemmodlab: A Cheminformatics Modeling Laboratory R Package for Fitting and Assessing Machine Learning Models. J. Cheminform. 2018, 10 (1).

2) **Ash, J.**; Fourches, D. *Characterizing the Chemical Space of ERK2 Kinase Inhibitors Using Descriptors Computed from Molecular Dynamics Trajectories.* J. Chem. Inf. Model. 2017, 57 (6), 1286–1299.

- Awarded ACS Editor's Choice.

1) Huang W.; Zhou G.; Marchand M.; **Ash J. R.**; Morris D.; Van Dooren P.; Brown J. M.; Gallivan K. A.; Wilgenbusch J. C. *TreeScaper: Visualizing and Extracting Phylogenetic Signal from Sets of Trees.* Mol. Biol. Evol. 2016, 33 (12), 3314–3316.

Patents

Ash, J. R.; Gotwalt, C. M., Lancaster, L. C. *Analytic system with extrapolation control in interactive graphical prediction evaluation.* US Patent 10,963,804. 2021. Patent document **here.**

Selected Presentations

(When available, titles link to presentations)

JMP Discovery Summit Europe — *Virtual*

PRESENTATION — *Jan. 2021*

Lancaster, L, **Ash JR**, Gotwalt, C. *Controlling Extrapolation in the Prediction Profiler in JMP Pro 16.*.

JMP Discovery Summit America — *Virtual*

PRESENTATION — *Oct. 2020*

Ash JR. *Fault Detection and Diagnosis of the Tennessee Eastman Process using Multivariate Control Charts.*.

Joint Statistical Meetings — *Virtual*

PRESENTATION — *Aug. 2020*

Ash JR, Lancaster L. *Methods for Helping Users Avoid Extrapolation when Making Predictions with Statistical and Machine Learning Models.*

Bioinformatics Ph. D. Defense — *Raleigh, NC*

PRESENTATION — *June 2021*

Ash JR *Methods Development for Quantitative Structure-Activity Relationships.*.

International Conference on Statistical Distributions and Applications — *Grand Rapids, MI*

POSTER — *Oct. 2019*

Ash JR, Hughes-Oliver JM. *Confidence Bands and Hypothesis Test Methods for Recall and Precision Curves at Extremely Small Fractions with Applications to Drug Discovery.*.

American Chemical Society Conference — *Boston, MA*

PRESENTATION — *Aug. 2018*

Ash JR, Kuenemann MA, Rotroff D, Motsinger-Reif A, and Fourches D. *Structure-Based Approach to Exploring and Modeling Trait-Associated Metabolite Profiles.*

POSTER

Ash JR, Hughes-Oliver JM and Fourches D. *Molecular Modeling of Differential ERK1/2-Ligand Dynamic Interactions*.

- ACS Division of Chemical Information Scholarship of Excellence.

American Chemical Society Conference — *Washington, DC*

PRESENTATION — *Aug. 2017*

Ash JR and Fourches D. *Characterizing the Chemical Space of Kinase Inhibitors Using Molecular Descriptors Computed from MD Trajectories.*

POSTER

Ash JR, Kuenemann MA, and Fourches D. *Cheminformatics Approach to Exploring and Modeling Trait-Associated Metabolic Profiles.*

- ACS Division of Chemical Information Scholarship of Excellence.

American Chemical Society Conference — *Philadelphia, PA*

POSTER — *Aug. 2016*

Ash JR and Fourches D. *Leveraging GPU-Accelerated Molecular Dynamics Simulations to Compute and Analyze the 4D Chemical Descriptor Space of ERK2 Kinase Inhibitors.*

- Also presented at German Conference on Cheminformatics. Fulda, Germany. November 2016.

SAMSI Bioinformatics Transition Workshop — *RTP, NC*

PRESENTATION — *May 2015*

Larson G, **Ash JR**, Thorne J, Schmidler S. *Improving the Biological Realism of Insertions and Deletions in a Bayesian Model for Simultaneous Estimation of Alignment and Phylogeny.*.

Evolution Conference *Raleigh, NC*

Poster *July 2014*

Ash JR, Huang W, Zhou G, Wilgenbusch J, Gallivan K, Marchand M, and Brown J. *Community Detection on Networks of Topologies and Bipartitions Identifies Conflicting Phylogenetic Signal.*

The Center of Learning and Memory Conference *Austin, TX*

Poster *April 2013*

Ash, JR*, Taylor W*, Siegel J, Gray R, Johnston J, Chitwood R, *Advances in Trace Eyelid Conditioning in Mice.* *Contributed equally.

- Also presented at the Society of Neuroscience Conference in San Diego, CA, November 2013.

Service

2017-2018 **President,** NCSU Genomic Sciences Graduate Student Association

2018 **Organizer,** First Annual NCSU Genomic Sciences and Biomath Research Symposium

2018-Pres. **Reviewer,** Journal of Cheminformatics.

References

- Jacqueline Hughes-Oliver, PhD Co-chair (hughesol@ncsu.edu)
- Denis Fourches, PhD Co-chair (dfourch@ncsu.edu)
- Jeffrey Thorne, PhD committee and StatAlign collaborator (thorne@ncsu.edu)
- Jeremy Brown, TreeScaper collaborator (jembrown@lsu.edu)
- Eric Chi, PhD committee and co-manifold collaborator (eric_chi@ncsu.edu)